



## wwPDB EM Validation Summary Report ⓘ

Apr 11, 2026 – 11:44 AM UTC

PDB ID : 9E5C / pdb\_00009e5c  
EMDB ID : EMD-47524  
Title : Cryo-EM structure of 96 nm repeat of microtubule doublet from *T. brucei* flagellum  
Authors : Xia, X.; Shimogawa, M.M.; Wang, H.; Liu, S.; Wijono, A.; Langousis, G.; Kassem, A.M.; Wohlschlegel, J.A.; Hill, K.; Zhou, Z.H.  
Deposited on : 2024-10-28  
Resolution : 3.20 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.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : **FAILED**  
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 : **NOT EXECUTED**  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.



## 2 Entry composition

There are 160 unique types of molecules in this entry. The entry contains 3895227 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called EF-hand domain-containing family member C2.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1   | 0A    | 662      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 5390  | 3423 | 929  | 1014 | 24 |         |       |
| 1   | 0B    | 734      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 5972  | 3782 | 1036 | 1125 | 29 |         |       |
| 1   | 0C    | 730      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 5933  | 3757 | 1026 | 1121 | 29 |         |       |
| 1   | 0D    | 662      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 5390  | 3423 | 929  | 1014 | 24 |         |       |
| 1   | 0E    | 734      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 5972  | 3782 | 1036 | 1125 | 29 |         |       |
| 1   | 0F    | 730      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 5933  | 3757 | 1026 | 1121 | 29 |         |       |

- Molecule 2 is a protein called EF-hand domain-containing family member C2.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 2   | 0G    | 730      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 5862  | 3718 | 1025 | 1088 | 31 |         |       |
| 2   | 0H    | 730      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 5862  | 3718 | 1025 | 1088 | 31 |         |       |
| 2   | 0I    | 730      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 5862  | 3718 | 1025 | 1088 | 31 |         |       |

- Molecule 3 is a protein called Rib72 protein-like protein.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 3   | 0J    | 665      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5389  | 3412 | 938 | 1011 | 28 |         |       |
| 3   | 0K    | 665      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5389  | 3412 | 938 | 1011 | 28 |         |       |
| 3   | 0L    | 665      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5389  | 3412 | 938 | 1011 | 28 |         |       |

- Molecule 4 is a protein called CMF34/CARP4.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 4   | 0M    | 758      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6157  | 3875 | 1093 | 1162 | 27 |         |       |
| 4   | 0N    | 758      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6157  | 3875 | 1093 | 1162 | 27 |         |       |

- Molecule 5 is a protein called Flagellar protofilament ribbon protein, putative.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | 0O    | 193      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1673  | 1019 | 327 | 319 | 8  |         |       |
| 5   | 0P    | 363      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3131  | 1907 | 616 | 594 | 14 |         |       |
| 5   | 0Q    | 361      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3116  | 1899 | 614 | 591 | 12 |         |       |
| 5   | 0R    | 236      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2036  | 1237 | 405 | 386 | 8  |         |       |
| 5   | 0S    | 347      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3014  | 1834 | 597 | 569 | 14 |         |       |
| 5   | 0T    | 309      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2687  | 1635 | 529 | 513 | 10 |         |       |

- Molecule 6 is a protein called Cilia- and flagella-associated protein 53.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6   | 0U    | 32       | Total | C    | N   | O   |    | 0       | 0     |
|     |       |          | 277   | 174  | 55  | 48  |    |         |       |
| 6   | 0V    | 456      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3874  | 2350 | 786 | 723 | 15 |         |       |
| 6   | 0W    | 456      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3874  | 2350 | 786 | 723 | 15 |         |       |
| 6   | 0X    | 290      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2454  | 1478 | 500 | 465 | 11 |         |       |

- Molecule 7 is a protein called Meiosis-specific nuclear structural protein 1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7   | 0Y    | 153      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1299  | 795  | 251 | 251 | 2 |         |       |
| 7   | 0Z    | 423      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3586  | 2179 | 705 | 693 | 9 |         |       |
| 7   | 1A    | 423      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3586  | 2179 | 705 | 693 | 9 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | 1B    | 126      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1052  | 636 | 209 | 201 | 6 |         |       |

- Molecule 8 is a protein called KIAA1430 homologue.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | 0a    | 96       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 828   | 505 | 167 | 152 | 4 |         |       |
| 8   | 0b    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1155  | 706 | 234 | 210 | 5 |         |       |
| 8   | 0c    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1155  | 706 | 234 | 210 | 5 |         |       |
| 8   | 0d    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1155  | 706 | 234 | 210 | 5 |         |       |
| 8   | 0e    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1155  | 706 | 234 | 210 | 5 |         |       |
| 8   | 0f    | 38       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 327   | 201 | 67  | 58  | 1 |         |       |

- Molecule 9 is a protein called Starmaker.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | 0g    | 72       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 643   | 395 | 130 | 116 | 2 |         |       |
| 9   | 0h    | 72       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 643   | 395 | 130 | 116 | 2 |         |       |
| 9   | 0i    | 72       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 643   | 395 | 130 | 116 | 2 |         |       |
| 9   | 0j    | 72       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 643   | 395 | 130 | 116 | 2 |         |       |
| 9   | 0k    | 72       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 643   | 395 | 130 | 116 | 2 |         |       |
| 9   | 0l    | 72       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 643   | 395 | 130 | 116 | 2 |         |       |
| 9   | 0m    | 72       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 643   | 395 | 130 | 116 | 2 |         |       |
| 9   | 0n    | 72       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 643   | 395 | 130 | 116 | 2 |         |       |
| 9   | 0o    | 72       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 643   | 395 | 130 | 116 | 2 |         |       |
| 9   | 0p    | 72       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 643   | 395 | 130 | 116 | 2 |         |       |

- Molecule 10 is a protein called LIM zinc-binding domain-containing protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | 0q    | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 731   | 450 | 131 | 142 | 8 |         |       |

- Molecule 11 is a protein called Sperm-tail PG-rich repeat.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 11  | 0r    | 77       | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 613   | 391  | 114 | 106 | 2 |         |       |
| 11  | 0s    | 207      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1606  | 1018 | 292 | 293 | 3 |         |       |

- Molecule 12 is a protein called MOP84A.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 12  | 0t    | 470      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3548  | 2199 | 631 | 697 | 21 |         |       |

- Molecule 13 is a protein called Leucine-rich repeat protein (LRRP).

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 13  | 0u    | 483      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3730  | 2318 | 679 | 710 | 23 |         |       |

- Molecule 14 is a protein called Coiled-coil domain-containing protein 39.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 14  | 0v    | 419      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3443  | 2081 | 674 | 677 | 11 |         |       |
| 14  | 0w    | 487      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3966  | 2414 | 768 | 766 | 18 |         |       |

- Molecule 15 is a protein called Coiled-coil domain-containing protein 40.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 15  | 0x    | 421      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3425  | 2107 | 614 | 691 | 13 |         |       |
| 15  | 0y    | 459      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3706  | 2277 | 671 | 738 | 20 |         |       |

- Molecule 16 is a protein called Cilia- and flagella-associated protein 299.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 16  | 0z    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1848  | 1170 | 325 | 351 | 2 |         |       |

- Molecule 17 is a protein called Nucleoside diphosphate kinase, putative.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 17  | 1C    | 332      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2587  | 1637 | 446 | 484 | 20 |         |       |
| 17  | 1D    | 332      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2587  | 1637 | 446 | 484 | 20 |         |       |
| 17  | 1G    | 332      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2587  | 1637 | 446 | 484 | 20 |         |       |

- Molecule 18 is a protein called Nucleoside diphosphate kinase, putative.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 18  | 1E    | 343      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2685  | 1703 | 472 | 493 | 17 |         |       |
| 18  | 1F    | 343      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2685  | 1703 | 472 | 493 | 17 |         |       |

- Molecule 19 is a protein called EF-hand domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 19  | 1H    | 419      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3331  | 2094 | 584 | 638 | 15 |         |       |
| 19  | 1I    | 419      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3331  | 2094 | 584 | 638 | 15 |         |       |

- Molecule 20 is a protein called EF-hand domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 20  | 1J    | 414      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3295  | 2050 | 603 | 624 | 18 |         |       |
| 20  | 1K    | 414      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3295  | 2050 | 603 | 624 | 18 |         |       |

- Molecule 21 is a protein called Cyclic nucleotide-binding domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 21  | 1L    | 306      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2446  | 1557 | 422 | 454 | 13 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 21  | 1M    | 306      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2446  | 1557 | 422 | 454 | 13 |         |       |

- Molecule 22 is a protein called TbMIP23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | 1N    | 170      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1262  | 795 | 219 | 241 | 7 |         |       |
| 22  | 1O    | 170      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1262  | 795 | 219 | 241 | 7 |         |       |

- Molecule 23 is a protein called FAP141.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | 1P    | 105      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 837   | 503 | 167 | 162 | 5 |         |       |
| 23  | 1Q    | 105      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 837   | 503 | 167 | 162 | 5 |         |       |

- Molecule 24 is a protein called EF-hand domain-containing protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | 1R    | 181      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1457  | 935 | 250 | 267 | 5 |         |       |
| 24  | 1S    | 181      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1457  | 935 | 250 | 267 | 5 |         |       |

- Molecule 25 is a protein called Calpain-like cysteine peptidase, putative.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 25  | 1T    | 269      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2100  | 1327 | 366 | 392 | 15 |         |       |
| 25  | 1U    | 269      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2100  | 1327 | 366 | 392 | 15 |         |       |
| 25  | 1V    | 269      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2100  | 1327 | 366 | 392 | 15 |         |       |

- Molecule 26 is a protein called EF-hand domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 26  | 1W    | 472      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3717  | 2352 | 651 | 692 | 22 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 26  | 1X    | 472      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3717  | 2352 | 651 | 692 | 22 |         |       |

- Molecule 27 is a protein called Calcium-binding protein, putative.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 27  | 1Y    | 357      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2921  | 1842 | 511 | 552 | 16 |         |       |
| 27  | 1Z    | 357      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2921  | 1842 | 511 | 552 | 16 |         |       |

- Molecule 28 is a protein called Cilia- and flagella-associated protein 58 central coiled coil domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 28  | 1a    | 509      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4224  | 2582 | 796 | 823 | 23 |         |       |

- Molecule 29 is a protein called Cilia- and flagella-associated protein 58 central coiled coil domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 29  | 1b    | 517      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4282  | 2632 | 829 | 803 | 18 |         |       |

- Molecule 30 is a protein called CMF5.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 30  | 1c    | 972      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 7724  | 4829 | 1382 | 1477 | 36 |         |       |

- Molecule 31 is a protein called CMF6.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 31  | 1d    | 958      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 7575  | 4739 | 1359 | 1438 | 39 |         |       |

- Molecule 32 is a protein called CCDC113/CCDC96 coiled-coil domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 32  | 1e    | 328      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2755  | 1690 | 534 | 516 | 15 |         |       |

- Molecule 33 is a protein called Cilia- and flagella-associated protein 263.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 33  | 1f    | 333      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2738  | 1678 | 519 | 527 | 14 |         |       |

- Molecule 34 is a protein called DRC1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 34  | 1g    | 570      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4747  | 2921 | 882 | 925 | 19 |         |       |

- Molecule 35 is a protein called Dynein regulatory complex subunit 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 35  | 1h    | 438      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3589  | 2210 | 647 | 715 | 17 |         |       |

- Molecule 36 is a protein called Dynein regulatory complex subunit 3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 36  | 1i    | 535      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4420  | 2768 | 794 | 841 | 17 |         |       |

- Molecule 37 is a protein called Trypanin-related protein, putative.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 37  | 1j    | 424      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3544  | 2189 | 663 | 675 | 17 |         |       |

- Molecule 38 is a protein called Trypanin.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 38  | 1k    | 420      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3534  | 2173 | 666 | 681 | 14 |         |       |

- Molecule 39 is a protein called Leucine-rich repeat protein (LRRP).



| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 39  | 1l    | 392      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3071  | 1939 | 538 | 583 | 11 |         |       |

- Molecule 40 is a protein called Transglutaminase-like domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 40  | 1m    | 484      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4013  | 2567 | 710 | 717 | 19 |         |       |

- Molecule 41 is a protein called DRC9.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 41  | 1n    | 410      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3266  | 2020 | 609 | 628 | 9 |         |       |

- Molecule 42 is a protein called Dynein regulatory complex protein 10.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 42  | 1o    | 416      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3311  | 2040 | 579 | 676 | 16 |         |       |

- Molecule 43 is a protein called ATPase AAA-type core domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 43  | 1p    | 553      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4417  | 2785 | 782 | 820 | 30 |         |       |

- Molecule 44 is a protein called Cilia- and flagella-associated protein 43.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 44  | 1r    | 1383     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10942 | 6862 | 1928 | 2079 | 73 |         |       |

- Molecule 45 is a protein called Cilia- and flagella-associated protein 44.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 45  | 1t    | 1298     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10371 | 6524 | 1830 | 1957 | 60 |         |       |

- Molecule 46 is a protein called EF-hand domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 46  | 2A    | 276      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2253  | 1422 | 411 | 409 | 11 |         |       |
| 46  | 2B    | 276      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2253  | 1422 | 411 | 409 | 11 |         |       |
| 46  | 2C    | 218      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1766  | 1113 | 322 | 322 | 9  |         |       |

- Molecule 47 is a protein called Peptidyl-prolyl cis-trans isomerase.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 47  | 2D    | 247      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1908  | 1188 | 346 | 360 | 14 |         |       |
| 47  | 2E    | 247      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1908  | 1188 | 346 | 360 | 14 |         |       |
| 47  | 2F    | 247      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1908  | 1188 | 346 | 360 | 14 |         |       |

- Molecule 48 is a protein called EF-hand domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 48  | 2G    | 298      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2371  | 1516 | 415 | 427 | 13 |         |       |
| 48  | 2H    | 298      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2371  | 1516 | 415 | 427 | 13 |         |       |
| 48  | 2I    | 298      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2371  | 1516 | 415 | 427 | 13 |         |       |

- Molecule 49 is a protein called FAP107/MC11.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 49  | 2J    | 237      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1880  | 1180 | 325 | 363 | 12 |         |       |
| 49  | 2K    | 237      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1880  | 1180 | 325 | 363 | 12 |         |       |
| 49  | 2L    | 237      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1880  | 1180 | 325 | 363 | 12 |         |       |

- Molecule 50 is a protein called T. brucei spp.-specific protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 50  | 2M    | 234      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1862  | 1148 | 338 | 366 | 10 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 50  | 2N    | 234      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1862  | 1148 | 338 | 366 | 10 |         |       |
| 50  | 2O    | 149      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1190  | 728  | 226 | 232 | 4  |         |       |

- Molecule 51 is a protein called FAP95/MC6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51  | 2P    | 165      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1287  | 808 | 234 | 239 | 6 |         |       |
| 51  | 2Q    | 165      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1287  | 808 | 234 | 239 | 6 |         |       |

- Molecule 52 is a protein called FAP129.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 52  | 2R    | 258      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2005  | 1242 | 371 | 379 | 13 |         |       |
| 52  | 2S    | 258      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2005  | 1242 | 371 | 379 | 13 |         |       |
| 52  | 2T    | 258      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2005  | 1242 | 371 | 379 | 13 |         |       |

- Molecule 53 is a protein called T. brucei spp.-specific protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 53  | 2U    | 292      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2311  | 1433 | 422 | 450 | 6 |         |       |
| 53  | 2V    | 375      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2968  | 1848 | 540 | 572 | 8 |         |       |
| 53  | 2W    | 375      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2968  | 1848 | 540 | 572 | 8 |         |       |

- Molecule 54 is a protein called FAP21.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 54  | 2X    | 371      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2921  | 1801 | 561 | 536 | 23 |         |       |
| 54  | 2Y    | 371      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2921  | 1801 | 561 | 536 | 23 |         |       |
| 54  | 2Z    | 127      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 991   | 597  | 205 | 182 | 7  |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 54  | 3D    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 802   | 494 | 150 | 149 | 9 |         |       |

- Molecule 55 is a protein called RSP1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 55  | 2a    | 322      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2609  | 1649 | 450 | 493 | 17 |         |       |
| 55  | 2b    | 322      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2609  | 1649 | 450 | 493 | 17 |         |       |
| 55  | 2c    | 322      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2609  | 1649 | 450 | 493 | 17 |         |       |
| 55  | 2d    | 322      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2609  | 1649 | 450 | 493 | 17 |         |       |

- Molecule 56 is a protein called RSP2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 56  | 2e    | 507      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3972  | 2457 | 718 | 782 | 15 |         |       |
| 56  | 2f    | 507      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3972  | 2457 | 718 | 782 | 15 |         |       |
| 56  | 2g    | 507      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3972  | 2457 | 718 | 782 | 15 |         |       |
| 56  | 2h    | 507      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3972  | 2457 | 718 | 782 | 15 |         |       |

- Molecule 57 is a protein called Radial spoke protein 3, putative.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 57  | 2i    | 165      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1413  | 887  | 259 | 262 | 5 |         |       |
| 57  | 2j    | 280      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2352  | 1462 | 442 | 441 | 7 |         |       |
| 57  | 2k    | 215      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1815  | 1136 | 324 | 350 | 5 |         |       |
| 57  | 2l    | 218      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1835  | 1149 | 329 | 352 | 5 |         |       |

- Molecule 58 is a protein called Flagellar radial spoke component, putative.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 58  | 2m    | 527      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4232  | 2656 | 702 | 854 | 20 |         |       |
| 58  | 2n    | 527      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4232  | 2656 | 702 | 854 | 20 |         |       |
| 58  | 2o    | 527      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4232  | 2656 | 702 | 854 | 20 |         |       |
| 58  | 2p    | 527      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4232  | 2656 | 702 | 854 | 20 |         |       |

- Molecule 59 is a protein called Flagellar radial spoke protein-like, putative.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 59  | 2q    | 494      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3881  | 2454 | 655 | 760 | 12 |         |       |
| 59  | 2r    | 494      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3881  | 2454 | 655 | 760 | 12 |         |       |
| 59  | 2s    | 494      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3881  | 2454 | 655 | 760 | 12 |         |       |
| 59  | 2t    | 469      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3679  | 2330 | 629 | 708 | 12 |         |       |

- Molecule 60 is a protein called RSP8.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 60  | 2u    | 429      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3322  | 2108 | 580 | 617 | 17 |         |       |

- Molecule 61 is a protein called Radial spoke head protein 9 homolog.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 61  | 2v    | 297      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2390  | 1528 | 408 | 444 | 10 |         |       |
| 61  | 2w    | 297      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2390  | 1528 | 408 | 444 | 10 |         |       |
| 61  | 2x    | 297      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2390  | 1528 | 408 | 444 | 10 |         |       |
| 61  | 2y    | 297      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2390  | 1528 | 408 | 444 | 10 |         |       |

- Molecule 62 is a protein called Radial spoke protein RSP9.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 62  | 2z    | 310      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2451  | 1563 | 411 | 466 | 11 |         |       |
| 62  | 3a    | 279      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2199  | 1416 | 376 | 397 | 10 |         |       |
| 62  | 3b    | 310      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2451  | 1563 | 411 | 466 | 11 |         |       |
| 62  | 3c    | 272      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2145  | 1381 | 368 | 386 | 10 |         |       |

- Molecule 63 is a protein called Flagellar associated protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 63  | 3A    | 205      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1620  | 1004 | 305 | 303 | 8  |         |       |
| 63  | 3B    | 305      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2388  | 1483 | 447 | 448 | 10 |         |       |
| 63  | 3C    | 305      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2388  | 1483 | 447 | 448 | 10 |         |       |

- Molecule 64 is a protein called TbRib26b.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 64  | 3E    | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 953   | 598 | 170 | 182 | 3 |         |       |
| 64  | 3F    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 772   | 492 | 132 | 146 | 2 |         |       |
| 64  | 3G    | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 953   | 598 | 170 | 182 | 3 |         |       |
| 64  | 3H    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 772   | 492 | 132 | 146 | 2 |         |       |
| 64  | 3I    | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 953   | 598 | 170 | 182 | 3 |         |       |

- Molecule 65 is a protein called EF-hand domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 65  | 3J    | 650      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5268  | 3330 | 951 | 972 | 15 |         |       |
| 65  | 3K    | 556      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4482  | 2828 | 816 | 827 | 11 |         |       |
| 65  | 3L    | 94       | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 786   | 502  | 135 | 145 | 4  |         |       |

- Molecule 66 is a protein called PACRGA.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 66  | 3M    | 277      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2223  | 1425 | 399 | 393 | 6 |         |       |
| 66  | 3N    | 277      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2223  | 1425 | 399 | 393 | 6 |         |       |
| 66  | 3O    | 277      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2223  | 1425 | 399 | 393 | 6 |         |       |
| 66  | 3P    | 277      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2223  | 1425 | 399 | 393 | 6 |         |       |
| 66  | 3Q    | 277      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2223  | 1425 | 399 | 393 | 6 |         |       |
| 66  | 3R    | 277      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2223  | 1425 | 399 | 393 | 6 |         |       |
| 66  | 3S    | 277      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2223  | 1425 | 399 | 393 | 6 |         |       |
| 66  | 3T    | 277      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2223  | 1425 | 399 | 393 | 6 |         |       |

- Molecule 67 is a protein called PACRGB.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 67  | 3U    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1819  | 1174 | 311 | 329 | 5 |         |       |
| 67  | 3V    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1819  | 1174 | 311 | 329 | 5 |         |       |
| 67  | 3W    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1819  | 1174 | 311 | 329 | 5 |         |       |
| 67  | 3X    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1819  | 1174 | 311 | 329 | 5 |         |       |
| 67  | 3Y    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1819  | 1174 | 311 | 329 | 5 |         |       |

- Molecule 68 is a protein called Cilia- and flagella-associated protein 20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 68  | 3Z    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1537  | 985 | 271 | 273 | 8 |         |       |
| 68  | 4A    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1537  | 985 | 271 | 273 | 8 |         |       |
| 68  | 4B    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1537  | 985 | 271 | 273 | 8 |         |       |
| 68  | 4C    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1537  | 985 | 271 | 273 | 8 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 68  | 4D    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1537  | 985 | 271 | 273 | 8 |         |       |
| 68  | 4E    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1537  | 985 | 271 | 273 | 8 |         |       |
| 68  | 4F    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1537  | 985 | 271 | 273 | 8 |         |       |
| 68  | 4G    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1537  | 985 | 271 | 273 | 8 |         |       |
| 68  | 4H    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1537  | 985 | 271 | 273 | 8 |         |       |
| 68  | 4I    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1537  | 985 | 271 | 273 | 8 |         |       |
| 68  | 4J    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1537  | 985 | 271 | 273 | 8 |         |       |
| 68  | 4K    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1537  | 985 | 271 | 273 | 8 |         |       |
| 68  | 4L    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1537  | 985 | 271 | 273 | 8 |         |       |
| 68  | 4M    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1537  | 985 | 271 | 273 | 8 |         |       |
| 68  | 4N    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1537  | 985 | 271 | 273 | 8 |         |       |

- Molecule 69 is a protein called Phosphatidylinositol 4-phosphate 5-kinase.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 69  | 3d    | 675      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5388  | 3380 | 969 | 1023 | 16 |         |       |
| 69  | 3e    | 675      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5388  | 3380 | 969 | 1023 | 16 |         |       |
| 69  | 3f    | 675      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5388  | 3380 | 969 | 1023 | 16 |         |       |
| 69  | 3g    | 675      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5388  | 3380 | 969 | 1023 | 16 |         |       |

- Molecule 70 is a protein called Cyclophilin type peptidyl-prolyl cis-trans isomerase, putative.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 70  | 3h    | 310      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2453  | 1538 | 426 | 466 | 23 |         |       |
| 70  | 3i    | 310      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2453  | 1538 | 426 | 466 | 23 |         |       |



- Molecule 71 is a protein called RSP14.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 71  | 3j    | 380      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3009  | 1900 | 526 | 562 | 21 |         |       |

- Molecule 72 is a protein called Leucine-rich repeat protein (LRRP).

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 72  | 3k    | 364      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2743  | 1715 | 479 | 534 | 15 |         |       |

- Molecule 73 is a protein called Chaperone protein DNAJ, putative.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 73  | 3l    | 302      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2354  | 1487 | 413 | 448 | 6 |         |       |
| 73  | 3m    | 289      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2252  | 1420 | 397 | 429 | 6 |         |       |
| 73  | 3o    | 302      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2354  | 1487 | 413 | 448 | 6 |         |       |
| 73  | 3p    | 289      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2252  | 1420 | 397 | 429 | 6 |         |       |

- Molecule 74 is a protein called Nucleoside diphosphate kinase.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 74  | 3q    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1769  | 1121 | 320 | 320 | 8 |         |       |
| 74  | 3r    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1769  | 1121 | 320 | 320 | 8 |         |       |
| 74  | 3s    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1769  | 1121 | 320 | 320 | 8 |         |       |
| 74  | 3t    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1769  | 1121 | 320 | 320 | 8 |         |       |

- Molecule 75 is a protein called Dynein light chain.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 75  | 3u    | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 715   | 465 | 116 | 131 | 3 |         |       |
| 75  | 3v    | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 715   | 465 | 116 | 131 | 3 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 75  | 3w    | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 722   | 469 | 117 | 133 | 3 |         |       |
| 75  | 3x    | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 715   | 465 | 116 | 131 | 3 |         |       |
| 75  | 3y    | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 715   | 465 | 116 | 131 | 3 |         |       |
| 75  | 3z    | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 715   | 465 | 116 | 131 | 3 |         |       |
| 75  | 4a    | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 715   | 465 | 116 | 131 | 3 |         |       |
| 75  | 4b    | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 715   | 465 | 116 | 131 | 3 |         |       |
| 75  | 4c    | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 717   | 467 | 116 | 131 | 3 |         |       |
| 75  | 4d    | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 717   | 467 | 116 | 131 | 3 |         |       |
| 75  | 4e    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 710   | 463 | 115 | 129 | 3 |         |       |
| 75  | 4f    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 710   | 463 | 115 | 129 | 3 |         |       |
| 75  | 4g    | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 717   | 467 | 116 | 131 | 3 |         |       |
| 75  | 4h    | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 717   | 467 | 116 | 131 | 3 |         |       |
| 75  | 4i    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 710   | 463 | 115 | 129 | 3 |         |       |
| 75  | 4j    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 710   | 463 | 115 | 129 | 3 |         |       |
| 75  | 4k    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 710   | 463 | 115 | 129 | 3 |         |       |
| 75  | 4l    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 710   | 463 | 115 | 129 | 3 |         |       |
| 75  | 4m    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 710   | 463 | 115 | 129 | 3 |         |       |
| 75  | 4n    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 710   | 463 | 115 | 129 | 3 |         |       |
| 75  | 5s    | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 715   | 465 | 116 | 131 | 3 |         |       |
| 75  | 5t    | 89       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 728   | 472 | 118 | 135 | 3 |         |       |
| 75  | 5u    | 84       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 687   | 449 | 109 | 126 | 3 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 75  | 5v    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 707   | 461 | 115 | 128 | 3 |         |       |
| 75  | 5w    | 90       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 736   | 477 | 119 | 136 | 4 |         |       |
| 75  | 5x    | 90       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 736   | 477 | 119 | 136 | 4 |         |       |
| 75  | 7k    | 89       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 728   | 472 | 118 | 135 | 3 |         |       |
| 75  | 7n    | 84       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 687   | 449 | 109 | 126 | 3 |         |       |
| 75  | 7o    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 707   | 461 | 115 | 128 | 3 |         |       |
| 75  | 7p    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 707   | 461 | 115 | 128 | 3 |         |       |
| 75  | 8k    | 89       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 728   | 472 | 118 | 135 | 3 |         |       |
| 75  | 8n    | 84       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 687   | 449 | 109 | 126 | 3 |         |       |
| 75  | 8o    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 707   | 461 | 115 | 128 | 3 |         |       |
| 75  | 8p    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 707   | 461 | 115 | 128 | 3 |         |       |
| 75  | 9k    | 89       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 728   | 472 | 118 | 135 | 3 |         |       |
| 75  | 9n    | 84       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 687   | 449 | 109 | 126 | 3 |         |       |
| 75  | 9o    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 707   | 461 | 115 | 128 | 3 |         |       |
| 75  | 9p    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 707   | 461 | 115 | 128 | 3 |         |       |

- Molecule 76 is a protein called Cilia- and flagella-associated protein 52.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 76  | 4O    | 620      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4671  | 2918 | 821 | 901 | 31 |         |       |
| 76  | 4P    | 627      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4727  | 2953 | 829 | 914 | 31 |         |       |
| 76  | 4Q    | 627      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4727  | 2953 | 829 | 914 | 31 |         |       |
| 76  | 4R    | 620      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4671  | 2918 | 821 | 901 | 31 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 76  | 4S    | 627      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4727  | 2953 | 829 | 914 | 31 |         |       |
| 76  | 4T    | 627      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4727  | 2953 | 829 | 914 | 31 |         |       |
| 76  | 4U    | 620      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4671  | 2918 | 821 | 901 | 31 |         |       |

- Molecule 77 is a protein called Enkurin domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 77  | 4V    | 240      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1867  | 1166 | 339 | 358 | 4 |         |       |
| 77  | 4W    | 240      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1867  | 1166 | 339 | 358 | 4 |         |       |
| 77  | 4X    | 240      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1867  | 1166 | 339 | 358 | 4 |         |       |
| 77  | 4Y    | 240      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1867  | 1166 | 339 | 358 | 4 |         |       |
| 77  | 4Z    | 240      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1867  | 1166 | 339 | 358 | 4 |         |       |

- Molecule 78 is a protein called Cytochrome b5 domain-containing protein 1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 78  | 4o    | 220      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1802  | 1139 | 302 | 352 | 9 |         |       |
| 78  | 4p    | 220      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1802  | 1139 | 302 | 352 | 9 |         |       |

- Molecule 79 is a protein called Leucine-rich repeat protein (LRRP).

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 79  | 4q    | 852      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6513  | 4052 | 1149 | 1276 | 36 |         |       |
| 79  | 4r    | 852      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6513  | 4052 | 1149 | 1276 | 36 |         |       |

- Molecule 80 is a protein called VWFA domain-containing protein.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 80  | 4s    | 809      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6179  | 3905 | 1079 | 1154 | 41 |         |       |

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| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 80  | 4t    | 809      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6179  | 3905 | 1079 | 1154 | 41 |         |       |

- Molecule 81 is a protein called TbRSP63.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 81  | 4u    | 501      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3934  | 2439 | 702 | 770 | 23 |         |       |
| 81  | 4v    | 501      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3934  | 2439 | 702 | 770 | 23 |         |       |

- Molecule 82 is a protein called IQ and ubiquitin-like domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 82  | 4w    | 512      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4141  | 2593 | 775 | 757 | 16 |         |       |

- Molecule 83 is a protein called Calmodulin.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 83  | 4x    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 839   | 501 | 160 | 176 | 2 |         |       |

- Molecule 84 is a protein called MORN repeat-containing protein 3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 84  | 4y    | 661      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5306  | 3343 | 952 | 984 | 27 |         |       |

- Molecule 85 is a protein called Cilia- and flagella-associated protein 206.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 85  | 4z    | 528      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4132  | 2595 | 726 | 785 | 26 |         |       |

- Molecule 86 is a protein called Enkurin domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 86  | 5A    | 229      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1905  | 1207 | 344 | 347 | 7 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 86  | 5B    | 229      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1905  | 1207 | 344 | 347 | 7 |         |       |

- Molecule 87 is a protein called MC4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 87  | 5C    | 279      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2217  | 1384 | 418 | 404 | 11 |         |       |
| 87  | 5D    | 275      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2186  | 1366 | 412 | 398 | 10 |         |       |
| 87  | 5E    | 275      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2186  | 1366 | 412 | 398 | 10 |         |       |
| 87  | 5F    | 279      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2217  | 1384 | 418 | 404 | 11 |         |       |
| 87  | 5G    | 275      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2186  | 1366 | 412 | 398 | 10 |         |       |
| 87  | 5H    | 275      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2186  | 1366 | 412 | 398 | 10 |         |       |
| 87  | 5I    | 279      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2217  | 1384 | 418 | 404 | 11 |         |       |
| 87  | 5J    | 173      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1370  | 849  | 266 | 247 | 8  |         |       |

- Molecule 88 is a protein called Cilia- and flagella-associated protein 45.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 88  | 5K    | 153      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1308  | 790  | 260 | 249 | 9  |         |       |
| 88  | 5S    | 165      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1369  | 821  | 260 | 275 | 13 |         |       |
| 88  | 5T    | 459      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3875  | 2336 | 762 | 753 | 24 |         |       |
| 88  | 5U    | 459      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3875  | 2336 | 762 | 753 | 24 |         |       |
| 88  | 5V    | 295      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2465  | 1490 | 478 | 482 | 15 |         |       |
| 88  | 5W    | 473      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3981  | 2402 | 783 | 772 | 24 |         |       |
| 88  | 5X    | 382      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3253  | 1966 | 638 | 632 | 17 |         |       |

- Molecule 89 is a protein called CCDC81 HU domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 89  | 5L    | 239      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1911  | 1207 | 342 | 348 | 14 |         |       |
| 89  | 5M    | 239      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1911  | 1207 | 342 | 348 | 14 |         |       |

- Molecule 90 is a protein called MC5.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 90  | 5N    | 238      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1900  | 1188 | 349 | 355 | 8 |         |       |
| 90  | 5O    | 238      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1900  | 1188 | 349 | 355 | 8 |         |       |
| 90  | 5P    | 238      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1900  | 1188 | 349 | 355 | 8 |         |       |
| 90  | 5Q    | 238      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1900  | 1188 | 349 | 355 | 8 |         |       |
| 90  | 5R    | 238      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1900  | 1188 | 349 | 355 | 8 |         |       |

- Molecule 91 is a protein called Trichohyalin-plectin-homology domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 91  | 5Y    | 408      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3422  | 2084 | 668 | 652 | 18 |         |       |
| 91  | 5Z    | 465      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3907  | 2378 | 757 | 751 | 21 |         |       |
| 91  | 6A    | 262      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2236  | 1357 | 437 | 429 | 13 |         |       |

- Molecule 92 is a protein called TbRSP62.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 92  | 5a    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1256  | 783 | 231 | 237 | 5 |         |       |

- Molecule 93 is a protein called Cilia- and flagella-associated protein 91.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 93  | 5b    | 172      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1419  | 876 | 270 | 267 | 6 |         |       |

- Molecule 94 is a protein called Cilia- and flagella-associated protein 251.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 94  | 5c    | 918      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 7136  | 4531 | 1227 | 1343 | 35 |         |       |

- Molecule 95 is a protein called Cilia- and flagella-associated protein 61 N-terminal domain-containing protein.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 95  | 5d    | 1274     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10191 | 6477 | 1738 | 1929 | 47 |         |       |

- Molecule 96 is a protein called DUF4200 domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 96  | 5e    | 225      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1895  | 1154 | 373 | 362 | 6 |         |       |

- Molecule 97 is a protein called DUF4200 domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 97  | 5f    | 322      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2649  | 1636 | 481 | 519 | 13 |         |       |

- Molecule 98 is a protein called Leucine-rich repeat-containing protein 51.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 98  | 5g    | 435      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3510  | 2220 | 618 | 654 | 18 |         |       |

- Molecule 99 is a protein called IDAf-alpha.

| Mol | Chain | Residues | Atoms |       |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|-----|---------|-------|
| 99  | 5h    | 1379     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 11265 | 7169  | 1969 | 2076 | 51  |         |       |
| 99  | 5i    | 3336     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 26792 | 17002 | 4620 | 5021 | 149 |         |       |

- Molecule 100 is a protein called Dynein heavy chain, putative.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 100 | 5j    | 1336     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10917 | 6902 | 1939 | 2025 | 51 |         |       |

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| Mol | Chain | Residues | Atoms |       |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|-----|---------|-------|
| 100 | 5k    | 3425     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 27648 | 17529 | 4783 | 5192 | 144 |         |       |

- Molecule 101 is a protein called Dynein axonemal intermediate chain 4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 101 | 5l    | 435      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3410  | 2133 | 590 | 666 | 21 |         |       |

- Molecule 102 is a protein called IC140.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 102 | 5m    | 477      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3788  | 2392 | 690 | 686 | 20 |         |       |

- Molecule 103 is a protein called IC97/Casc1 N-terminal domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 103 | 5n    | 645      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5223  | 3319 | 902 | 976 | 26 |         |       |

- Molecule 104 is a protein called FAP120.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 104 | 5o    | 337      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2622  | 1621 | 473 | 512 | 16 |         |       |

- Molecule 105 is a protein called Dynein light chain, putative.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 105 | 5p    | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 929   | 583 | 167 | 172 | 7 |         |       |
| 105 | 7i    | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 929   | 583 | 167 | 172 | 7 |         |       |
| 105 | 8i    | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 929   | 583 | 167 | 172 | 7 |         |       |
| 105 | 9i    | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 929   | 583 | 167 | 172 | 7 |         |       |

- Molecule 106 is a protein called Dynein light chain roadblock.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 106 | 5q    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 784   | 500 | 139 | 144 | 1 |         |       |
| 106 | 7l    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 784   | 500 | 139 | 144 | 1 |         |       |
| 106 | 8l    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 784   | 500 | 139 | 144 | 1 |         |       |
| 106 | 9l    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 784   | 500 | 139 | 144 | 1 |         |       |

- Molecule 107 is a protein called Dynein light chain roadblock.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 107 | 5r    | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 756   | 470 | 138 | 145 | 3 |         |       |
| 107 | 7m    | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 756   | 470 | 138 | 145 | 3 |         |       |
| 107 | 8m    | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 756   | 470 | 138 | 145 | 3 |         |       |
| 107 | 9m    | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 756   | 470 | 138 | 145 | 3 |         |       |

- Molecule 108 is a protein called Dynein light chain, putative.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 108 | 5y    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 823   | 533 | 133 | 153 | 4 |         |       |
| 108 | 7q    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 823   | 533 | 133 | 153 | 4 |         |       |
| 108 | 8q    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 823   | 533 | 133 | 153 | 4 |         |       |
| 108 | 9q    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 823   | 533 | 133 | 153 | 4 |         |       |

- Molecule 109 is a protein called Trichohyalin-plectin-homology domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 109 | 6B    | 93       | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 786   | 487  | 155 | 142 | 2  |         |       |
| 109 | 6C    | 318      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2691  | 1646 | 523 | 508 | 14 |         |       |
| 109 | 6D    | 318      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2691  | 1646 | 523 | 508 | 14 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 109 | 6E    | 80       | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 699   | 429  | 133 | 135 | 2  |         |       |
| 109 | 6F    | 344      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2892  | 1769 | 564 | 545 | 14 |         |       |
| 109 | 6G    | 347      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2912  | 1780 | 567 | 551 | 14 |         |       |
| 109 | 6H    | 180      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1538  | 931  | 303 | 296 | 8  |         |       |
| 109 | 6I    | 239      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1975  | 1209 | 384 | 372 | 10 |         |       |
| 109 | 6J    | 346      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2905  | 1775 | 566 | 550 | 14 |         |       |
| 109 | 6K    | 285      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2394  | 1457 | 467 | 458 | 12 |         |       |
| 109 | 6L    | 141      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1161  | 721  | 225 | 213 | 2  |         |       |
| 109 | 6M    | 347      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2912  | 1780 | 567 | 551 | 14 |         |       |
| 109 | 6N    | 347      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2912  | 1780 | 567 | 551 | 14 |         |       |
| 109 | 6O    | 253      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2146  | 1307 | 417 | 410 | 12 |         |       |
| 109 | 6P    | 253      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2146  | 1307 | 417 | 410 | 12 |         |       |
| 109 | 6Q    | 163      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1406  | 852  | 276 | 270 | 8  |         |       |

- Molecule 110 is a protein called STOP axonemal protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 110 | 6R    | 151      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1199  | 765  | 212 | 217 | 5  |         |       |
| 110 | 6S    | 228      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1816  | 1155 | 318 | 332 | 11 |         |       |
| 110 | 6T    | 177      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1415  | 902  | 243 | 261 | 9  |         |       |
| 110 | 6U    | 98       | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 776   | 492  | 138 | 141 | 5  |         |       |
| 110 | 6V    | 231      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1846  | 1168 | 331 | 336 | 11 |         |       |
| 110 | 6W    | 231      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1846  | 1168 | 331 | 336 | 11 |         |       |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 110 | 6X    | 51       | Total<br>401  | C<br>250  | N<br>70  | O<br>76  | S<br>5  | 0       | 0     |
| 110 | 6Y    | 229      | Total<br>1819 | C<br>1152 | N<br>322 | O<br>334 | S<br>11 | 0       | 0     |
| 110 | 6Z    | 229      | Total<br>1819 | C<br>1152 | N<br>322 | O<br>334 | S<br>11 | 0       | 0     |
| 110 | 7A    | 112      | Total<br>886  | C<br>559  | N<br>158 | O<br>163 | S<br>6  | 0       | 0     |
| 110 | 7B    | 179      | Total<br>1430 | C<br>912  | N<br>251 | O<br>262 | S<br>5  | 0       | 0     |
| 110 | 7C    | 239      | Total<br>1907 | C<br>1212 | N<br>334 | O<br>350 | S<br>11 | 0       | 0     |
| 110 | 7D    | 178      | Total<br>1424 | C<br>907  | N<br>246 | O<br>262 | S<br>9  | 0       | 0     |
| 110 | 7E    | 106      | Total<br>839  | C<br>530  | N<br>147 | O<br>157 | S<br>5  | 0       | 0     |
| 110 | 7F    | 228      | Total<br>1814 | C<br>1148 | N<br>321 | O<br>334 | S<br>11 | 0       | 0     |
| 110 | 7G    | 228      | Total<br>1814 | C<br>1148 | N<br>321 | O<br>334 | S<br>11 | 0       | 0     |
| 110 | 7H    | 101      | Total<br>798  | C<br>503  | N<br>144 | O<br>145 | S<br>6  | 0       | 0     |
| 110 | 7I    | 237      | Total<br>1884 | C<br>1193 | N<br>336 | O<br>344 | S<br>11 | 0       | 0     |
| 110 | 7J    | 237      | Total<br>1884 | C<br>1193 | N<br>336 | O<br>344 | S<br>11 | 0       | 0     |
| 110 | 7K    | 51       | Total<br>401  | C<br>253  | N<br>75  | O<br>71  | S<br>2  | 0       | 0     |
| 110 | 9Z    | 43       | Total<br>337  | C<br>213  | N<br>64  | O<br>59  | S<br>1  | 0       | 0     |

- Molecule 111 is a protein called Dynein heavy chain, putative.

| Mol | Chain | Residues | Atoms          |            |           |           |          | AltConf | Trace |
|-----|-------|----------|----------------|------------|-----------|-----------|----------|---------|-------|
| 111 | 6a    | 4058     | Total<br>32697 | C<br>20810 | N<br>5575 | O<br>6136 | S<br>176 | 0       | 0     |

- Molecule 112 is a protein called Dynein heavy chain, putative.

| Mol | Chain | Residues | Atoms          |            |           |           |          | AltConf | Trace |
|-----|-------|----------|----------------|------------|-----------|-----------|----------|---------|-------|
| 112 | 6b    | 4055     | Total<br>32697 | C<br>20834 | N<br>5572 | O<br>6089 | S<br>202 | 0       | 0     |

- Molecule 113 is a protein called Dynein heavy chain, putative.

| Mol | Chain | Residues | Atoms |       |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|-----|---------|-------|
| 113 | 6c    | 3929     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 31436 | 19931 | 5406 | 5916 | 183 |         |       |

- Molecule 114 is a protein called Dynein heavy chain, putative.

| Mol | Chain | Residues | Atoms |       |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|-----|---------|-------|
| 114 | 6d    | 4002     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 31959 | 20295 | 5495 | 6005 | 164 |         |       |

- Molecule 115 is a protein called Dynein heavy chain, putative.

| Mol | Chain | Residues | Atoms |       |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|-----|---------|-------|
| 115 | 6e    | 4089     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 32835 | 20894 | 5595 | 6161 | 185 |         |       |

- Molecule 116 is a protein called Actin A.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 116 | 6f    | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2905  | 1835 | 492 | 556 | 22 |         |       |
| 116 | 6g    | 371      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2896  | 1830 | 491 | 553 | 22 |         |       |

- Molecule 117 is a protein called Actin-like protein, putative.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 117 | 6h    | 393      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3040  | 1901 | 539 | 578 | 22 |         |       |

- Molecule 118 is a protein called Actin, putative.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 118 | 6i    | 412      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3215  | 2021 | 571 | 602 | 21 |         |       |

- Molecule 119 is a protein called Actin, putative.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 119 | 6j    | 392      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3038  | 1921 | 525 | 573 | 19 |         |       |

- Molecule 120 is a protein called Dynein arm light chain, axonemal, putative.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 120 | 6k    | 168      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1383  | 854  | 248 | 273 | 8 |         |       |
| 120 | 6l    | 214      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1770  | 1109 | 310 | 343 | 8 |         |       |
| 120 | 6m    | 221      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1825  | 1142 | 321 | 354 | 8 |         |       |

- Molecule 121 is a protein called 33 kDa inner dynein arm light chain, axonemal, putative.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 121 | 6n    | 195      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1621  | 1004 | 303 | 308 | 6 |         |       |

- Molecule 122 is a protein called Dynein arm light chain, axonemal, putative.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 122 | 6o    | 243      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1959  | 1224 | 365 | 362 | 8 |         |       |

- Molecule 123 is a protein called Dynein arm light chain, axonemal, putative.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 123 | 6p    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1370  | 846 | 258 | 258 | 8 |         |       |

- Molecule 124 is a protein called Protein TAX-1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 124 | 6q    | 338      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2687  | 1714 | 467 | 496 | 10 |         |       |

- Molecule 125 is a protein called Tetratricopeptide repeat protein 29.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 125 | 6r    | 364      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1816 | 517 | 554 | 19 |         |       |

- Molecule 126 is a protein called Tetratricopeptide repeat protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 126 | 6s    | 370      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2835  | 1774 | 523 | 517 | 21 |         |       |

- Molecule 127 is a protein called Centrin, putative.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 127 | 6t    | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1226  | 772 | 205 | 244 | 5 |         |       |

- Molecule 128 is a protein called Centrin, putative.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 128 | 6u    | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1206  | 760 | 206 | 235 | 5 |         |       |

- Molecule 129 is a protein called MC8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 129 | 7L    | 154      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1293  | 822 | 224 | 238 | 9 |         |       |
| 129 | 7M    | 154      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1293  | 822 | 224 | 238 | 9 |         |       |

- Molecule 130 is a protein called MC3.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 130 | 7N    | 163      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1338  | 844 | 232 | 252 | 10 |         |       |
| 130 | 7O    | 163      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1338  | 844 | 232 | 252 | 10 |         |       |
| 130 | 7P    | 163      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1338  | 844 | 232 | 252 | 10 |         |       |

- Molecule 131 is a protein called FAP90.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 131 | 7Q    | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1281  | 794 | 235 | 244 | 8 |         |       |
| 131 | 7R    | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1281  | 794 | 235 | 244 | 8 |         |       |
| 131 | 7S    | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1281  | 794 | 235 | 244 | 8 |         |       |

- Molecule 132 is a protein called PBP36.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 132 | 7T    | 161      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1288  | 821  | 240 | 222 | 5  |         |       |
| 132 | 7U    | 298      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2408  | 1525 | 452 | 421 | 10 |         |       |
| 132 | 8L    | 238      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1938  | 1226 | 367 | 338 | 7  |         |       |

- Molecule 133 is a protein called Enkurin domain-containing protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 133 | 7V    | 239      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1920  | 1191 | 366 | 352 | 11 |         |       |
| 133 | 7W    | 238      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1906  | 1183 | 363 | 347 | 13 |         |       |
| 133 | 7X    | 231      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1844  | 1145 | 349 | 337 | 13 |         |       |
| 133 | 7Y    | 239      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1920  | 1191 | 366 | 352 | 11 |         |       |
| 133 | 7Z    | 238      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1906  | 1183 | 363 | 347 | 13 |         |       |
| 133 | 8A    | 231      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1844  | 1145 | 349 | 337 | 13 |         |       |
| 133 | 8B    | 239      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1920  | 1191 | 366 | 352 | 11 |         |       |
| 133 | 8C    | 238      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1906  | 1183 | 363 | 347 | 13 |         |       |

- Molecule 134 is a protein called Dynein heavy chain, putative.

| Mol | Chain | Residues | Atoms |       |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|-----|---------|-------|
| 134 | 7a    | 3423     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 27522 | 17521 | 4745 | 5105 | 151 |         |       |
| 134 | 7e    | 4629     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 37310 | 23753 | 6431 | 6935 | 191 |         |       |
| 134 | 8e    | 4629     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 37310 | 23753 | 6431 | 6935 | 191 |         |       |
| 134 | 9e    | 4629     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 37310 | 23753 | 6431 | 6935 | 191 |         |       |

- Molecule 135 is a protein called Dynein heavy chain, putative.



| Mol | Chain | Residues | Atoms |       |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|-----|---------|-------|
| 135 | 7b    | 3366     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 27000 | 17185 | 4608 | 5047 | 160 |         |       |
| 135 | 7f    | 4591     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 36840 | 23385 | 6285 | 6962 | 208 |         |       |
| 135 | 8f    | 4591     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 36840 | 23385 | 6285 | 6962 | 208 |         |       |
| 135 | 9f    | 4591     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 36840 | 23385 | 6285 | 6962 | 208 |         |       |

- Molecule 136 is a protein called TbDC65.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 136 | 7c    | 340      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2790  | 1756 | 517 | 504 | 13 |         |       |
| 136 | 8c    | 340      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2790  | 1756 | 517 | 504 | 13 |         |       |
| 136 | 9c    | 340      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2790  | 1756 | 517 | 504 | 13 |         |       |

- Molecule 137 is a protein called TbDC13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 137 | 7d    | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 662   | 425 | 123 | 107 | 7 |         |       |
| 137 | 8d    | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 662   | 425 | 123 | 107 | 7 |         |       |
| 137 | 9d    | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 662   | 425 | 123 | 107 | 7 |         |       |

- Molecule 138 is a protein called Dynein, putative.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 138 | 7g    | 533      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4236  | 2662 | 743 | 812 | 19 |         |       |
| 138 | 8g    | 533      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4236  | 2662 | 743 | 812 | 19 |         |       |
| 138 | 9g    | 533      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4236  | 2662 | 743 | 812 | 19 |         |       |

- Molecule 139 is a protein called Dynein intermediate chain, putative.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 139 | 7h    | 609      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4830  | 3046 | 835 | 920 | 29 |         |       |
| 139 | 8h    | 609      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4830  | 3046 | 835 | 920 | 29 |         |       |
| 139 | 9h    | 609      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4830  | 3046 | 835 | 920 | 29 |         |       |

- Molecule 140 is a protein called Dynein light chain.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 140 | 7j    | 105      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 855   | 547 | 139 | 158 | 11 |         |       |
| 140 | 8j    | 105      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 855   | 547 | 139 | 158 | 11 |         |       |
| 140 | 9j    | 105      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 855   | 547 | 139 | 158 | 11 |         |       |

- Molecule 141 is a protein called Dynein light chain.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 141 | 7r    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 776   | 484 | 140 | 147 | 5 |         |       |
| 141 | 8r    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 776   | 484 | 140 | 147 | 5 |         |       |
| 141 | 9r    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 776   | 484 | 140 | 147 | 5 |         |       |

- Molecule 142 is a protein called Outer dynein arm docking complex.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 142 | 7s    | 164      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1320  | 823  | 229 | 262 | 6 |         |       |
| 142 | 8s    | 327      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2670  | 1645 | 501 | 518 | 6 |         |       |
| 142 | 9a    | 180      | Total | C    | N   | O   |   | 0       | 0     |
|     |       |          | 1504  | 916  | 305 | 283 |   |         |       |
| 142 | 9s    | 344      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2824  | 1739 | 534 | 545 | 6 |         |       |

- Molecule 143 is a protein called ODAD1 central coiled coil region domain-containing protein.

| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 143 | 7t    | 179      | Total<br>1441 | C<br>888  | N<br>260 | O<br>288 | S<br>5  | 0       | 0     |
| 143 | 8t    | 339      | Total<br>2727 | C<br>1662 | N<br>501 | O<br>552 | S<br>12 | 0       | 0     |
| 143 | 9b    | 181      | Total<br>1450 | C<br>871  | N<br>273 | O<br>299 | S<br>7  | 0       | 0     |
| 143 | 9t    | 360      | Total<br>2891 | C<br>1759 | N<br>533 | O<br>587 | S<br>12 | 0       | 0     |

- Molecule 144 is a protein called Enkurin domain-containing protein.

| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 144 | 8D    | 249      | Total<br>2017 | C<br>1253 | N<br>377 | O<br>376 | S<br>11 | 0       | 0     |
| 144 | 8E    | 120      | Total<br>990  | C<br>609  | N<br>183 | O<br>193 | S<br>5  | 0       | 0     |
| 144 | 8F    | 239      | Total<br>1937 | C<br>1202 | N<br>360 | O<br>364 | S<br>11 | 0       | 0     |
| 144 | 8G    | 249      | Total<br>2017 | C<br>1253 | N<br>377 | O<br>376 | S<br>11 | 0       | 0     |
| 144 | 8H    | 120      | Total<br>990  | C<br>609  | N<br>183 | O<br>193 | S<br>5  | 0       | 0     |
| 144 | 8I    | 239      | Total<br>1937 | C<br>1202 | N<br>360 | O<br>364 | S<br>11 | 0       | 0     |
| 144 | 8J    | 249      | Total<br>2017 | C<br>1253 | N<br>377 | O<br>376 | S<br>11 | 0       | 0     |
| 144 | 8K    | 120      | Total<br>990  | C<br>609  | N<br>183 | O<br>193 | S<br>5  | 0       | 0     |

- Molecule 145 is a protein called PON3.

| Mol | Chain | Residues | Atoms        |          |          |          |        | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|-------|
| 145 | 8M    | 100      | Total<br>824 | C<br>509 | N<br>158 | O<br>149 | S<br>8 | 0       | 0     |
| 145 | 8N    | 108      | Total<br>889 | C<br>548 | N<br>171 | O<br>162 | S<br>8 | 0       | 0     |
| 145 | 8O    | 104      | Total<br>858 | C<br>528 | N<br>167 | O<br>155 | S<br>8 | 0       | 0     |
| 145 | 8P    | 100      | Total<br>824 | C<br>509 | N<br>158 | O<br>149 | S<br>8 | 0       | 0     |
| 145 | 8Q    | 108      | Total<br>889 | C<br>548 | N<br>171 | O<br>162 | S<br>8 | 0       | 0     |
| 145 | 8R    | 104      | Total<br>858 | C<br>528 | N<br>167 | O<br>155 | S<br>8 | 0       | 0     |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 145 | 8S    | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 824   | 509 | 158 | 149 | 8 |         |       |
| 145 | 8T    | 108      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 889   | 548 | 171 | 162 | 8 |         |       |

- Molecule 146 is a protein called PON4.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 146 | 8U    | 40       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 327   | 199 | 60  | 67  | 1  |         |       |
| 146 | 8V    | 131      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1054  | 633 | 203 | 208 | 10 |         |       |
| 146 | 8W    | 40       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 327   | 199 | 60  | 67  | 1  |         |       |
| 146 | 8X    | 40       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 327   | 199 | 60  | 67  | 1  |         |       |
| 146 | 8Y    | 131      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1054  | 633 | 203 | 208 | 10 |         |       |
| 146 | 8Z    | 40       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 327   | 199 | 60  | 67  | 1  |         |       |
| 146 | 9A    | 40       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 327   | 199 | 60  | 67  | 1  |         |       |
| 146 | 9B    | 116      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 942   | 564 | 181 | 187 | 10 |         |       |

- Molecule 147 is a protein called MC7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 147 | 9C    | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1642  | 1020 | 321 | 293 | 8 |         |       |
| 147 | 9D    | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1642  | 1020 | 321 | 293 | 8 |         |       |
| 147 | 9E    | 33       | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 274   | 177  | 46  | 50  | 1 |         |       |

- Molecule 148 is a protein called FAP96C/MC15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 148 | 9F    | 28       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 223   | 143 | 39  | 39  | 2 |         |       |
| 148 | 9G    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1218  | 770 | 211 | 229 | 8 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 148 | 9H    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1218  | 770 | 211 | 229 | 8 |         |       |
| 148 | 9I    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 798   | 499 | 141 | 154 | 4 |         |       |

- Molecule 149 is a protein called FAP96B.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 149 | 9J    | 173      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1432  | 926  | 252 | 246 | 8  |         |       |
| 149 | 9K    | 275      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2269  | 1458 | 402 | 398 | 11 |         |       |
| 149 | 9L    | 253      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2071  | 1328 | 364 | 368 | 11 |         |       |

- Molecule 150 is a protein called MOP23A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 150 | 9M    | 160      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1380  | 847 | 261 | 270 | 2 |         |       |
| 150 | 9N    | 160      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1380  | 847 | 261 | 270 | 2 |         |       |
| 150 | 9O    | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1373  | 843 | 260 | 268 | 2 |         |       |
| 150 | 9P    | 160      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1380  | 847 | 261 | 270 | 2 |         |       |
| 150 | 9Q    | 160      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1380  | 847 | 261 | 270 | 2 |         |       |
| 150 | 9R    | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1373  | 843 | 260 | 268 | 2 |         |       |
| 150 | 9S    | 160      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1380  | 847 | 261 | 270 | 2 |         |       |

- Molecule 151 is a protein called MOP23B.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 151 | 9T    | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1193  | 730 | 230 | 229 | 4 |         |       |
| 151 | 9U    | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1193  | 730 | 230 | 229 | 4 |         |       |
| 151 | 9V    | 132      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1091  | 669 | 210 | 208 | 4 |         |       |

- Molecule 152 is a protein called MOP23C.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 152 | 9W    | 71       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 583   | 368 | 100 | 113 | 2 |         |       |
| 152 | 9X    | 71       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 583   | 368 | 100 | 113 | 2 |         |       |
| 152 | 9Y    | 71       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 583   | 368 | 100 | 113 | 2 |         |       |

- Molecule 153 is a protein called Tubulin beta chain.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 153 | AA    | 430      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3372  | 2114 | 575 | 652 | 31 |         |       |
| 153 | AC    | 430      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3372  | 2114 | 575 | 652 | 31 |         |       |
| 153 | AE    | 430      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3372  | 2114 | 575 | 652 | 31 |         |       |
| 153 | AG    | 430      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3372  | 2114 | 575 | 652 | 31 |         |       |
| 153 | AI    | 430      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3372  | 2114 | 575 | 652 | 31 |         |       |
| 153 | AK    | 430      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3372  | 2114 | 575 | 652 | 31 |         |       |
| 153 | AM    | 430      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3372  | 2114 | 575 | 652 | 31 |         |       |
| 153 | AO    | 430      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3372  | 2114 | 575 | 652 | 31 |         |       |
| 153 | AQ    | 430      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3372  | 2114 | 575 | 652 | 31 |         |       |
| 153 | AS    | 430      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3372  | 2114 | 575 | 652 | 31 |         |       |
| 153 | AU    | 430      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3372  | 2114 | 575 | 652 | 31 |         |       |
| 153 | AW    | 430      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3372  | 2114 | 575 | 652 | 31 |         |       |
| 153 | AY    | 430      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3372  | 2114 | 575 | 652 | 31 |         |       |
| 153 | Aa    | 430      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3372  | 2114 | 575 | 652 | 31 |         |       |
| 153 | Ac    | 430      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3372  | 2114 | 575 | 652 | 31 |         |       |
| 153 | Ae    | 430      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3372  | 2114 | 575 | 652 | 31 |         |       |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 153 | Ag    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | Ai    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | Ak    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | Am    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | Ao    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | BA    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | BC    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | BG    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | BI    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | BK    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | BM    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | BO    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | BQ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | BS    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | BU    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | BW    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | BY    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | CA    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | CC    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | CE    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | CH    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 153 | CK    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | CM    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | CO    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | CQ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | CS    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | CU    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | CW    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | CY    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | DA    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | DC    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | DE    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | DG    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | DI    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | DK    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | DN    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | DP    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | DR    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | DT    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | DV    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | DX    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | DZ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 153 | EB    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | ED    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | EF    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | EH    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | EJ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | EL    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | EN    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | ER    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | ET    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | EV    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | EX    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | EZ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | FB    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | FD    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | FF    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | FH    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | FJ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | FL    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | FN    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | FP    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | FR    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 153 | FT    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | FV    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | FX    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | FZ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | GB    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | GD    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | GF    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | GH    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | GJ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | GL    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | GN    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | GP    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | GR    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | GT    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | GV    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | GX    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | GZ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | HB    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | HD    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | HF    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | HH    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 153 | HJ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | HL    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | HN    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | HP    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | HR    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | HT    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | HV    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | HX    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | HZ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | IB    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | ID    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | IF    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | IH    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | IJ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | IL    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | IN    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | IP    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | IR    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | IT    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | IV    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | IX    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 153 | IZ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | JB    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | JD    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | JF    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | JG    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | JI    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | JK    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | JM    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | JO    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | JQ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | JS    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | JU    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | JW    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | JY    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | KA    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | KC    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | KE    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | KG    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | KI    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | KK    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | KM    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 153 | KO    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | KQ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | KS    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | KU    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | KW    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | KY    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | LA    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | LC    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | LE    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | LG    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | LI    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | LK    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | LM    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | LO    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | LQ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | LS    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | LU    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | LW    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | LY    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | MA    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | MC    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 153 | ME    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | MG    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | MI    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | MK    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | MM    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | MO    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | MQ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | MU    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | MW    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | MY    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | NA    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | NC    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | NE    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | NG    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | NI    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | NK    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | NM    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | NO    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | NQ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | NS    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | NU    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 153 | NY    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | OA    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | OC    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | OE    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | OG    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | OI    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | OK    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | OM    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | OO    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | OQ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | OS    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | OU    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | OW    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | OY    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | PA    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | PD    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | PF    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | PH    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | PJ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | PL    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | PN    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 153 | PP    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | PR    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | PT    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | PV    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | PX    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | PZ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | QB    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | QD    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | QF    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | QH    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | QJ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | QL    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | QN    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | QP    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | QR    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | QT    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | QV    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | QX    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | QZ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | RB    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | RD    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 153 | RF    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | RH    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | RJ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | RL    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | RN    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | RP    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | RR    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | RT    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | RV    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | RX    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | RZ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | SB    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | SD    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | SF    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | SH    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | SJ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | SL    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | SN    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | SP    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | SR    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | ST    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 153 | SV    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | SX    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | SZ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | TB    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | TD    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | TF    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | TH    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | TJ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | TL    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | TN    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | TP    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | TS    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | TU    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | TW    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | TY    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | UA    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | UC    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | UE    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | UG    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | UI    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | UK    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 153 | UM    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | UO    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | UQ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | US    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | UU    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | UX    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | UZ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | VB    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | VD    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | VF    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | VH    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | VJ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | VL    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | VN    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | VP    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | VR    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | VT    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | VV    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | VX    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | VZ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | WB    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 153 | WD    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | WF    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | WH    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | WJ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | WL    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | WN    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | WP    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | WR    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | WT    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | WV    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | WX    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | WZ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | XB    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | XD    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | XF    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | XH    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | XJ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | XL    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | XN    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | XP    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | XR    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 153 | XT    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | XV    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | XX    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | XZ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | YB    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | YD    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | YF    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | YH    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | YK    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | YM    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | YO    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | YQ    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | YS    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | YU    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | YW    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | YY    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | ZA    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | ZC    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | ZE    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | ZG    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |
| 153 | ZI    | 430      | Total<br>3372 | C<br>2114 | N<br>575 | O<br>652 | S<br>31 | 0       | 0     |

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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 153 | ZK    | 430      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3372  | 2114 | 575 | 652 | 31 |         |       |
| 153 | ZM    | 430      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3372  | 2114 | 575 | 652 | 31 |         |       |
| 153 | ZO    | 430      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3372  | 2114 | 575 | 652 | 31 |         |       |
| 153 | ZQ    | 430      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3372  | 2114 | 575 | 652 | 31 |         |       |
| 153 | ZS    | 430      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3372  | 2114 | 575 | 652 | 31 |         |       |
| 153 | ZU    | 430      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3372  | 2114 | 575 | 652 | 31 |         |       |
| 153 | ZW    | 430      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3372  | 2114 | 575 | 652 | 31 |         |       |
| 153 | ZY    | 430      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3372  | 2114 | 575 | 652 | 31 |         |       |

- Molecule 154 is a protein called Tubulin alpha chain.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 154 | AB    | 442      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3421  | 2158 | 582 | 660 | 21 |         |       |
| 154 | AD    | 442      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3421  | 2158 | 582 | 660 | 21 |         |       |
| 154 | AF    | 442      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3421  | 2158 | 582 | 660 | 21 |         |       |
| 154 | AH    | 442      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3421  | 2158 | 582 | 660 | 21 |         |       |
| 154 | AJ    | 442      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3421  | 2158 | 582 | 660 | 21 |         |       |
| 154 | AL    | 442      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3421  | 2158 | 582 | 660 | 21 |         |       |
| 154 | AN    | 442      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3421  | 2158 | 582 | 660 | 21 |         |       |
| 154 | AP    | 442      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3421  | 2158 | 582 | 660 | 21 |         |       |
| 154 | AR    | 442      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3421  | 2158 | 582 | 660 | 21 |         |       |
| 154 | AT    | 442      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3421  | 2158 | 582 | 660 | 21 |         |       |
| 154 | AV    | 442      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3421  | 2158 | 582 | 660 | 21 |         |       |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 154 | AX    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | AZ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | Ab    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | Ad    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | Af    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | Ah    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | Aj    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | Al    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | An    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | Ap    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | BB    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | BD    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | BF    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | BH    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | BJ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | BL    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | BN    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | BP    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | BR    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | BT    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | BV    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 154 | BX    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | BZ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | CB    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | CD    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | CF    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | CI    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | CJ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | CL    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | CN    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | CP    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | CR    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | CT    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | CV    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | CX    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | CZ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | DB    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | DD    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | DF    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | DH    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | DJ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | DL    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 154 | DM    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | DO    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | DQ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | DS    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | DU    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | DW    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | DY    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | EA    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | EC    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | EE    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | EG    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | EI    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | EK    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | EM    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | EO    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | EQ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | ES    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | EU    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | EW    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | EY    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | FA    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 154 | FC    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | FE    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | FG    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | FI    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | FK    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | FM    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | FO    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | FQ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | FS    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | FW    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | FY    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | GA    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | GC    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | GE    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | GG    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | GI    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | GK    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | GM    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | GO    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | GQ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | GS    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 154 | GU    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | GW    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | HA    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | HC    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | HE    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | HG    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | HI    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | HK    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | HM    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | HO    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | HQ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | HS    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | HU    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | HW    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | HY    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | IA    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | IE    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | IG    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | II    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | IK    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | IM    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 154 | IO    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | IQ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | IS    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | IU    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | IW    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | IY    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | JA    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | JC    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | JE    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | JH    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | JJ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | JL    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | JN    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | JP    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | JR    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | JT    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | JV    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | JX    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | JZ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | KB    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | KD    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 154 | KF    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | KH    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | KJ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | KL    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | KN    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | KP    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | KR    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | KT    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | KV    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | KX    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | KZ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | LB    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | LD    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | LF    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | LH    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | LJ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | LL    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | LN    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | LP    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | LR    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | LT    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 154 | LV    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | LX    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | LZ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | MB    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | MD    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | MF    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | MH    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | MJ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | ML    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | MN    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | MP    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | MR    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | MT    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | MV    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | MX    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | MZ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | NB    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | ND    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | NF    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | NH    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | NJ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 154 | NL    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | NN    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | NP    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | NR    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | NT    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | NV    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | NX    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | NZ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | OB    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | OD    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | OF    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | OH    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | OJ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | OL    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | ON    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | OP    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | OR    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | OT    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | OV    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | OX    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | OZ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 154 | PC    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | PE    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | PG    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | PI    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | PK    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | PM    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | PO    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | PQ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | PS    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | PU    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | PW    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | PY    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | QA    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | QC    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | QE    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | QG    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | QI    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | QK    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | QM    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | QO    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | QQ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 154 | QS    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | QU    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | QW    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | QY    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | RA    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | RC    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | RE    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | RG    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | RI    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | RK    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | RM    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | RO    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | RQ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | RS    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | RU    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | RW    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | RY    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | SA    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | SC    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | SE    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | SG    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 154 | SI    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | SK    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | SM    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | SO    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | SQ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | SS    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | SU    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | SW    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | SY    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | TA    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | TC    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | TE    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | TG    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | TI    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | TK    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | TM    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | TO    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | TQ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | TR    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | TT    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | TV    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 154 | TX    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | TZ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | UB    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | UD    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | UF    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | UH    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | UJ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | UL    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | UN    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | UP    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | UR    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | UT    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | UW    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | UY    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | VA    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | VC    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | VE    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | VG    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | VI    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | VK    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | VM    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 154 | VO    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | VQ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | VS    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | VU    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | VW    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | VY    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | WA    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | WC    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | WE    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | WG    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | WI    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | WK    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | WM    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | WO    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | WQ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | WS    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | WU    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | WW    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | WY    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | XA    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | XC    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 154 | XE    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | XG    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | XI    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | XK    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | XM    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | XO    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | XQ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | XS    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | XU    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | XW    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | XY    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | YA    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | YC    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | YE    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | YG    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | YJ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | YL    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | YN    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | YP    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | YR    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | YT    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 154 | YV    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | YX    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | YZ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | ZB    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | ZD    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | ZF    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | ZH    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | ZJ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | ZL    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | ZN    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | ZP    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | ZR    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | ZT    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | ZV    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | ZX    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |
| 154 | ZZ    | 442      | Total<br>3421 | C<br>2158 | N<br>582 | O<br>660 | S<br>21 | 0       | 0     |

- Molecule 155 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 155 | 0q    | 2        | Total<br>2 | Zn<br>2 | 0       |
| 155 | 5C    | 2        | Total<br>2 | Zn<br>2 | 0       |
| 155 | 5E    | 1        | Total<br>1 | Zn<br>1 | 0       |

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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 155 | 5F    | 2        | Total<br>2 | Zn<br>2 | 0       |
| 155 | 5H    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 155 | 5I    | 2        | Total<br>2 | Zn<br>2 | 0       |
| 155 | 5L    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 155 | 5M    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 155 | 7V    | 2        | Total<br>2 | Zn<br>2 | 0       |
| 155 | 7W    | 2        | Total<br>2 | Zn<br>2 | 0       |
| 155 | 7X    | 3        | Total<br>3 | Zn<br>3 | 0       |
| 155 | 7Y    | 2        | Total<br>2 | Zn<br>2 | 0       |
| 155 | 7Z    | 2        | Total<br>2 | Zn<br>2 | 0       |
| 155 | 7d    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 155 | 8A    | 3        | Total<br>3 | Zn<br>3 | 0       |
| 155 | 8B    | 2        | Total<br>2 | Zn<br>2 | 0       |
| 155 | 8C    | 3        | Total<br>3 | Zn<br>3 | 0       |
| 155 | 8D    | 3        | Total<br>3 | Zn<br>3 | 0       |
| 155 | 8F    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 155 | 8G    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 155 | 8J    | 2        | Total<br>2 | Zn<br>2 | 0       |
| 155 | 8M    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 155 | 8N    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 155 | 8O    | 1        | Total<br>1 | Zn<br>1 | 0       |

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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 155 | 8P    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 155 | 8Q    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 155 | 8R    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 155 | 8S    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 155 | 8T    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 155 | 8V    | 3        | Total<br>3 | Zn<br>3 | 0       |
| 155 | 8Y    | 3        | Total<br>3 | Zn<br>3 | 0       |
| 155 | 8d    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 155 | 9B    | 3        | Total<br>3 | Zn<br>3 | 0       |
| 155 | 9d    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 155 | LP    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 155 | LV    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 155 | MB    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 155 | MD    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 155 | MN    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 155 | MV    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 155 | MX    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 155 | NF    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 155 | NH    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 155 | NJ    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 155 | NR    | 1        | Total<br>1 | Zn<br>1 | 0       |

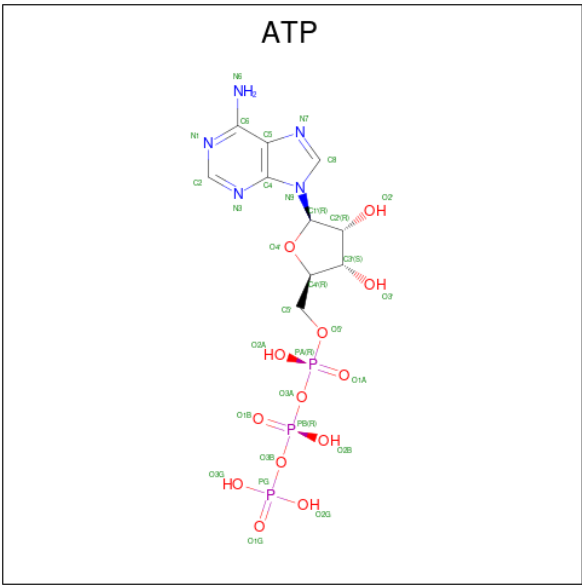
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| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
|     |       |          | Total | Zn |         |
| 155 | NV    | 1        | 1     | 1  | 0       |

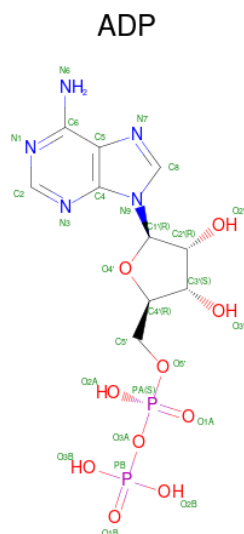
- Molecule 156 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



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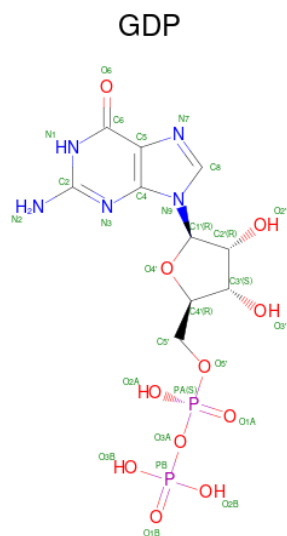
| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 156 | 7f    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 156 | 7f    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 156 | 8e    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 156 | 8e    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 156 | 8e    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 156 | 8f    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 156 | 8f    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 156 | 8f    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 156 | 9e    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 156 | 9e    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 156 | 9e    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 156 | 9f    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 156 | 9f    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 156 | 9f    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |

- Molecule 157 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 157 | 7a    | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 157 | 7b    | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 157 | 7e    | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 157 | 7f    | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 157 | 8e    | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 157 | 8f    | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 157 | 9e    | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 157 | 9f    | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |

- Molecule 158 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$ ).



| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 158 | AA    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | AC    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | AE    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | AG    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | AI    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | AK    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | AM    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | AO    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | AQ    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | AS    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | AU    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | AW    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | AY    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | Aa    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |

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| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 158 | Ac    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | Ae    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | Ag    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | Ai    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | Ak    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | Am    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | Ao    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | BA    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | BC    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | BG    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | BI    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | BK    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | BM    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | BO    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | BQ    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | BS    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | BU    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | BW    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | BY    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | CA    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | CC    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |

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| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 158 | CE    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | CH    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | CK    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | CM    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | CO    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | CQ    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | CS    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | CU    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | CW    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | CY    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | DA    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | DC    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | DE    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | DG    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | DI    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | DK    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | DN    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | DP    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | DR    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | DT    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | DV    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |

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| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 158 | DX    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | DZ    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | EB    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | ED    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | EF    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | EH    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | EJ    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | EL    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | EN    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | ER    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | ET    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | EV    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | EX    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | EZ    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | FB    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | FD    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | FF    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | FH    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | FJ    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | FL    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | FN    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |

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| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 158 | FP    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | FR    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | FT    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | FV    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | FX    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | FZ    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | GB    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | GD    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | GF    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | GH    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | GJ    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | GL    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | GN    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | GP    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | GR    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | GT    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | GV    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | GX    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | GZ    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | HB    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | HD    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |

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| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 158 | HF    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | HH    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | HJ    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | HL    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | HN    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | HP    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | HR    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | HT    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | HV    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | HX    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | HZ    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | IB    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | ID    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | IF    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | IH    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | IJ    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | IL    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | IN    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | IP    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | IR    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | IT    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |

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| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 158 | IV    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | IX    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | IZ    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | JB    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | JD    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | JF    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | JG    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | JI    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | JK    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | JM    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | JO    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | JQ    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | JS    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | JU    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | JW    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | JY    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | KA    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | KC    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | KE    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | KG    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | KI    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |

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| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 158 | KK    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | KM    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | KO    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | KQ    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | KS    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | KU    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | KW    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | KY    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | LA    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | LC    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | LE    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | LG    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | LI    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | LK    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | LM    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | LO    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | LQ    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | LS    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | LU    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | LW    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | LY    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |

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| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 158 | MA    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | MC    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | ME    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | MG    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | MI    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | MK    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | MM    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | MO    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | MQ    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | MU    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | MW    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | MY    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | NA    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | NC    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | NE    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | NG    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | NI    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | NK    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | NM    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | NO    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | NQ    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |

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| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 158 | NS    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | NU    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | NY    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | OA    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | OC    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | OE    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | OG    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | OI    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | OK    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | OM    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | OO    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | OQ    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | OS    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | OU    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | OW    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | OY    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | PA    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | PD    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | PF    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | PH    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | PJ    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |

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| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 158 | PL    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | PN    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | PP    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | PR    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | PT    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | PV    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | PX    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | PZ    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | QB    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | QD    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | QF    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | QH    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | QJ    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | QL    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | QN    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | QP    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | QR    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | QT    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | QV    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | QX    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | QZ    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |

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| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 158 | RB    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | RD    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | RF    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | RH    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | RJ    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | RL    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | RN    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | RP    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | RR    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | RT    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | RV    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | RX    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | RZ    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | SB    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | SD    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | SF    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | SH    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | SJ    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | SL    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | SN    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | SP    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |

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| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 158 | SR    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | ST    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | SV    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | SX    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | SZ    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | TB    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | TD    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | TF    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | TH    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | TJ    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | TL    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | TN    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | TP    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | TS    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | TU    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | TW    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | TY    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | UA    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | UC    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | UE    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | UG    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |

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| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 158 | UI    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | UK    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | UM    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | UO    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | UQ    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | US    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | UU    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | UX    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | UZ    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | VB    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | VD    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | VF    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | VH    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | VJ    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | VL    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | VN    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | VP    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | VR    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | VT    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | VV    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | VX    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |

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| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 158 | VZ    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | WB    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | WD    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | WF    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | WH    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | WJ    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | WL    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | WN    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | WP    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | WR    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | WT    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | WV    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | WX    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | WZ    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | XB    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | XD    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | XF    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | XH    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | XJ    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | XL    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | XN    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |

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| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 158 | XP    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | XR    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | XT    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | XV    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | XX    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | XZ    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | YB    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | YD    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | YF    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | YH    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | YK    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | YM    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | YO    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | YQ    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | YS    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | YU    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | YW    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | YY    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | ZA    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | ZC    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |
| 158 | ZE    | 1        | Total<br>28 | C<br>10 | N<br>5 | O<br>11 | P<br>2 | 0       |

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| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 158 | ZG    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | ZI    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | ZK    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | ZM    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | ZO    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | ZQ    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | ZS    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | ZU    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | ZW    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |
| 158 | ZY    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 28    | 10 | 5 | 11 | 2 |         |

- Molecule 159 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 159 | AB    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 159 | AD    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 159 | AF    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 159 | AH    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 159 | AJ    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 159 | AL    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 159 | AN    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 159 | AP    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 159 | AR    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 159 | AT    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | AV    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | AX    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | AZ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | Ab    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | Ad    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | Af    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | Ah    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | Aj    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | Al    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | An    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | Ap    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | BB    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | BD    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | BF    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | BH    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | BJ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | BL    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | BN    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | BP    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | BR    | 1        | Total<br>1 | Mg<br>1 | 0       |

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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 159 | BT    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | BV    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | BX    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | BZ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | CB    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | CD    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | CF    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | CI    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | CJ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | CL    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | CN    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | CP    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | CR    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | CT    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | CV    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | CX    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | CZ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | DB    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | DD    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | DF    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | DH    | 1        | Total<br>1 | Mg<br>1 | 0       |

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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 159 | DJ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | DL    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | DM    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | DO    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | DQ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | DS    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | DU    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | DW    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | DY    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | EA    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | EC    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | EE    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | EG    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | EI    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | EK    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | EM    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | EO    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | EQ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | ES    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | EU    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | EW    | 1        | Total<br>1 | Mg<br>1 | 0       |

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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 159 | EZ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | FA    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | FC    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | FE    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | FG    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | FI    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | FL    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | FM    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | FO    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | FQ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | FS    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | FW    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | FY    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | GA    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | GC    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | GE    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | GG    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | GI    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | GK    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | GM    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | GO    | 1        | Total<br>1 | Mg<br>1 | 0       |

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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 159 | GQ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | GS    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | GU    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | GW    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | HA    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | HC    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | HE    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | HG    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | HI    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | HK    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | HM    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | HO    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | HQ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | HS    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | HU    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | HW    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | HY    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | IA    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | IE    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | IG    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | II    | 1        | Total<br>1 | Mg<br>1 | 0       |

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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 159 | IK    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | IM    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | IO    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | IQ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | IS    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | IU    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | IW    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | IY    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | JA    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | JC    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | JE    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | JH    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | JJ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | JL    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | JN    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | JP    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | JR    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | JT    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | JV    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | JX    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | JZ    | 1        | Total<br>1 | Mg<br>1 | 0       |

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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 159 | KB    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | KD    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | KF    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | KH    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | KJ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | KL    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | KN    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | KP    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | KR    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | KT    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | KV    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | KX    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | KZ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | LB    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | LD    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | LF    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | LH    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | LJ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | LL    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | LN    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | LP    | 1        | Total<br>1 | Mg<br>1 | 0       |

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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 159 | LR    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | LT    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | LV    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | LX    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | LZ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | MB    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | MD    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | MF    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | MH    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | MJ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | ML    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | MN    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | MP    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | MR    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | MT    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | MV    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | MX    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | MZ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | NB    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | ND    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | NF    | 1        | Total<br>1 | Mg<br>1 | 0       |

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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 159 | NH    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | NJ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | NL    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | NN    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | NP    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | NR    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | NT    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | NV    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | NX    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | NZ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | OB    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | OD    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | OF    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | OH    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | OJ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | OL    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | ON    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | OP    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | OR    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | OT    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | OV    | 1        | Total<br>1 | Mg<br>1 | 0       |

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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 159 | OX    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | OZ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | PC    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | PE    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | PG    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | PI    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | PK    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | PM    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | PO    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | PQ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | PS    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | PU    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | PW    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | PY    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | QA    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | QC    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | QE    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | QG    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | QI    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | QK    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | QM    | 1        | Total<br>1 | Mg<br>1 | 0       |

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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 159 | QO    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | QQ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | QS    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | QU    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | QW    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | QY    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | RA    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | RC    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | RE    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | RG    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | RI    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | RK    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | RM    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | RO    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | RQ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | RS    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | RU    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | RW    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | RY    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | SA    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | SC    | 1        | Total<br>1 | Mg<br>1 | 0       |

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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 159 | SE    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | SG    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | SI    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | SK    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | SM    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | SO    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | SQ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | SS    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | SU    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | SW    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | SY    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | TA    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | TC    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | TE    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | TG    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | TI    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | TK    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | TM    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | TO    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | TQ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | TR    | 1        | Total<br>1 | Mg<br>1 | 0       |

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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 159 | TT    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | TV    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | TX    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | TZ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | UB    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | UD    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | UF    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | UH    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | UJ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | UL    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | UN    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | UP    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | UR    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | UT    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | UW    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | UY    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | VA    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | VC    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | VE    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | VG    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | VI    | 1        | Total<br>1 | Mg<br>1 | 0       |

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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 159 | VK    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | VM    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | VO    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | VQ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | VS    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | VU    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | VW    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | VY    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | WA    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | WC    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | WE    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | WG    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | WI    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | WK    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | WM    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | WO    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | WQ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | WS    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | WU    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | WW    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | WY    | 1        | Total<br>1 | Mg<br>1 | 0       |

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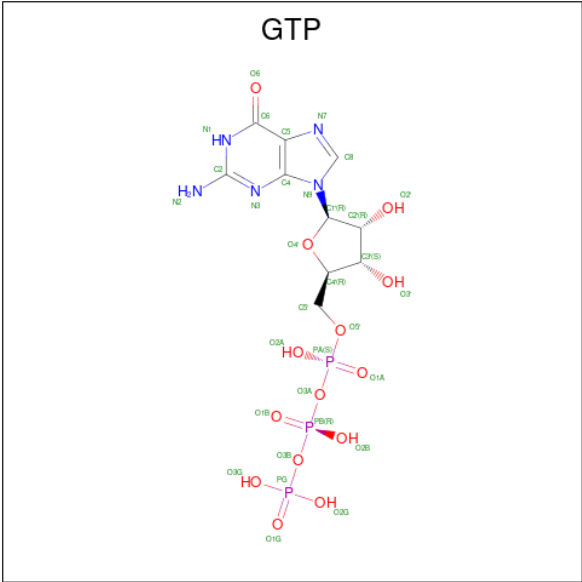
| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 159 | XA    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | XC    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | XE    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | XG    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | XI    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | XK    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | XM    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | XO    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | XQ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | XS    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | XU    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | XW    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | XY    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | YA    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | YC    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | YE    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | YG    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | YJ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | YL    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | YN    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | YP    | 1        | Total<br>1 | Mg<br>1 | 0       |

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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 159 | YR    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | YT    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | YV    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | YX    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | YZ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | ZB    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | ZD    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | ZF    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | ZH    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | ZJ    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | ZL    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | ZN    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | ZP    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | ZR    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | ZT    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | ZV    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | ZX    | 1        | Total<br>1 | Mg<br>1 | 0       |
| 159 | ZZ    | 1        | Total<br>1 | Mg<br>1 | 0       |

- Molecule 160 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 160 | AB    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 160 | AD    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 160 | AF    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 160 | AH    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 160 | AJ    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 160 | AL    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 160 | AN    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 160 | AP    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 160 | AR    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 160 | AT    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 160 | AV    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 160 | AX    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 160 | AZ    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |
| 160 | Ab    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |

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| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 160 | Ad    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | Af    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | Ah    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | Aj    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | Al    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | An    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | Ap    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | BB    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | BD    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | BF    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | BH    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | BJ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | BL    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | BN    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | BP    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | BR    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | BT    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | BV    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | BX    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | BZ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | CB    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |

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| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 160 | CD    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | CF    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | CI    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | CJ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | CL    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | CN    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | CP    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | CR    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | CT    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | CV    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | CX    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | CZ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | DB    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | DD    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | DF    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | DH    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | DJ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | DL    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | DM    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | DO    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | DQ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |

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| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 160 | DS    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | DU    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | DW    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | DY    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | EA    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | EC    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | EE    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | EG    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | EI    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | EK    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | EM    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | EO    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | EQ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | ES    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | EU    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | EW    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | EY    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | FA    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | FC    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | FE    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | FG    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |

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| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 160 | FI    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | FK    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | FM    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | FO    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | FQ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | FS    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | FW    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | FY    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | GA    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | GC    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | GE    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | GG    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | GI    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | GK    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | GM    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | GO    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | GQ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | GS    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | GU    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | GW    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | HA    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |

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| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 160 | HC    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | HE    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | HG    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | HI    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | HK    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | HM    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | HO    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | HQ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | HS    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | HU    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | HW    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | HY    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | IA    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | IE    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | IG    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | II    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | IK    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | IM    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | IO    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | IQ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | IS    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |

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| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 160 | IU    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | IW    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | IY    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | JA    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | JC    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | JE    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | JH    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | JJ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | JL    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | JN    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | JP    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | JR    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | JT    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | JV    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | JX    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | JZ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | KB    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | KD    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | KF    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | KH    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | KJ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |

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| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 160 | KL    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | KN    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | KP    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | KR    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | KT    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | KV    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | KX    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | KZ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | LB    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | LD    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | LF    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | LH    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | LJ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | LL    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | LN    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | LP    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | LR    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | LT    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | LV    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | LX    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | LZ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |

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| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 160 | MB    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | MD    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | MF    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | MH    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | MJ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | ML    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | MN    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | MP    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | MR    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | MT    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | MV    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | MX    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | MZ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | NB    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | ND    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | NF    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | NH    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | NJ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | NL    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | NN    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | NP    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |

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| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 160 | NR    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | NT    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | NV    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | NX    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | NZ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | OB    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | OD    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | OF    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | OH    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | OJ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | OL    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | ON    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | OP    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | OR    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | OT    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | OV    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | OX    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | OZ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | PC    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | PE    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | PG    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |

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| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 160 | PI    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | PK    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | PM    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | PO    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | PQ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | PS    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | PU    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | PW    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | PY    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | QA    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | QC    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | QE    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | QG    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | QI    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | QK    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | QM    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | QO    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | QQ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | QS    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | QU    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | QW    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |

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| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 160 | QY    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | RA    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | RC    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | RE    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | RG    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | RI    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | RK    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | RM    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | RO    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | RQ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | RS    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | RU    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | RW    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | RY    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | SA    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | SC    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | SE    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | SG    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | SI    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | SK    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | SM    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |

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| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 160 | SO    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | SQ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | SS    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | SU    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | SW    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | SY    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | TA    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | TC    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | TE    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | TG    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | TI    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | TK    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | TM    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | TO    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | TQ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | TR    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | TT    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | TV    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | TX    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | TZ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | UB    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |

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| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 160 | UD    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | UF    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | UH    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | UJ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | UL    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | UN    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | UP    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | UR    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | UT    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | UW    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | UY    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | VA    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | VC    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | VE    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | VG    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | VI    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | VK    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | VM    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | VO    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | VQ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | VS    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |

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| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 160 | VU    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | VW    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | VY    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | WA    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | WC    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | WE    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | WG    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | WI    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | WK    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | WM    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | WO    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | WQ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | WS    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | WU    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | WW    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | WY    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | XA    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | XC    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | XE    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | XG    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | XI    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |

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| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 160 | XK    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | XM    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | XO    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | XQ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | XS    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | XU    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | XW    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | XY    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | YA    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | YC    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | YE    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | YG    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | YJ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | YL    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | YN    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | YP    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | YR    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | YT    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | YV    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | YX    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | YZ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |

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| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 160 | ZB    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | ZD    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | ZF    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | ZH    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | ZJ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | ZL    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | ZN    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | ZP    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | ZR    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | ZT    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | ZV    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | ZX    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |
| 160 | ZZ    | 1        | Total<br>32 | C<br>10 | N<br>5 | O<br>14 | P<br>3 | 0       |

MolProbity failed to run properly - this section is therefore empty.

### 3 Experimental information

| Property                             | Value                         | Source    |
|--------------------------------------|-------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE               | Depositor |
| Imposed symmetry                     | POINT, C1                     | Depositor |
| Number of particles used             | 244497                        | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF             | Depositor |
| CTF correction method                | PHASE FLIPPING ONLY           | Depositor |
| Microscope                           | TFS KRIOS                     | Depositor |
| Voltage (kV)                         | 300                           | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                            | Depositor |
| Minimum defocus (nm)                 | 1600                          | Depositor |
| Maximum defocus (nm)                 | 2400                          | Depositor |
| Magnification                        | 81000                         | Depositor |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value                    | 2.426                         | Depositor |
| Minimum map value                    | 0.000                         | Depositor |
| Average map value                    | 0.015                         | Depositor |
| Map value standard deviation         | 0.077                         | Depositor |
| Recommended contour level            | 0.15                          | Depositor |
| Map size ( $\text{\AA}$ )            | 836.0, 946.0, 1320.0          | wwPDB     |
| Map dimensions                       | 760, 860, 1200                | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0              | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.1, 1.1, 1.1                 | Depositor |

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

MolProbity failed to run properly - this section is therefore empty.

### 4.3 Torsion angles [i](#)

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

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

### 4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 4.6 Ligand geometry [i](#)

Of 1125 ligands modelled in this entry, 412 are monoatomic - leaving 713 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 160 | GTP  | UT    | 501  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.96 | 4 (8%)   |
| 160 | GTP  | PY    | 602  | 159  | 33,34,34     | 0.67 | 0        | 50,54,54    | 0.94 | 4 (8%)   |
| 160 | GTP  | MV    | 502  | 159  | 33,34,34     | 0.71 | 0        | 50,54,54    | 0.96 | 4 (8%)   |
| 160 | GTP  | ZD    | 501  | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.96 | 3 (6%)   |
| 158 | GDP  | CE    | 501  | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 160 | GTP  | MP    | 501  | 159  | 33,34,34     | 0.72 | 0        | 50,54,54    | 0.95 | 4 (8%)   |
| 158 | GDP  | FZ    | 501  | -    | 29,30,30     | 1.17 | 3 (10%)  | 45,47,47    | 1.76 | 5 (11%)  |
| 158 | GDP  | ZS    | 501  | -    | 29,30,30     | 0.82 | 0        | 45,47,47    | 0.86 | 0        |
| 160 | GTP  | WM    | 602  | 159  | 33,34,34     | 0.67 | 0        | 50,54,54    | 0.91 | 3 (6%)   |
| 160 | GTP  | FE    | 501  | 159  | 33,34,34     | 0.66 | 0        | 50,54,54    | 0.92 | 3 (6%)   |
| 160 | GTP  | LP    | 502  | 159  | 33,34,34     | 0.71 | 0        | 50,54,54    | 0.95 | 3 (6%)   |
| 160 | GTP  | XM    | 602  | 159  | 33,34,34     | 0.53 | 0        | 50,54,54    | 0.56 | 0        |
| 158 | GDP  | Ao    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.93 | 2 (4%)   |
| 158 | GDP  | WP    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.87 | 2 (4%)   |
| 160 | GTP  | OH    | 501  | 159  | 33,34,34     | 0.67 | 0        | 50,54,54    | 0.96 | 3 (6%)   |
| 158 | GDP  | UM    | 501  | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.85 | 2 (4%)   |
| 158 | GDP  | WB    | 501  | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.85 | 2 (4%)   |
| 160 | GTP  | QG    | 602  | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.97 | 4 (8%)   |
| 160 | GTP  | JL    | 501  | 159  | 33,34,34     | 0.93 | 2 (6%)   | 50,54,54    | 0.89 | 0        |
| 158 | GDP  | IZ    | 501  | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.91 | 2 (4%)   |
| 158 | GDP  | FN    | 501  | -    | 29,30,30     | 0.49 | 0        | 45,47,47    | 0.88 | 2 (4%)   |
| 158 | GDP  | MW    | 501  | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.88 | 2 (4%)   |
| 160 | GTP  | Ap    | 501  | 159  | 33,34,34     | 0.67 | 0        | 50,54,54    | 0.97 | 3 (6%)   |
| 158 | GDP  | ZQ    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.93 | 2 (4%)   |
| 158 | GDP  | EV    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.93 | 2 (4%)   |
| 160 | GTP  | KF    | 602  | 159  | 33,34,34     | 0.67 | 0        | 50,54,54    | 0.93 | 3 (6%)   |
| 160 | GTP  | HK    | 501  | 159  | 33,34,34     | 0.65 | 0        | 50,54,54    | 0.95 | 3 (6%)   |
| 158 | GDP  | QD    | 501  | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.91 | 2 (4%)   |
| 160 | GTP  | ZR    | 602  | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.97 | 4 (8%)   |
| 156 | ATP  | 7e    | 4704 | -    | 32,33,33     | 0.48 | 0        | 48,52,52    | 0.40 | 0        |
| 160 | GTP  | AL    | 602  | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.99 | 4 (8%)   |
| 158 | GDP  | IJ    | 501  | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.92 | 2 (4%)   |
| 158 | GDP  | HB    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.49 | 0        |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 160 | GTP  | JE    | 501  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.96 | 4 (8%)   |
| 160 | GTP  | OT    | 602  | 159  | 33,34,34     | 0.65 | 0        | 50,54,54    | 0.97 | 3 (6%)   |
| 160 | GTP  | SE    | 501  | 159  | 33,34,34     | 0.72 | 0        | 50,54,54    | 0.96 | 3 (6%)   |
| 160 | GTP  | KX    | 501  | 159  | 33,34,34     | 0.74 | 0        | 50,54,54    | 0.95 | 3 (6%)   |
| 160 | GTP  | EA    | 501  | 159  | 33,34,34     | 0.66 | 0        | 50,54,54    | 0.93 | 3 (6%)   |
| 160 | GTP  | WC    | 501  | 159  | 33,34,34     | 0.64 | 0        | 50,54,54    | 0.93 | 3 (6%)   |
| 158 | GDP  | FH    | 501  | -    | 29,30,30     | 1.20 | 3 (10%)  | 45,47,47    | 1.76 | 6 (13%)  |
| 158 | GDP  | RB    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 158 | GDP  | IP    | 501  | -    | 29,30,30     | 1.16 | 3 (10%)  | 45,47,47    | 1.75 | 6 (13%)  |
| 160 | GTP  | VY    | 501  | 159  | 33,34,34     | 0.67 | 0        | 50,54,54    | 0.93 | 3 (6%)   |
| 160 | GTP  | PU    | 602  | 159  | 33,34,34     | 0.71 | 0        | 50,54,54    | 0.92 | 3 (6%)   |
| 160 | GTP  | QI    | 602  | 159  | 33,34,34     | 0.88 | 2 (6%)   | 50,54,54    | 1.59 | 8 (16%)  |
| 160 | GTP  | SO    | 501  | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.96 | 3 (6%)   |
| 160 | GTP  | LB    | 501  | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.95 | 4 (8%)   |
| 158 | GDP  | RF    | 501  | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.91 | 2 (4%)   |
| 158 | GDP  | FV    | 501  | -    | 29,30,30     | 1.19 | 3 (10%)  | 45,47,47    | 1.76 | 6 (13%)  |
| 160 | GTP  | MZ    | 602  | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.96 | 4 (8%)   |
| 158 | GDP  | JB    | 501  | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.91 | 2 (4%)   |
| 160 | GTP  | Ab    | 501  | 159  | 33,34,34     | 0.67 | 0        | 50,54,54    | 0.98 | 4 (8%)   |
| 156 | ATP  | 9f    | 4701 | -    | 32,33,33     | 0.49 | 1 (3%)   | 48,52,52    | 0.29 | 0        |
| 158 | GDP  | MI    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.91 | 2 (4%)   |
| 160 | GTP  | TT    | 602  | 159  | 33,34,34     | 0.72 | 0        | 50,54,54    | 0.95 | 3 (6%)   |
| 158 | GDP  | MU    | 501  | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 160 | GTP  | GA    | 602  | 159  | 33,34,34     | 0.90 | 0        | 50,54,54    | 1.56 | 9 (18%)  |
| 160 | GTP  | YC    | 501  | 159  | 33,34,34     | 0.71 | 0        | 50,54,54    | 0.98 | 4 (8%)   |
| 158 | GDP  | OC    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.92 | 2 (4%)   |
| 158 | GDP  | ZG    | 501  | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 158 | GDP  | JK    | 501  | -    | 29,30,30     | 1.14 | 3 (10%)  | 45,47,47    | 1.73 | 6 (13%)  |
| 158 | GDP  | KK    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.92 | 2 (4%)   |
| 160 | GTP  | DJ    | 501  | 159  | 33,34,34     | 0.67 | 0        | 50,54,54    | 0.97 | 3 (6%)   |
| 160 | GTP  | DS    | 602  | 159  | 33,34,34     | 0.88 | 0        | 50,54,54    | 1.55 | 8 (16%)  |
| 160 | GTP  | SU    | 501  | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.95 | 3 (6%)   |
| 160 | GTP  | SQ    | 602  | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.94 | 3 (6%)   |
| 158 | GDP  | OU    | 501  | -    | 29,30,30     | 0.49 | 0        | 45,47,47    | 0.91 | 2 (4%)   |
| 158 | GDP  | UO    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.89 | 2 (4%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 160 | GTP  | LZ    | 501 | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.95 | 3 (6%)   |
| 160 | GTP  | FS    | 602 | 159  | 33,34,34     | 0.67 | 0        | 50,54,54    | 0.97 | 3 (6%)   |
| 158 | GDP  | ZC    | 501 | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.91 | 2 (4%)   |
| 160 | GTP  | UL    | 602 | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.95 | 3 (6%)   |
| 160 | GTP  | GO    | 501 | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.95 | 3 (6%)   |
| 160 | GTP  | XG    | 602 | 159  | 33,34,34     | 0.71 | 0        | 50,54,54    | 0.96 | 4 (8%)   |
| 160 | GTP  | JX    | 501 | 159  | 33,34,34     | 0.85 | 0        | 50,54,54    | 1.55 | 8 (16%)  |
| 158 | GDP  | SL    | 501 | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.95 | 2 (4%)   |
| 160 | GTP  | JV    | 501 | 159  | 33,34,34     | 0.87 | 1 (3%)   | 50,54,54    | 1.54 | 8 (16%)  |
| 158 | GDP  | VF    | 501 | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.88 | 2 (4%)   |
| 160 | GTP  | MN    | 502 | 159  | 33,34,34     | 0.71 | 0        | 50,54,54    | 0.96 | 3 (6%)   |
| 158 | GDP  | NA    | 501 | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.93 | 2 (4%)   |
| 160 | GTP  | Ad    | 602 | 159  | 33,34,34     | 0.86 | 1 (3%)   | 50,54,54    | 1.59 | 8 (16%)  |
| 160 | GTP  | ZJ    | 501 | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.93 | 3 (6%)   |
| 158 | GDP  | DZ    | 501 | -    | 29,30,30     | 0.49 | 0        | 45,47,47    | 0.85 | 2 (4%)   |
| 158 | GDP  | BO    | 501 | -    | 29,30,30     | 1.17 | 3 (10%)  | 45,47,47    | 1.78 | 6 (13%)  |
| 158 | GDP  | NG    | 501 | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 158 | GDP  | RD    | 501 | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.88 | 2 (4%)   |
| 158 | GDP  | ZE    | 501 | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.91 | 2 (4%)   |
| 158 | GDP  | FF    | 501 | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.88 | 2 (4%)   |
| 158 | GDP  | CW    | 501 | -    | 29,30,30     | 1.16 | 3 (10%)  | 45,47,47    | 1.73 | 6 (13%)  |
| 160 | GTP  | WI    | 602 | 159  | 33,34,34     | 0.66 | 0        | 50,54,54    | 0.88 | 3 (6%)   |
| 158 | GDP  | NE    | 501 | -    | 29,30,30     | 0.54 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 158 | GDP  | FJ    | 501 | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.93 | 2 (4%)   |
| 158 | GDP  | NM    | 501 | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.92 | 2 (4%)   |
| 158 | GDP  | Aa    | 501 | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.93 | 2 (4%)   |
| 160 | GTP  | HW    | 501 | 159  | 33,34,34     | 0.65 | 0        | 50,54,54    | 0.95 | 3 (6%)   |
| 160 | GTP  | SS    | 602 | 159  | 33,34,34     | 0.90 | 2 (6%)   | 50,54,54    | 1.06 | 3 (6%)   |
| 158 | GDP  | BC    | 501 | -    | 29,30,30     | 1.17 | 3 (10%)  | 45,47,47    | 1.75 | 6 (13%)  |
| 160 | GTP  | BJ    | 602 | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.96 | 4 (8%)   |
| 158 | GDP  | ER    | 501 | -    | 29,30,30     | 1.15 | 3 (10%)  | 45,47,47    | 1.69 | 6 (13%)  |
| 158 | GDP  | LG    | 501 | -    | 29,30,30     | 0.54 | 0        | 45,47,47    | 0.93 | 2 (4%)   |
| 160 | GTP  | TO    | 501 | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.94 | 3 (6%)   |
| 160 | GTP  | FK    | 501 | 159  | 33,34,34     | 0.64 | 0        | 50,54,54    | 0.98 | 3 (6%)   |
| 158 | GDP  | CY    | 501 | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.90 | 2 (4%)   |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 158 | GDP  | KM    | 501  | -    | 29,30,30     | 0.56 | 0        | 45,47,47    | 0.99 | 2 (4%)   |
| 158 | GDP  | LM    | 501  | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 158 | GDP  | TH    | 501  | -    | 29,30,30     | 0.57 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 160 | GTP  | ZP    | 501  | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.98 | 3 (6%)   |
| 160 | GTP  | NR    | 502  | 159  | 33,34,34     | 0.71 | 0        | 50,54,54    | 0.95 | 4 (8%)   |
| 160 | GTP  | ON    | 501  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.97 | 3 (6%)   |
| 158 | GDP  | XZ    | 501  | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.87 | 2 (4%)   |
| 158 | GDP  | CK    | 501  | -    | 29,30,30     | 1.15 | 3 (10%)  | 45,47,47    | 1.72 | 6 (13%)  |
| 160 | GTP  | DW    | 602  | 159  | 33,34,34     | 0.87 | 0        | 50,54,54    | 1.56 | 8 (16%)  |
| 158 | GDP  | EJ    | 501  | -    | 29,30,30     | 0.49 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 160 | GTP  | TQ    | 602  | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.99 | 3 (6%)   |
| 160 | GTP  | NV    | 503  | 159  | 33,34,34     | 0.67 | 0        | 50,54,54    | 0.95 | 3 (6%)   |
| 158 | GDP  | VD    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 158 | GDP  | AM    | 501  | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.92 | 2 (4%)   |
| 156 | ATP  | 7f    | 4702 | -    | 32,33,33     | 0.43 | 0        | 48,52,52    | 0.29 | 0        |
| 160 | GTP  | FO    | 602  | 159  | 33,34,34     | 0.65 | 0        | 50,54,54    | 0.96 | 3 (6%)   |
| 160 | GTP  | MD    | 502  | 159  | 33,34,34     | 0.72 | 0        | 50,54,54    | 0.95 | 3 (6%)   |
| 160 | GTP  | MX    | 502  | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.97 | 3 (6%)   |
| 160 | GTP  | KL    | 602  | 159  | 33,34,34     | 0.73 | 0        | 50,54,54    | 0.98 | 3 (6%)   |
| 158 | GDP  | TS    | 501  | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.96 | 2 (4%)   |
| 158 | GDP  | FD    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.85 | 2 (4%)   |
| 160 | GTP  | TE    | 501  | 159  | 33,34,34     | 0.66 | 0        | 50,54,54    | 0.98 | 3 (6%)   |
| 160 | GTP  | LH    | 501  | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.97 | 3 (6%)   |
| 160 | GTP  | ZH    | 501  | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.98 | 4 (8%)   |
| 160 | GTP  | BN    | 602  | 159  | 33,34,34     | 0.87 | 1 (3%)   | 50,54,54    | 1.60 | 8 (16%)  |
| 158 | GDP  | TD    | 501  | -    | 29,30,30     | 0.49 | 0        | 45,47,47    | 0.93 | 2 (4%)   |
| 160 | GTP  | CR    | 501  | 159  | 33,34,34     | 0.67 | 0        | 50,54,54    | 0.94 | 3 (6%)   |
| 160 | GTP  | DD    | 501  | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.92 | 3 (6%)   |
| 158 | GDP  | CS    | 501  | -    | 29,30,30     | 1.14 | 3 (10%)  | 45,47,47    | 1.73 | 6 (13%)  |
| 158 | GDP  | RR    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.94 | 2 (4%)   |
| 158 | GDP  | NS    | 501  | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 158 | GDP  | QV    | 501  | -    | 29,30,30     | 0.54 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 160 | GTP  | BP    | 501  | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.98 | 3 (6%)   |
| 160 | GTP  | VU    | 501  | 159  | 33,34,34     | 0.65 | 0        | 50,54,54    | 0.92 | 3 (6%)   |
| 160 | GTP  | ML    | 602  | 159  | 33,34,34     | 0.71 | 0        | 50,54,54    | 0.96 | 3 (6%)   |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 160 | GTP  | UR    | 501  | 159  | 33,34,34     | 0.73 | 0        | 50,54,54    | 0.95 | 3 (6%)   |
| 158 | GDP  | UZ    | 501  | -    | 29,30,30     | 0.49 | 0        | 45,47,47    | 0.87 | 2 (4%)   |
| 160 | GTP  | CT    | 602  | 159  | 33,34,34     | 0.88 | 1 (3%)   | 50,54,54    | 1.57 | 8 (16%)  |
| 158 | GDP  | BM    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 160 | GTP  | CV    | 501  | 159  | 33,34,34     | 0.88 | 1 (3%)   | 50,54,54    | 1.58 | 8 (16%)  |
| 158 | GDP  | UC    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 160 | GTP  | EU    | 501  | 159  | 33,34,34     | 0.66 | 0        | 50,54,54    | 0.95 | 3 (6%)   |
| 160 | GTP  | PI    | 602  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.92 | 3 (6%)   |
| 158 | GDP  | OE    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 160 | GTP  | YX    | 602  | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.94 | 3 (6%)   |
| 160 | GTP  | AP    | 602  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.96 | 3 (6%)   |
| 158 | GDP  | WT    | 501  | -    | 29,30,30     | 0.54 | 0        | 45,47,47    | 0.87 | 2 (4%)   |
| 158 | GDP  | MG    | 501  | -    | 29,30,30     | 0.54 | 0        | 45,47,47    | 0.94 | 2 (4%)   |
| 160 | GTP  | FY    | 501  | 159  | 33,34,34     | 0.87 | 0        | 50,54,54    | 1.59 | 8 (16%)  |
| 160 | GTP  | AX    | 501  | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.97 | 4 (8%)   |
| 158 | GDP  | NY    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.94 | 2 (4%)   |
| 158 | GDP  | TF    | 501  | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 160 | GTP  | UB    | 501  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.96 | 3 (6%)   |
| 156 | ATP  | 8f    | 4702 | -    | 32,33,33     | 0.46 | 0        | 48,52,52    | 0.35 | 0        |
| 160 | GTP  | AJ    | 501  | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.96 | 3 (6%)   |
| 160 | GTP  | RW    | 501  | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.94 | 3 (6%)   |
| 160 | GTP  | EO    | 501  | 159  | 33,34,34     | 0.64 | 0        | 50,54,54    | 0.95 | 4 (8%)   |
| 158 | GDP  | JG    | 501  | -    | 29,30,30     | 1.17 | 3 (10%)  | 45,47,47    | 1.71 | 6 (13%)  |
| 158 | GDP  | PV    | 501  | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 158 | GDP  | IH    | 501  | -    | 29,30,30     | 1.16 | 3 (10%)  | 45,47,47    | 1.74 | 6 (13%)  |
| 160 | GTP  | BL    | 501  | 159  | 33,34,34     | 0.67 | 0        | 50,54,54    | 0.98 | 4 (8%)   |
| 160 | GTP  | FQ    | 501  | 159  | 33,34,34     | 0.65 | 0        | 50,54,54    | 0.93 | 3 (6%)   |
| 158 | GDP  | KC    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.86 | 2 (4%)   |
| 157 | ADP  | 8e    | 4701 | -    | 28,29,29     | 1.39 | 4 (14%)  | 43,45,45    | 1.81 | 8 (18%)  |
| 158 | GDP  | LW    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.91 | 2 (4%)   |
| 158 | GDP  | GV    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 158 | GDP  | QF    | 501  | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.88 | 2 (4%)   |
| 160 | GTP  | SG    | 501  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.97 | 3 (6%)   |
| 158 | GDP  | HV    | 501  | -    | 29,30,30     | 0.48 | 0        | 45,47,47    | 0.91 | 2 (4%)   |
| 160 | GTP  | GI    | 501  | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.97 | 3 (6%)   |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 160 | GTP  | GM    | 501  | 159  | 33,34,34     | 0.71 | 0        | 50,54,54    | 0.97 | 3 (6%)   |
| 158 | GDP  | MQ    | 501  | -    | 29,30,30     | 1.14 | 3 (10%)  | 45,47,47    | 1.72 | 6 (13%)  |
| 156 | ATP  | 8e    | 4703 | -    | 32,33,33     | 0.40 | 0        | 48,52,52    | 0.32 | 0        |
| 160 | GTP  | LD    | 602  | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.95 | 4 (8%)   |
| 158 | GDP  | WR    | 501  | -    | 29,30,30     | 0.54 | 0        | 45,47,47    | 0.88 | 2 (4%)   |
| 160 | GTP  | EW    | 501  | 159  | 33,34,34     | 0.93 | 1 (3%)   | 50,54,54    | 0.97 | 2 (4%)   |
| 158 | GDP  | GR    | 501  | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.94 | 2 (4%)   |
| 160 | GTP  | VS    | 501  | 159  | 33,34,34     | 0.66 | 0        | 50,54,54    | 0.90 | 3 (6%)   |
| 158 | GDP  | WL    | 501  | -    | 29,30,30     | 1.14 | 3 (10%)  | 45,47,47    | 1.69 | 6 (13%)  |
| 158 | GDP  | HN    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.49 | 0        |
| 160 | GTP  | PE    | 602  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.94 | 4 (8%)   |
| 158 | GDP  | ZW    | 501  | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.94 | 2 (4%)   |
| 160 | GTP  | CN    | 602  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.96 | 3 (6%)   |
| 160 | GTP  | II    | 501  | 159  | 33,34,34     | 0.96 | 3 (9%)   | 50,54,54    | 0.95 | 2 (4%)   |
| 160 | GTP  | QQ    | 501  | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.95 | 3 (6%)   |
| 160 | GTP  | IQ    | 501  | 159  | 33,34,34     | 0.89 | 2 (6%)   | 50,54,54    | 1.57 | 9 (18%)  |
| 158 | GDP  | BW    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.88 | 2 (4%)   |
| 158 | GDP  | WH    | 501  | -    | 29,30,30     | 0.54 | 0        | 45,47,47    | 0.88 | 2 (4%)   |
| 158 | GDP  | XN    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.88 | 2 (4%)   |
| 160 | GTP  | Aj    | 501  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.97 | 4 (8%)   |
| 158 | GDP  | DE    | 501  | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 158 | GDP  | LC    | 501  | -    | 29,30,30     | 0.54 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 158 | GDP  | VN    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.87 | 2 (4%)   |
| 160 | GTP  | WK    | 602  | 159  | 33,34,34     | 0.65 | 0        | 50,54,54    | 0.93 | 3 (6%)   |
| 160 | GTP  | OX    | 602  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.95 | 3 (6%)   |
| 158 | GDP  | BS    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 160 | GTP  | CI    | 501  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.95 | 4 (8%)   |
| 160 | GTP  | NH    | 502  | 159  | 33,34,34     | 0.71 | 0        | 50,54,54    | 0.97 | 4 (8%)   |
| 160 | GTP  | KR    | 602  | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.96 | 4 (8%)   |
| 160 | GTP  | JH    | 602  | 159  | 33,34,34     | 0.86 | 0        | 50,54,54    | 1.55 | 8 (16%)  |
| 160 | GTP  | NN    | 501  | 159  | 33,34,34     | 0.71 | 0        | 50,54,54    | 0.96 | 3 (6%)   |
| 158 | GDP  | CM    | 501  | -    | 29,30,30     | 0.49 | 0        | 45,47,47    | 0.92 | 2 (4%)   |
| 158 | GDP  | OQ    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 160 | GTP  | LL    | 501  | 159  | 33,34,34     | 0.71 | 0        | 50,54,54    | 0.98 | 4 (8%)   |
| 156 | ATP  | 9e    | 5004 | -    | 32,33,33     | 0.50 | 1 (3%)   | 48,52,52    | 0.46 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 160 | GTP  | ZZ    | 501 | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.97 | 3 (6%)   |
| 160 | GTP  | NP    | 501 | 159  | 33,34,34     | 0.71 | 0        | 50,54,54    | 0.95 | 4 (8%)   |
| 160 | GTP  | WG    | 501 | 159  | 33,34,34     | 1.01 | 2 (6%)   | 50,54,54    | 0.96 | 3 (6%)   |
| 158 | GDP  | ZI    | 501 | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.88 | 2 (4%)   |
| 160 | GTP  | VQ    | 501 | 159  | 33,34,34     | 0.66 | 0        | 50,54,54    | 0.92 | 3 (6%)   |
| 158 | GDP  | TW    | 501 | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.94 | 2 (4%)   |
| 160 | GTP  | TA    | 602 | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.97 | 3 (6%)   |
| 160 | GTP  | FM    | 501 | 159  | 33,34,34     | 0.66 | 0        | 50,54,54    | 0.96 | 4 (8%)   |
| 160 | GTP  | JA    | 501 | 159  | 33,34,34     | 0.71 | 0        | 50,54,54    | 0.99 | 4 (8%)   |
| 158 | GDP  | SZ    | 501 | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.92 | 2 (4%)   |
| 160 | GTP  | RC    | 501 | 159  | 33,34,34     | 0.71 | 0        | 50,54,54    | 0.96 | 4 (8%)   |
| 160 | GTP  | PO    | 602 | 159  | 33,34,34     | 0.72 | 0        | 50,54,54    | 0.92 | 3 (6%)   |
| 158 | GDP  | RT    | 501 | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.91 | 2 (4%)   |
| 160 | GTP  | OD    | 602 | 159  | 33,34,34     | 0.66 | 0        | 50,54,54    | 0.97 | 3 (6%)   |
| 160 | GTP  | FG    | 501 | 159  | 33,34,34     | 0.89 | 0        | 50,54,54    | 1.58 | 8 (16%)  |
| 158 | GDP  | XR    | 501 | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.93 | 2 (4%)   |
| 158 | GDP  | TU    | 501 | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 158 | GDP  | OW    | 501 | -    | 29,30,30     | 0.49 | 0        | 45,47,47    | 0.93 | 2 (4%)   |
| 158 | GDP  | AG    | 501 | -    | 29,30,30     | 0.82 | 0        | 45,47,47    | 0.83 | 1 (2%)   |
| 160 | GTP  | BV    | 602 | 159  | 33,34,34     | 0.67 | 0        | 50,54,54    | 0.95 | 4 (8%)   |
| 158 | GDP  | XV    | 501 | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 158 | GDP  | UE    | 501 | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.94 | 2 (4%)   |
| 160 | GTP  | GC    | 602 | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.95 | 3 (6%)   |
| 158 | GDP  | TJ    | 501 | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 158 | GDP  | NI    | 501 | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.88 | 2 (4%)   |
| 160 | GTP  | IO    | 501 | 159  | 33,34,34     | 0.92 | 2 (6%)   | 50,54,54    | 0.96 | 2 (4%)   |
| 160 | GTP  | JR    | 602 | 159  | 33,34,34     | 0.87 | 0        | 50,54,54    | 1.56 | 8 (16%)  |
| 158 | GDP  | KW    | 501 | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.88 | 2 (4%)   |
| 160 | GTP  | RK    | 602 | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.94 | 3 (6%)   |
| 158 | GDP  | IB    | 501 | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.94 | 2 (4%)   |
| 158 | GDP  | XF    | 501 | -    | 29,30,30     | 1.16 | 3 (10%)  | 45,47,47    | 1.74 | 6 (13%)  |
| 160 | GTP  | YE    | 602 | 159  | 33,34,34     | 0.71 | 0        | 50,54,54    | 0.97 | 4 (8%)   |
| 158 | GDP  | QT    | 501 | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.91 | 2 (4%)   |
| 160 | GTP  | ZF    | 602 | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.97 | 4 (8%)   |
| 158 | GDP  | BA    | 501 | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.91 | 2 (4%)   |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 158 | GDP  | GF    | 501  | -    | 29,30,30     | 0.49 | 0        | 45,47,47    | 0.95 | 2 (4%)   |
| 158 | GDP  | PL    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 160 | GTP  | XA    | 501  | 159  | 33,34,34     | 0.65 | 0        | 50,54,54    | 0.93 | 3 (6%)   |
| 158 | GDP  | Ag    | 501  | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.91 | 2 (4%)   |
| 160 | GTP  | HY    | 501  | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 1.00 | 4 (8%)   |
| 158 | GDP  | Am    | 501  | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.91 | 2 (4%)   |
| 158 | GDP  | Ai    | 501  | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.94 | 2 (4%)   |
| 158 | GDP  | QR    | 501  | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.86 | 2 (4%)   |
| 160 | GTP  | KB    | 501  | 159  | 33,34,34     | 0.66 | 0        | 50,54,54    | 0.94 | 3 (6%)   |
| 158 | GDP  | ZA    | 501  | -    | 29,30,30     | 0.54 | 0        | 45,47,47    | 0.91 | 2 (4%)   |
| 160 | GTP  | RE    | 501  | 159  | 33,34,34     | 0.71 | 0        | 50,54,54    | 0.97 | 4 (8%)   |
| 160 | GTP  | XI    | 602  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.95 | 4 (8%)   |
| 160 | GTP  | DL    | 501  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.94 | 3 (6%)   |
| 158 | GDP  | JY    | 501  | -    | 29,30,30     | 1.15 | 3 (10%)  | 45,47,47    | 1.72 | 6 (13%)  |
| 160 | GTP  | RG    | 501  | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.96 | 4 (8%)   |
| 160 | GTP  | RM    | 501  | 159  | 33,34,34     | 0.72 | 0        | 50,54,54    | 0.98 | 3 (6%)   |
| 156 | ATP  | 7a    | 4704 | -    | 32,33,33     | 0.45 | 0        | 48,52,52    | 0.39 | 0        |
| 160 | GTP  | DB    | 501  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.92 | 3 (6%)   |
| 160 | GTP  | CL    | 501  | 159  | 33,34,34     | 0.87 | 1 (3%)   | 50,54,54    | 1.56 | 8 (16%)  |
| 158 | GDP  | XP    | 501  | -    | 29,30,30     | 0.54 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 158 | GDP  | SP    | 501  | -    | 29,30,30     | 0.54 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 157 | ADP  | 7e    | 4701 | -    | 28,29,29     | 1.40 | 4 (14%)  | 43,45,45    | 1.83 | 8 (18%)  |
| 160 | GTP  | YJ    | 602  | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.97 | 4 (8%)   |
| 158 | GDP  | XJ    | 501  | -    | 29,30,30     | 0.79 | 0        | 45,47,47    | 0.83 | 0        |
| 160 | GTP  | PK    | 501  | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.94 | 3 (6%)   |
| 158 | GDP  | Ae    | 501  | -    | 29,30,30     | 0.81 | 0        | 45,47,47    | 0.86 | 1 (2%)   |
| 156 | ATP  | 8e    | 4704 | -    | 32,33,33     | 0.50 | 1 (3%)   | 48,52,52    | 0.37 | 0        |
| 158 | GDP  | OM    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.88 | 2 (4%)   |
| 160 | GTP  | RU    | 501  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.96 | 3 (6%)   |
| 158 | GDP  | XB    | 501  | -    | 29,30,30     | 0.49 | 0        | 45,47,47    | 0.88 | 2 (4%)   |
| 158 | GDP  | YQ    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.93 | 2 (4%)   |
| 160 | GTP  | XW    | 602  | 159  | 33,34,34     | 0.74 | 0        | 50,54,54    | 0.95 | 4 (8%)   |
| 158 | GDP  | LY    | 501  | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.91 | 2 (4%)   |
| 160 | GTP  | VO    | 501  | 159  | 33,34,34     | 1.02 | 3 (9%)   | 50,54,54    | 0.92 | 3 (6%)   |
| 158 | GDP  | HL    | 501  | -    | 29,30,30     | 1.16 | 3 (10%)  | 45,47,47    | 1.75 | 5 (11%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 158 | GDP  | PZ    | 501  | -    | 29,30,30     | 0.55 | 0        | 45,47,47    | 0.91 | 2 (4%)   |
| 158 | GDP  | WJ    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.85 | 2 (4%)   |
| 160 | GTP  | ES    | 501  | 159  | 33,34,34     | 0.89 | 0        | 50,54,54    | 1.55 | 9 (18%)  |
| 157 | ADP  | 9f    | 4702 | -    | 28,29,29     | 1.38 | 5 (17%)  | 43,45,45    | 1.80 | 10 (23%) |
| 158 | GDP  | HZ    | 501  | -    | 29,30,30     | 0.49 | 0        | 45,47,47    | 0.49 | 0        |
| 158 | GDP  | AW    | 501  | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.87 | 2 (4%)   |
| 160 | GTP  | EG    | 501  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.93 | 3 (6%)   |
| 160 | GTP  | DO    | 501  | 159  | 33,34,34     | 0.88 | 0        | 50,54,54    | 1.57 | 8 (16%)  |
| 160 | GTP  | EC    | 501  | 159  | 33,34,34     | 0.89 | 1 (3%)   | 50,54,54    | 1.59 | 8 (16%)  |
| 158 | GDP  | PF    | 501  | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 160 | GTP  | EI    | 501  | 159  | 33,34,34     | 0.66 | 0        | 50,54,54    | 0.93 | 3 (6%)   |
| 158 | GDP  | PX    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.88 | 2 (4%)   |
| 158 | GDP  | TN    | 501  | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 158 | GDP  | KA    | 501  | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.86 | 2 (4%)   |
| 158 | GDP  | VX    | 501  | -    | 29,30,30     | 0.49 | 0        | 45,47,47    | 0.88 | 2 (4%)   |
| 158 | GDP  | ZY    | 501  | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.94 | 2 (4%)   |
| 160 | GTP  | CF    | 501  | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.96 | 4 (8%)   |
| 158 | GDP  | YY    | 501  | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.91 | 2 (4%)   |
| 160 | GTP  | EE    | 501  | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.93 | 3 (6%)   |
| 158 | GDP  | KO    | 501  | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 158 | GDP  | HF    | 501  | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.94 | 2 (4%)   |
| 158 | GDP  | YM    | 501  | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 160 | GTP  | BR    | 501  | 159  | 33,34,34     | 0.84 | 0        | 50,54,54    | 1.58 | 8 (16%)  |
| 160 | GTP  | FC    | 501  | 159  | 33,34,34     | 0.65 | 0        | 50,54,54    | 0.96 | 3 (6%)   |
| 160 | GTP  | UF    | 501  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.95 | 3 (6%)   |
| 160 | GTP  | GS    | 602  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.99 | 4 (8%)   |
| 160 | GTP  | TX    | 602  | 159  | 33,34,34     | 0.96 | 3 (9%)   | 50,54,54    | 1.00 | 3 (6%)   |
| 160 | GTP  | JP    | 602  | 159  | 33,34,34     | 0.88 | 1 (3%)   | 50,54,54    | 1.54 | 9 (18%)  |
| 160 | GTP  | QU    | 602  | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.97 | 4 (8%)   |
| 160 | GTP  | OJ    | 602  | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.98 | 3 (6%)   |
| 160 | GTP  | RY    | 602  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.98 | 3 (6%)   |
| 160 | GTP  | SC    | 602  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.95 | 3 (6%)   |
| 160 | GTP  | YN    | 501  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.95 | 3 (6%)   |
| 160 | GTP  | Af    | 501  | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.99 | 4 (8%)   |
| 158 | GDP  | IV    | 501  | -    | 29,30,30     | 1.17 | 3 (10%)  | 45,47,47    | 1.74 | 6 (13%)  |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 158 | GDP  | JU    | 501 | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 160 | GTP  | AI    | 602 | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.96 | 3 (6%)   |
| 158 | GDP  | DN    | 501 | -    | 29,30,30     | 1.15 | 3 (10%)  | 45,47,47    | 1.69 | 6 (13%)  |
| 160 | GTP  | OL    | 602 | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.94 | 3 (6%)   |
| 158 | GDP  | UX    | 501 | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 158 | GDP  | LS    | 501 | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 158 | GDP  | JD    | 501 | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.87 | 2 (4%)   |
| 158 | GDP  | NU    | 501 | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.87 | 2 (4%)   |
| 160 | GTP  | DF    | 501 | 159  | 33,34,34     | 0.67 | 0        | 50,54,54    | 0.96 | 4 (8%)   |
| 160 | GTP  | WE    | 602 | 159  | 33,34,34     | 0.90 | 0        | 50,54,54    | 1.52 | 8 (16%)  |
| 160 | GTP  | WW    | 501 | 159  | 33,34,34     | 0.66 | 0        | 50,54,54    | 0.93 | 3 (6%)   |
| 158 | GDP  | RL    | 501 | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.93 | 2 (4%)   |
| 158 | GDP  | DX    | 501 | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 160 | GTP  | VC    | 501 | 159  | 33,34,34     | 1.07 | 3 (9%)   | 50,54,54    | 1.07 | 4 (8%)   |
| 160 | GTP  | OP    | 501 | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.99 | 3 (6%)   |
| 158 | GDP  | DV    | 501 | -    | 29,30,30     | 1.16 | 3 (10%)  | 45,47,47    | 1.73 | 6 (13%)  |
| 158 | GDP  | PH    | 501 | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.85 | 2 (4%)   |
| 158 | GDP  | TP    | 501 | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.96 | 2 (4%)   |
| 160 | GTP  | ZV    | 602 | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.95 | 3 (6%)   |
| 158 | GDP  | PR    | 501 | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 160 | GTP  | OV    | 501 | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.98 | 3 (6%)   |
| 160 | GTP  | MB    | 502 | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.95 | 3 (6%)   |
| 160 | GTP  | FW    | 602 | 159  | 33,34,34     | 0.89 | 0        | 50,54,54    | 1.60 | 8 (16%)  |
| 158 | GDP  | EB    | 501 | -    | 29,30,30     | 1.15 | 4 (13%)  | 45,47,47    | 1.71 | 6 (13%)  |
| 160 | GTP  | EY    | 501 | 159  | 33,34,34     | 0.65 | 0        | 50,54,54    | 0.98 | 3 (6%)   |
| 160 | GTP  | NT    | 602 | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.96 | 4 (8%)   |
| 158 | GDP  | RX    | 501 | -    | 29,30,30     | 0.49 | 0        | 45,47,47    | 0.95 | 2 (4%)   |
| 160 | GTP  | IY    | 501 | 159  | 33,34,34     | 0.73 | 0        | 50,54,54    | 0.98 | 4 (8%)   |
| 160 | GTP  | WU    | 501 | 159  | 33,34,34     | 0.65 | 0        | 50,54,54    | 0.88 | 3 (6%)   |
| 158 | GDP  | IL    | 501 | -    | 29,30,30     | 1.16 | 3 (10%)  | 45,47,47    | 1.73 | 6 (13%)  |
| 158 | GDP  | EZ    | 602 | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 158 | GDP  | AQ    | 501 | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.93 | 2 (4%)   |
| 160 | GTP  | NZ    | 602 | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.94 | 3 (6%)   |
| 158 | GDP  | BK    | 501 | -    | 29,30,30     | 0.49 | 0        | 45,47,47    | 0.88 | 2 (4%)   |
| 160 | GTP  | IS    | 501 | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.97 | 4 (8%)   |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 158 | GDP  | AI    | 501  | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.93 | 2 (4%)   |
| 158 | GDP  | LU    | 501  | -    | 29,30,30     | 0.54 | 0        | 45,47,47    | 0.93 | 2 (4%)   |
| 160 | GTP  | UN    | 602  | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.97 | 4 (8%)   |
| 158 | GDP  | NC    | 501  | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 156 | ATP  | 9e    | 5001 | -    | 32,33,33     | 0.49 | 0        | 48,52,52    | 0.35 | 0        |
| 160 | GTP  | KV    | 602  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.94 | 3 (6%)   |
| 160 | GTP  | HI    | 602  | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.93 | 3 (6%)   |
| 160 | GTP  | IK    | 602  | 159  | 33,34,34     | 0.88 | 1 (3%)   | 50,54,54    | 1.60 | 8 (16%)  |
| 160 | GTP  | QY    | 501  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.97 | 4 (8%)   |
| 158 | GDP  | YS    | 501  | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.91 | 2 (4%)   |
| 160 | GTP  | HM    | 602  | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.99 | 4 (8%)   |
| 160 | GTP  | NB    | 501  | 159  | 33,34,34     | 0.72 | 0        | 50,54,54    | 0.95 | 3 (6%)   |
| 158 | GDP  | XD    | 501  | -    | 29,30,30     | 0.55 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 160 | GTP  | BZ    | 501  | 159  | 33,34,34     | 0.71 | 0        | 50,54,54    | 0.97 | 4 (8%)   |
| 160 | GTP  | TC    | 501  | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.94 | 3 (6%)   |
| 160 | GTP  | HG    | 501  | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.98 | 3 (6%)   |
| 160 | GTP  | ZN    | 602  | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.97 | 3 (6%)   |
| 160 | GTP  | GU    | 602  | 159  | 33,34,34     | 0.71 | 0        | 50,54,54    | 0.98 | 3 (6%)   |
| 156 | ATP  | 7e    | 4702 | -    | 32,33,33     | 0.42 | 0        | 48,52,52    | 0.31 | 0        |
| 156 | ATP  | 9e    | 5003 | -    | 32,33,33     | 0.45 | 0        | 48,52,52    | 0.31 | 0        |
| 158 | GDP  | YF    | 501  | -    | 29,30,30     | 0.54 | 0        | 45,47,47    | 0.91 | 2 (4%)   |
| 158 | GDP  | YU    | 501  | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.91 | 2 (4%)   |
| 160 | GTP  | An    | 602  | 159  | 33,34,34     | 0.67 | 0        | 50,54,54    | 0.98 | 4 (8%)   |
| 158 | GDP  | DC    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 160 | GTP  | GK    | 602  | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.96 | 3 (6%)   |
| 158 | GDP  | EX    | 501  | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.92 | 2 (4%)   |
| 160 | GTP  | ZB    | 501  | 159  | 33,34,34     | 0.71 | 0        | 50,54,54    | 0.93 | 4 (8%)   |
| 160 | GTP  | DU    | 501  | 159  | 33,34,34     | 0.87 | 0        | 50,54,54    | 1.55 | 8 (16%)  |
| 158 | GDP  | CQ    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 160 | GTP  | AT    | 501  | 159  | 33,34,34     | 0.67 | 0        | 50,54,54    | 0.96 | 3 (6%)   |
| 160 | GTP  | ZX    | 501  | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.96 | 4 (8%)   |
| 158 | GDP  | VZ    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.88 | 2 (4%)   |
| 158 | GDP  | VJ    | 501  | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.88 | 2 (4%)   |
| 158 | GDP  | QH    | 501  | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 160 | GTP  | ZT    | 602  | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.98 | 4 (8%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 160 | GTP  | CD    | 602 | 159  | 33,34,34     | 0.67 | 0        | 50,54,54    | 0.96 | 3 (6%)   |
| 158 | GDP  | XT    | 501 | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 158 | GDP  | VL    | 501 | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.87 | 2 (4%)   |
| 160 | GTP  | MT    | 501 | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.95 | 4 (8%)   |
| 158 | GDP  | AS    | 501 | -    | 29,30,30     | 0.84 | 0        | 45,47,47    | 0.86 | 1 (2%)   |
| 160 | GTP  | IM    | 602 | 159  | 33,34,34     | 0.72 | 0        | 50,54,54    | 0.98 | 4 (8%)   |
| 160 | GTP  | KZ    | 602 | 159  | 33,34,34     | 0.89 | 1 (3%)   | 50,54,54    | 1.57 | 8 (16%)  |
| 160 | GTP  | BX    | 602 | 159  | 33,34,34     | 0.67 | 0        | 50,54,54    | 0.97 | 4 (8%)   |
| 158 | GDP  | PP    | 501 | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 158 | GDP  | OY    | 501 | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.88 | 2 (4%)   |
| 160 | GTP  | ZL    | 602 | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.95 | 3 (6%)   |
| 158 | GDP  | PT    | 501 | -    | 29,30,30     | 0.54 | 0        | 45,47,47    | 0.84 | 2 (4%)   |
| 158 | GDP  | RH    | 501 | -    | 29,30,30     | 0.55 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 160 | GTP  | XU    | 501 | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.96 | 4 (8%)   |
| 158 | GDP  | AK    | 501 | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.88 | 2 (4%)   |
| 160 | GTP  | NL    | 602 | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.96 | 4 (8%)   |
| 158 | GDP  | MA    | 501 | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 160 | GTP  | JC    | 501 | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.96 | 4 (8%)   |
| 158 | GDP  | NQ    | 501 | -    | 29,30,30     | 0.54 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 158 | GDP  | US    | 501 | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 160 | GTP  | CZ    | 501 | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.94 | 3 (6%)   |
| 158 | GDP  | DR    | 501 | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.93 | 2 (4%)   |
| 158 | GDP  | YD    | 501 | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.92 | 2 (4%)   |
| 160 | GTP  | JZ    | 501 | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.93 | 3 (6%)   |
| 160 | GTP  | MH    | 501 | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.95 | 4 (8%)   |
| 158 | GDP  | ME    | 501 | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 158 | GDP  | HR    | 501 | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.93 | 2 (4%)   |
| 158 | GDP  | YW    | 501 | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.88 | 2 (4%)   |
| 160 | GTP  | NX    | 501 | 159  | 33,34,34     | 0.67 | 0        | 50,54,54    | 0.99 | 3 (6%)   |
| 158 | GDP  | PD    | 501 | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.88 | 2 (4%)   |
| 160 | GTP  | XQ    | 501 | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.98 | 4 (8%)   |
| 158 | GDP  | BI    | 501 | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.87 | 2 (4%)   |
| 160 | GTP  | DH    | 501 | 159  | 33,34,34     | 0.66 | 0        | 50,54,54    | 0.95 | 3 (6%)   |
| 158 | GDP  | GX    | 501 | -    | 29,30,30     | 0.54 | 0        | 45,47,47    | 0.93 | 2 (4%)   |
| 158 | GDP  | WV    | 501 | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.85 | 2 (4%)   |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 158 | GDP  | Ak    | 501  | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.96 | 2 (4%)   |
| 157 | ADP  | 9e    | 5002 | -    | 28,29,29     | 1.39 | 4 (14%)  | 43,45,45    | 1.81 | 8 (18%)  |
| 158 | GDP  | SD    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.95 | 2 (4%)   |
| 160 | GTP  | EM    | 501  | 159  | 33,34,34     | 0.67 | 0        | 50,54,54    | 0.94 | 3 (6%)   |
| 160 | GTP  | GE    | 602  | 159  | 33,34,34     | 0.65 | 0        | 50,54,54    | 0.97 | 3 (6%)   |
| 160 | GTP  | RQ    | 501  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.96 | 3 (6%)   |
| 156 | ATP  | 9f    | 4704 | -    | 32,33,33     | 0.38 | 0        | 48,52,52    | 0.36 | 0        |
| 158 | GDP  | MC    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 158 | GDP  | SJ    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.94 | 2 (4%)   |
| 158 | GDP  | VB    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 160 | GTP  | VG    | 501  | 159  | 33,34,34     | 0.67 | 0        | 50,54,54    | 0.92 | 3 (6%)   |
| 160 | GTP  | XC    | 602  | 159  | 33,34,34     | 0.71 | 0        | 50,54,54    | 0.90 | 3 (6%)   |
| 158 | GDP  | HD    | 501  | -    | 29,30,30     | 1.14 | 3 (10%)  | 45,47,47    | 1.78 | 7 (15%)  |
| 158 | GDP  | KS    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.91 | 2 (4%)   |
| 160 | GTP  | KD    | 501  | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.94 | 4 (8%)   |
| 160 | GTP  | PQ    | 501  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.96 | 4 (8%)   |
| 158 | GDP  | FT    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.93 | 2 (4%)   |
| 158 | GDP  | GH    | 501  | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.92 | 2 (4%)   |
| 160 | GTP  | QA    | 602  | 159  | 33,34,34     | 0.73 | 0        | 50,54,54    | 0.92 | 3 (6%)   |
| 160 | GTP  | YL    | 602  | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.93 | 3 (6%)   |
| 160 | GTP  | HQ    | 602  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.99 | 4 (8%)   |
| 160 | GTP  | ND    | 501  | 159  | 33,34,34     | 0.72 | 0        | 50,54,54    | 0.96 | 3 (6%)   |
| 156 | ATP  | 7a    | 4702 | -    | 32,33,33     | 0.48 | 0        | 48,52,52    | 0.47 | 0        |
| 158 | GDP  | KY    | 501  | -    | 29,30,30     | 0.57 | 0        | 45,47,47    | 0.94 | 2 (4%)   |
| 158 | GDP  | QN    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 160 | GTP  | RO    | 602  | 159  | 33,34,34     | 0.67 | 0        | 50,54,54    | 0.97 | 4 (8%)   |
| 158 | GDP  | AU    | 501  | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.93 | 2 (4%)   |
| 160 | GTP  | QW    | 501  | 159  | 33,34,34     | 0.71 | 0        | 50,54,54    | 0.98 | 4 (8%)   |
| 157 | ADP  | 7b    | 4704 | -    | 28,29,29     | 1.38 | 5 (17%)  | 43,45,45    | 1.80 | 10 (23%) |
| 158 | GDP  | JM    | 501  | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 158 | GDP  | ID    | 501  | -    | 29,30,30     | 1.17 | 3 (10%)  | 45,47,47    | 1.76 | 6 (13%)  |
| 158 | GDP  | RJ    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.92 | 2 (4%)   |
| 160 | GTP  | AF    | 501  | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.97 | 4 (8%)   |
| 158 | GDP  | RP    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.94 | 2 (4%)   |
| 160 | GTP  | MJ    | 602  | 159  | 33,34,34     | 0.73 | 0        | 50,54,54    | 0.96 | 3 (6%)   |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 158 | GDP  | AY    | 501  | -    | 29,30,30     | 0.53 | 0           | 45,47,47    | 0.92 | 2 (4%)      |
| 158 | GDP  | YO    | 501  | -    | 29,30,30     | 0.54 | 0           | 45,47,47    | 0.90 | 2 (4%)      |
| 160 | GTP  | YR    | 501  | 159  | 33,34,34     | 0.67 | 0           | 50,54,54    | 0.96 | 3 (6%)      |
| 158 | GDP  | GD    | 501  | -    | 29,30,30     | 0.52 | 0           | 45,47,47    | 0.93 | 2 (4%)      |
| 160 | GTP  | XE    | 501  | 159  | 33,34,34     | 0.89 | 2 (6%)      | 50,54,54    | 1.59 | 8 (16%)     |
| 160 | GTP  | PG    | 501  | 159  | 33,34,34     | 0.70 | 0           | 50,54,54    | 0.93 | 3 (6%)      |
| 160 | GTP  | LN    | 501  | 159  | 33,34,34     | 0.69 | 0           | 50,54,54    | 0.95 | 4 (8%)      |
| 160 | GTP  | VM    | 602  | 159  | 33,34,34     | 0.67 | 0           | 50,54,54    | 0.92 | 3 (6%)      |
| 160 | GTP  | AZ    | 501  | 159  | 33,34,34     | 0.70 | 0           | 50,54,54    | 0.97 | 4 (8%)      |
| 158 | GDP  | OS    | 501  | -    | 29,30,30     | 0.51 | 0           | 45,47,47    | 0.90 | 2 (4%)      |
| 156 | ATP  | 7b    | 4701 | -    | 32,33,33     | 0.39 | 0           | 48,52,52    | 0.30 | 0           |
| 158 | GDP  | SV    | 501  | -    | 29,30,30     | 0.53 | 0           | 45,47,47    | 0.90 | 2 (4%)      |
| 160 | GTP  | LV    | 502  | 159  | 33,34,34     | 0.67 | 0           | 50,54,54    | 0.96 | 4 (8%)      |
| 158 | GDP  | LE    | 501  | -    | 29,30,30     | 0.50 | 0           | 45,47,47    | 0.92 | 2 (4%)      |
| 160 | GTP  | AV    | 501  | 159  | 33,34,34     | 0.68 | 0           | 50,54,54    | 0.94 | 3 (6%)      |
| 160 | GTP  | CP    | 602  | 159  | 33,34,34     | 0.68 | 0           | 50,54,54    | 0.94 | 3 (6%)      |
| 160 | GTP  | GW    | 501  | 159  | 33,34,34     | 0.70 | 0           | 50,54,54    | 0.97 | 3 (6%)      |
| 160 | GTP  | YP    | 602  | 159  | 33,34,34     | 0.70 | 0           | 50,54,54    | 0.91 | 3 (6%)      |
| 160 | GTP  | AD    | 501  | 159  | 33,34,34     | 0.88 | 1 (3%)      | 50,54,54    | 1.57 | 8 (16%)     |
| 158 | GDP  | IT    | 501  | -    | 29,30,30     | 1.17 | 3 (10%)     | 45,47,47    | 1.73 | 6 (13%)     |
| 158 | GDP  | ZM    | 501  | -    | 29,30,30     | 0.52 | 0           | 45,47,47    | 0.97 | 2 (4%)      |
| 158 | GDP  | CA    | 501  | -    | 29,30,30     | 0.50 | 0           | 45,47,47    | 0.93 | 2 (4%)      |
| 160 | GTP  | XO    | 602  | 159  | 33,34,34     | 0.88 | 1 (3%)      | 50,54,54    | 1.59 | 8 (16%)     |
| 158 | GDP  | JQ    | 501  | -    | 29,30,30     | 0.51 | 0           | 45,47,47    | 0.85 | 2 (4%)      |
| 160 | GTP  | QM    | 501  | 159  | 33,34,34     | 0.70 | 0           | 50,54,54    | 0.97 | 4 (8%)      |
| 158 | GDP  | RZ    | 501  | -    | 29,30,30     | 0.50 | 0           | 45,47,47    | 0.97 | 2 (4%)      |
| 158 | GDP  | UG    | 501  | -    | 29,30,30     | 0.50 | 0           | 45,47,47    | 0.89 | 2 (4%)      |
| 158 | GDP  | WZ    | 501  | -    | 29,30,30     | 0.52 | 0           | 45,47,47    | 0.86 | 2 (4%)      |
| 158 | GDP  | JW    | 501  | -    | 29,30,30     | 1.15 | 3 (10%)     | 45,47,47    | 1.73 | 6 (13%)     |
| 158 | GDP  | XL    | 501  | -    | 29,30,30     | 0.50 | 0           | 45,47,47    | 0.91 | 2 (4%)      |
| 156 | ATP  | 7b    | 4702 | -    | 32,33,33     | 0.39 | 0           | 48,52,52    | 0.29 | 0           |
| 158 | GDP  | MY    | 501  | -    | 29,30,30     | 0.52 | 0           | 45,47,47    | 0.92 | 2 (4%)      |
| 160 | GTP  | YZ    | 602  | 159  | 33,34,34     | 0.69 | 0           | 50,54,54    | 0.95 | 3 (6%)      |
| 158 | GDP  | ET    | 501  | -    | 29,30,30     | 1.17 | 3 (10%)     | 45,47,47    | 1.73 | 6 (13%)     |
| 160 | GTP  | UD    | 501  | 159  | 33,34,34     | 0.67 | 0           | 50,54,54    | 0.99 | 3 (6%)      |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 160 | GTP  | CB    | 501  | 159  | 33,34,34     | 0.67 | 0        | 50,54,54    | 0.96 | 4 (8%)   |
| 160 | GTP  | VW    | 501  | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.91 | 3 (6%)   |
| 158 | GDP  | VH    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.92 | 2 (4%)   |
| 160 | GTP  | MR    | 602  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.97 | 3 (6%)   |
| 158 | GDP  | KU    | 501  | -    | 29,30,30     | 0.55 | 0        | 45,47,47    | 0.91 | 2 (4%)   |
| 160 | GTP  | WO    | 501  | 159  | 33,34,34     | 0.65 | 0        | 50,54,54    | 0.92 | 3 (6%)   |
| 160 | GTP  | XY    | 501  | 159  | 33,34,34     | 0.54 | 0        | 50,54,54    | 0.56 | 0        |
| 158 | GDP  | KG    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 160 | GTP  | SW    | 501  | 159  | 33,34,34     | 0.67 | 0        | 50,54,54    | 0.94 | 3 (6%)   |
| 158 | GDP  | MO    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.92 | 2 (4%)   |
| 160 | GTP  | UJ    | 501  | 159  | 33,34,34     | 1.07 | 3 (9%)   | 50,54,54    | 0.95 | 3 (6%)   |
| 160 | GTP  | AR    | 602  | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.97 | 4 (8%)   |
| 160 | GTP  | BD    | 602  | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.96 | 4 (8%)   |
| 160 | GTP  | SA    | 501  | 159  | 33,34,34     | 1.01 | 2 (6%)   | 50,54,54    | 1.04 | 4 (8%)   |
| 160 | GTP  | WS    | 501  | 159  | 33,34,34     | 0.95 | 2 (6%)   | 50,54,54    | 0.94 | 2 (4%)   |
| 158 | GDP  | OO    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.92 | 2 (4%)   |
| 158 | GDP  | KQ    | 501  | -    | 29,30,30     | 0.54 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 160 | GTP  | EK    | 602  | 159  | 33,34,34     | 0.65 | 0        | 50,54,54    | 0.93 | 3 (6%)   |
| 156 | ATP  | 7f    | 4704 | -    | 32,33,33     | 0.41 | 0        | 48,52,52    | 0.30 | 0        |
| 160 | GTP  | JT    | 501  | 159  | 33,34,34     | 0.66 | 0        | 50,54,54    | 0.94 | 3 (6%)   |
| 160 | GTP  | QO    | 602  | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.96 | 4 (8%)   |
| 158 | GDP  | ZK    | 501  | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 160 | GTP  | RA    | 602  | 159  | 33,34,34     | 0.67 | 0        | 50,54,54    | 0.97 | 4 (8%)   |
| 160 | GTP  | IA    | 501  | 159  | 33,34,34     | 0.72 | 0        | 50,54,54    | 0.97 | 3 (6%)   |
| 160 | GTP  | EQ    | 602  | 159  | 33,34,34     | 0.65 | 0        | 50,54,54    | 0.96 | 3 (6%)   |
| 160 | GTP  | XK    | 501  | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.96 | 3 (6%)   |
| 158 | GDP  | IF    | 501  | -    | 29,30,30     | 1.16 | 3 (10%)  | 45,47,47    | 1.71 | 6 (13%)  |
| 158 | GDP  | VP    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.92 | 2 (4%)   |
| 158 | GDP  | EH    | 501  | -    | 29,30,30     | 0.48 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 156 | ATP  | 7e    | 4703 | -    | 32,33,33     | 0.48 | 0        | 48,52,52    | 0.47 | 0        |
| 158 | GDP  | GB    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.92 | 2 (4%)   |
| 158 | GDP  | HP    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.92 | 2 (4%)   |
| 158 | GDP  | GT    | 501  | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.94 | 2 (4%)   |
| 160 | GTP  | TK    | 501  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.98 | 4 (8%)   |
| 158 | GDP  | CH    | 501  | -    | 29,30,30     | 0.54 | 0        | 45,47,47    | 0.86 | 2 (4%)   |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 158 | GDP  | UK    | 501  | -    | 29,30,30     | 0.55 | 0           | 45,47,47    | 0.91 | 2 (4%)      |
| 158 | GDP  | EL    | 501  | -    | 29,30,30     | 0.48 | 0           | 45,47,47    | 0.86 | 2 (4%)      |
| 158 | GDP  | WN    | 501  | -    | 29,30,30     | 0.52 | 0           | 45,47,47    | 0.86 | 2 (4%)      |
| 157 | ADP  | 7a    | 4703 | -    | 28,29,29     | 1.38 | 4 (14%)     | 43,45,45    | 1.81 | 8 (18%)     |
| 160 | GTP  | YA    | 602  | 159  | 33,34,34     | 0.73 | 0           | 50,54,54    | 0.96 | 4 (8%)      |
| 160 | GTP  | QK    | 602  | 159  | 33,34,34     | 0.71 | 0           | 50,54,54    | 0.97 | 4 (8%)      |
| 160 | GTP  | WQ    | 602  | 159  | 33,34,34     | 0.69 | 0           | 50,54,54    | 0.89 | 3 (6%)      |
| 158 | GDP  | IN    | 501  | -    | 29,30,30     | 1.16 | 3 (10%)     | 45,47,47    | 1.72 | 6 (13%)     |
| 160 | GTP  | SI    | 501  | 159  | 33,34,34     | 0.70 | 0           | 50,54,54    | 0.94 | 3 (6%)      |
| 158 | GDP  | QX    | 501  | -    | 29,30,30     | 0.53 | 0           | 45,47,47    | 0.91 | 2 (4%)      |
| 158 | GDP  | DA    | 501  | -    | 29,30,30     | 0.50 | 0           | 45,47,47    | 0.91 | 2 (4%)      |
| 158 | GDP  | SN    | 501  | -    | 29,30,30     | 0.53 | 0           | 45,47,47    | 0.91 | 2 (4%)      |
| 158 | GDP  | GZ    | 501  | -    | 29,30,30     | 1.17 | 3 (10%)     | 45,47,47    | 1.75 | 6 (13%)     |
| 160 | GTP  | QE    | 501  | 159  | 33,34,34     | 0.69 | 0           | 50,54,54    | 0.93 | 3 (6%)      |
| 158 | GDP  | IR    | 501  | -    | 29,30,30     | 0.52 | 0           | 45,47,47    | 0.89 | 2 (4%)      |
| 158 | GDP  | DT    | 501  | -    | 29,30,30     | 1.15 | 3 (10%)     | 45,47,47    | 1.69 | 6 (13%)     |
| 160 | GTP  | OB    | 501  | 159  | 33,34,34     | 0.70 | 0           | 50,54,54    | 0.97 | 3 (6%)      |
| 160 | GTP  | HC    | 602  | 159  | 33,34,34     | 0.89 | 1 (3%)      | 50,54,54    | 1.60 | 8 (16%)     |
| 158 | GDP  | PN    | 501  | -    | 29,30,30     | 0.54 | 0           | 45,47,47    | 0.92 | 2 (4%)      |
| 158 | GDP  | QZ    | 501  | -    | 29,30,30     | 0.51 | 0           | 45,47,47    | 0.87 | 2 (4%)      |
| 160 | GTP  | TG    | 501  | 159  | 33,34,34     | 0.66 | 0           | 50,54,54    | 0.95 | 3 (6%)      |
| 158 | GDP  | FP    | 501  | -    | 29,30,30     | 0.50 | 0           | 45,47,47    | 0.87 | 2 (4%)      |
| 158 | GDP  | FR    | 501  | -    | 29,30,30     | 0.50 | 0           | 45,47,47    | 0.86 | 2 (4%)      |
| 160 | GTP  | VK    | 501  | 159  | 33,34,34     | 0.67 | 0           | 50,54,54    | 0.90 | 3 (6%)      |
| 160 | GTP  | SK    | 602  | 159  | 33,34,34     | 0.73 | 0           | 50,54,54    | 0.98 | 3 (6%)      |
| 158 | GDP  | HH    | 501  | -    | 29,30,30     | 0.49 | 0           | 45,47,47    | 0.91 | 2 (4%)      |
| 158 | GDP  | DG    | 501  | -    | 29,30,30     | 0.49 | 0           | 45,47,47    | 0.90 | 2 (4%)      |
| 158 | GDP  | WF    | 501  | -    | 29,30,30     | 1.16 | 3 (10%)     | 45,47,47    | 1.75 | 6 (13%)     |
| 160 | GTP  | VA    | 501  | 159  | 33,34,34     | 0.66 | 0           | 50,54,54    | 0.92 | 3 (6%)      |
| 158 | GDP  | BU    | 501  | -    | 29,30,30     | 1.18 | 3 (10%)     | 45,47,47    | 1.75 | 7 (15%)     |
| 158 | GDP  | CU    | 501  | -    | 29,30,30     | 1.16 | 3 (10%)     | 45,47,47    | 1.74 | 6 (13%)     |
| 158 | GDP  | UQ    | 501  | -    | 29,30,30     | 0.52 | 0           | 45,47,47    | 0.95 | 2 (4%)      |
| 156 | ATP  | 8f    | 4704 | -    | 32,33,33     | 0.53 | 1 (3%)      | 48,52,52    | 0.29 | 0           |
| 160 | GTP  | OR    | 602  | 159  | 33,34,34     | 0.67 | 0           | 50,54,54    | 0.96 | 3 (6%)      |
| 160 | GTP  | QS    | 501  | 159  | 33,34,34     | 0.71 | 0           | 50,54,54    | 0.96 | 4 (8%)      |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 158 | GDP  | QJ    | 501 | -    | 29,30,30     | 0.55 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 158 | GDP  | Ac    | 501 | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.93 | 2 (4%)   |
| 160 | GTP  | KJ    | 602 | 159  | 33,34,34     | 0.67 | 0        | 50,54,54    | 0.92 | 3 (6%)   |
| 158 | GDP  | YH    | 501 | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 160 | GTP  | KT    | 501 | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.94 | 3 (6%)   |
| 160 | GTP  | JJ    | 501 | 159  | 33,34,34     | 0.86 | 0        | 50,54,54    | 1.53 | 8 (16%)  |
| 160 | GTP  | OF    | 501 | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.95 | 3 (6%)   |
| 160 | GTP  | RI    | 501 | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.97 | 4 (8%)   |
| 158 | GDP  | UU    | 501 | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.92 | 2 (4%)   |
| 158 | GDP  | GP    | 501 | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 160 | GTP  | PW    | 501 | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.94 | 3 (6%)   |
| 158 | GDP  | FX    | 501 | -    | 29,30,30     | 1.16 | 3 (10%)  | 45,47,47    | 1.72 | 5 (11%)  |
| 158 | GDP  | WD    | 501 | -    | 29,30,30     | 1.17 | 3 (10%)  | 45,47,47    | 1.71 | 6 (13%)  |
| 158 | GDP  | YK    | 501 | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.88 | 2 (4%)   |
| 158 | GDP  | SF    | 501 | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 160 | GTP  | YT    | 602 | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.96 | 3 (6%)   |
| 160 | GTP  | GG    | 501 | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.99 | 4 (8%)   |
| 158 | GDP  | XH    | 501 | -    | 29,30,30     | 0.54 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 158 | GDP  | TL    | 501 | -    | 29,30,30     | 0.54 | 0        | 45,47,47    | 0.91 | 2 (4%)   |
| 160 | GTP  | KP    | 602 | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.95 | 4 (8%)   |
| 158 | GDP  | UA    | 501 | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.87 | 2 (4%)   |
| 160 | GTP  | BT    | 602 | 159  | 33,34,34     | 0.67 | 0        | 50,54,54    | 0.96 | 4 (8%)   |
| 158 | GDP  | ZU    | 501 | -    | 29,30,30     | 0.54 | 0        | 45,47,47    | 0.91 | 2 (4%)   |
| 160 | GTP  | BH    | 602 | 159  | 33,34,34     | 0.89 | 1 (3%)   | 50,54,54    | 1.58 | 8 (16%)  |
| 160 | GTP  | NF    | 502 | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.95 | 4 (8%)   |
| 158 | GDP  | NK    | 501 | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.92 | 2 (4%)   |
| 158 | GDP  | BY    | 501 | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.87 | 2 (4%)   |
| 160 | GTP  | TR    | 501 | 159  | 33,34,34     | 0.67 | 0        | 50,54,54    | 0.99 | 4 (8%)   |
| 158 | GDP  | HX    | 501 | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 158 | GDP  | SB    | 501 | -    | 29,30,30     | 0.49 | 0        | 45,47,47    | 0.96 | 2 (4%)   |
| 158 | GDP  | HT    | 501 | -    | 29,30,30     | 0.49 | 0        | 45,47,47    | 0.93 | 2 (4%)   |
| 158 | GDP  | SR    | 501 | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.95 | 2 (4%)   |
| 160 | GTP  | SM    | 501 | 159  | 33,34,34     | 0.67 | 0        | 50,54,54    | 0.96 | 3 (6%)   |
| 158 | GDP  | SH    | 501 | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.92 | 2 (4%)   |
| 158 | GDP  | AA    | 501 | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.92 | 2 (4%)   |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 160 | GTP  | HO    | 501  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.97 | 3 (6%)   |
| 158 | GDP  | UI    | 501  | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 160 | GTP  | HU    | 602  | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.95 | 3 (6%)   |
| 160 | GTP  | FI    | 602  | 159  | 33,34,34     | 0.90 | 1 (3%)   | 50,54,54    | 1.59 | 8 (16%)  |
| 156 | ATP  | 8e    | 4702 | -    | 32,33,33     | 0.43 | 0        | 48,52,52    | 0.45 | 0        |
| 158 | GDP  | CC    | 501  | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 160 | GTP  | XS    | 501  | 159  | 33,34,34     | 0.88 | 1 (3%)   | 50,54,54    | 1.59 | 8 (16%)  |
| 160 | GTP  | HE    | 602  | 159  | 33,34,34     | 0.90 | 1 (3%)   | 50,54,54    | 1.59 | 9 (18%)  |
| 160 | GTP  | VE    | 501  | 159  | 33,34,34     | 0.67 | 0        | 50,54,54    | 0.92 | 3 (6%)   |
| 160 | GTP  | TV    | 501  | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.97 | 4 (8%)   |
| 160 | GTP  | TZ    | 602  | 159  | 33,34,34     | 0.71 | 0        | 50,54,54    | 0.96 | 4 (8%)   |
| 158 | GDP  | LI    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.93 | 2 (4%)   |
| 158 | GDP  | SX    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 160 | GTP  | BF    | 602  | 159  | 33,34,34     | 0.84 | 0        | 50,54,54    | 1.58 | 8 (16%)  |
| 158 | GDP  | DI    | 501  | -    | 29,30,30     | 0.48 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 160 | GTP  | DM    | 501  | 159  | 33,34,34     | 0.64 | 0        | 50,54,54    | 0.93 | 3 (6%)   |
| 160 | GTP  | DY    | 501  | 159  | 33,34,34     | 0.64 | 0        | 50,54,54    | 0.93 | 3 (6%)   |
| 158 | GDP  | WX    | 501  | -    | 29,30,30     | 1.14 | 3 (10%)  | 45,47,47    | 1.69 | 6 (13%)  |
| 160 | GTP  | HA    | 501  | 159  | 33,34,34     | 0.88 | 2 (6%)   | 50,54,54    | 1.64 | 8 (16%)  |
| 158 | GDP  | YB    | 501  | -    | 29,30,30     | 0.54 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 160 | GTP  | OZ    | 501  | 159  | 33,34,34     | 0.71 | 0        | 50,54,54    | 0.97 | 3 (6%)   |
| 160 | GTP  | IG    | 501  | 159  | 33,34,34     | 0.87 | 1 (3%)   | 50,54,54    | 1.57 | 8 (16%)  |
| 158 | GDP  | HJ    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.91 | 2 (4%)   |
| 158 | GDP  | MK    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.91 | 2 (4%)   |
| 160 | GTP  | KN    | 602  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.99 | 4 (8%)   |
| 158 | GDP  | EF    | 501  | -    | 29,30,30     | 0.49 | 0        | 45,47,47    | 0.86 | 2 (4%)   |
| 158 | GDP  | DK    | 501  | -    | 29,30,30     | 0.49 | 0        | 45,47,47    | 0.92 | 2 (4%)   |
| 158 | GDP  | FL    | 602  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.88 | 2 (4%)   |
| 158 | GDP  | OI    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 160 | GTP  | BB    | 501  | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.94 | 3 (6%)   |
| 160 | GTP  | LR    | 501  | 159  | 33,34,34     | 0.72 | 0        | 50,54,54    | 0.94 | 3 (6%)   |
| 160 | GTP  | PM    | 602  | 159  | 33,34,34     | 0.67 | 0        | 50,54,54    | 0.94 | 4 (8%)   |
| 160 | GTP  | TI    | 501  | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.94 | 3 (6%)   |
| 156 | ATP  | 7a    | 4701 | -    | 32,33,33     | 0.45 | 0        | 48,52,52    | 0.32 | 0        |
| 160 | GTP  | WA    | 602  | 159  | 33,34,34     | 0.87 | 0        | 50,54,54    | 1.56 | 8 (16%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 158 | GDP  | JO    | 501  | -    | 29,30,30     | 0.52 | 0           | 45,47,47    | 0.87 | 2 (4%)      |
| 160 | GTP  | LF    | 602  | 159  | 33,34,34     | 0.68 | 0           | 50,54,54    | 0.95 | 3 (6%)      |
| 160 | GTP  | UH    | 501  | 159  | 33,34,34     | 0.70 | 0           | 50,54,54    | 0.97 | 4 (8%)      |
| 156 | ATP  | 8f    | 4703 | -    | 32,33,33     | 0.74 | 1 (3%)      | 48,52,52    | 0.33 | 0           |
| 160 | GTP  | VI    | 501  | 159  | 33,34,34     | 0.65 | 0           | 50,54,54    | 0.93 | 3 (6%)      |
| 160 | GTP  | AH    | 501  | 159  | 33,34,34     | 0.68 | 0           | 50,54,54    | 0.95 | 3 (6%)      |
| 158 | GDP  | BG    | 501  | -    | 29,30,30     | 0.52 | 0           | 45,47,47    | 0.90 | 2 (4%)      |
| 158 | GDP  | GL    | 501  | -    | 29,30,30     | 0.53 | 0           | 45,47,47    | 0.94 | 2 (4%)      |
| 160 | GTP  | UP    | 501  | 159  | 33,34,34     | 0.67 | 0           | 50,54,54    | 0.98 | 3 (6%)      |
| 158 | GDP  | OA    | 501  | -    | 29,30,30     | 0.50 | 0           | 45,47,47    | 0.87 | 2 (4%)      |
| 160 | GTP  | WY    | 602  | 159  | 33,34,34     | 0.66 | 0           | 50,54,54    | 0.92 | 3 (6%)      |
| 158 | GDP  | DP    | 501  | -    | 29,30,30     | 0.50 | 0           | 45,47,47    | 0.87 | 2 (4%)      |
| 158 | GDP  | RV    | 501  | -    | 29,30,30     | 0.50 | 0           | 45,47,47    | 0.91 | 2 (4%)      |
| 160 | GTP  | YV    | 602  | 159  | 33,34,34     | 0.69 | 0           | 50,54,54    | 0.98 | 4 (8%)      |
| 158 | GDP  | QB    | 501  | -    | 29,30,30     | 0.53 | 0           | 45,47,47    | 0.89 | 2 (4%)      |
| 158 | GDP  | ST    | 501  | -    | 29,30,30     | 0.53 | 0           | 45,47,47    | 0.92 | 2 (4%)      |
| 160 | GTP  | MF    | 602  | 159  | 33,34,34     | 0.70 | 0           | 50,54,54    | 0.97 | 3 (6%)      |
| 156 | ATP  | 7f    | 4703 | -    | 32,33,33     | 0.43 | 0           | 48,52,52    | 0.32 | 0           |
| 160 | GTP  | UW    | 602  | 159  | 33,34,34     | 0.65 | 0           | 50,54,54    | 0.93 | 3 (6%)      |
| 156 | ATP  | 9f    | 4703 | -    | 32,33,33     | 0.42 | 0           | 48,52,52    | 0.30 | 0           |
| 160 | GTP  | GQ    | 602  | 159  | 33,34,34     | 0.64 | 0           | 50,54,54    | 0.97 | 3 (6%)      |
| 158 | GDP  | AO    | 501  | -    | 29,30,30     | 1.16 | 3 (10%)     | 45,47,47    | 1.74 | 6 (13%)     |
| 158 | GDP  | CO    | 501  | -    | 29,30,30     | 0.51 | 0           | 45,47,47    | 0.91 | 2 (4%)      |
| 158 | GDP  | GJ    | 501  | -    | 29,30,30     | 0.52 | 0           | 45,47,47    | 0.91 | 2 (4%)      |
| 158 | GDP  | OK    | 501  | -    | 29,30,30     | 0.51 | 0           | 45,47,47    | 0.92 | 2 (4%)      |
| 158 | GDP  | MM    | 501  | -    | 29,30,30     | 0.52 | 0           | 45,47,47    | 0.90 | 2 (4%)      |
| 160 | GTP  | RS    | 501  | 159  | 33,34,34     | 0.71 | 0           | 50,54,54    | 0.96 | 3 (6%)      |
| 158 | GDP  | JS    | 501  | -    | 29,30,30     | 1.17 | 3 (10%)     | 45,47,47    | 1.72 | 6 (13%)     |
| 158 | GDP  | JI    | 501  | -    | 29,30,30     | 1.16 | 3 (10%)     | 45,47,47    | 1.71 | 6 (13%)     |
| 158 | GDP  | EN    | 501  | -    | 29,30,30     | 0.50 | 0           | 45,47,47    | 0.87 | 2 (4%)      |
| 158 | GDP  | ZO    | 501  | -    | 29,30,30     | 0.52 | 0           | 45,47,47    | 0.92 | 2 (4%)      |
| 160 | GTP  | DQ    | 501  | 159  | 33,34,34     | 0.66 | 0           | 50,54,54    | 0.95 | 4 (8%)      |
| 156 | ATP  | 7b    | 4703 | -    | 32,33,33     | 0.42 | 0           | 48,52,52    | 0.28 | 0           |
| 158 | GDP  | PA    | 501  | -    | 29,30,30     | 0.52 | 0           | 45,47,47    | 0.92 | 2 (4%)      |
| 160 | GTP  | IW    | 501  | 159  | 33,34,34     | 0.70 | 0           | 50,54,54    | 0.99 | 4 (8%)      |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 158 | GDP  | NO    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 160 | GTP  | PC    | 602  | 159  | 33,34,34     | 0.90 | 0        | 50,54,54    | 1.58 | 8 (16%)  |
| 160 | GTP  | FA    | 602  | 159  | 33,34,34     | 0.66 | 0        | 50,54,54    | 0.96 | 4 (8%)   |
| 160 | GTP  | CJ    | 501  | 159  | 33,34,34     | 0.67 | 0        | 50,54,54    | 0.95 | 3 (6%)   |
| 160 | GTP  | LJ    | 501  | 159  | 33,34,34     | 0.73 | 0        | 50,54,54    | 0.98 | 3 (6%)   |
| 160 | GTP  | IU    | 501  | 159  | 33,34,34     | 0.89 | 2 (6%)   | 50,54,54    | 1.60 | 8 (16%)  |
| 160 | GTP  | HS    | 501  | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.97 | 3 (6%)   |
| 158 | GDP  | LA    | 501  | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.87 | 2 (4%)   |
| 158 | GDP  | IX    | 501  | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 158 | GDP  | VR    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 158 | GDP  | XX    | 501  | -    | 29,30,30     | 0.46 | 0        | 45,47,47    | 0.92 | 2 (4%)   |
| 158 | GDP  | LQ    | 501  | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 158 | GDP  | AE    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 160 | GTP  | IE    | 501  | 159  | 33,34,34     | 0.88 | 2 (6%)   | 50,54,54    | 1.60 | 8 (16%)  |
| 158 | GDP  | TY    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 160 | GTP  | NJ    | 503  | 159  | 33,34,34     | 0.67 | 0        | 50,54,54    | 0.96 | 3 (6%)   |
| 160 | GTP  | UY    | 602  | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.91 | 3 (6%)   |
| 160 | GTP  | AN    | 501  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.98 | 3 (6%)   |
| 158 | GDP  | KE    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 160 | GTP  | Ah    | 501  | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.95 | 3 (6%)   |
| 157 | ADP  | 7f    | 4701 | -    | 28,29,29     | 1.38 | 5 (17%)  | 43,45,45    | 1.79 | 10 (23%) |
| 160 | GTP  | SY    | 602  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.98 | 3 (6%)   |
| 158 | GDP  | LO    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 160 | GTP  | CX    | 602  | 159  | 33,34,34     | 0.86 | 1 (3%)   | 50,54,54    | 1.55 | 8 (16%)  |
| 158 | GDP  | KI    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 160 | GTP  | TM    | 501  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.95 | 3 (6%)   |
| 158 | GDP  | OG    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 158 | GDP  | AC    | 501  | -    | 29,30,30     | 1.16 | 3 (10%)  | 45,47,47    | 1.75 | 6 (13%)  |
| 160 | GTP  | QC    | 501  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.95 | 4 (8%)   |
| 158 | GDP  | JF    | 501  | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 158 | GDP  | ED    | 501  | -    | 29,30,30     | 1.25 | 3 (10%)  | 45,47,47    | 1.73 | 6 (13%)  |
| 158 | GDP  | VT    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 158 | GDP  | BQ    | 501  | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 160 | GTP  | JN    | 501  | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.92 | 3 (6%)   |
| 158 | GDP  | RN    | 501  | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.95 | 2 (4%)   |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 157 | ADP  | 8f    | 4701 | -    | 28,29,29     | 1.38 | 5 (17%)  | 43,45,45    | 1.79 | 9 (20%)  |
| 158 | GDP  | PJ    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 158 | GDP  | QL    | 501  | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.91 | 2 (4%)   |
| 158 | GDP  | TB    | 501  | -    | 29,30,30     | 0.52 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 160 | GTP  | LX    | 501  | 159  | 33,34,34     | 0.71 | 0        | 50,54,54    | 0.96 | 3 (6%)   |
| 160 | GTP  | YG    | 602  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.95 | 4 (8%)   |
| 158 | GDP  | VV    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.89 | 2 (4%)   |
| 158 | GDP  | LK    | 501  | -    | 29,30,30     | 0.54 | 0        | 45,47,47    | 0.98 | 2 (4%)   |
| 160 | GTP  | LT    | 602  | 159  | 33,34,34     | 0.69 | 0        | 50,54,54    | 0.97 | 3 (6%)   |
| 160 | GTP  | KH    | 501  | 159  | 33,34,34     | 0.68 | 0        | 50,54,54    | 0.92 | 3 (6%)   |
| 158 | GDP  | QP    | 501  | -    | 29,30,30     | 0.53 | 0        | 45,47,47    | 0.88 | 2 (4%)   |
| 160 | GTP  | PS    | 501  | 159  | 33,34,34     | 0.70 | 0        | 50,54,54    | 0.92 | 3 (6%)   |
| 160 | GTP  | AB    | 602  | 159  | 33,34,34     | 0.88 | 1 (3%)   | 50,54,54    | 1.60 | 8 (16%)  |
| 158 | GDP  | GN    | 501  | -    | 29,30,30     | 0.50 | 0        | 45,47,47    | 0.90 | 2 (4%)   |
| 158 | GDP  | FB    | 501  | -    | 29,30,30     | 0.51 | 0        | 45,47,47    | 0.89 | 2 (4%)   |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 160 | GTP  | UT    | 501 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | PY    | 602 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | MV    | 502 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | ZD    | 501 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | CE    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | MP    | 501 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | FZ    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | ZS    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 160 | GTP  | WM    | 602 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | FE    | 501 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | LP    | 502 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | XM    | 602 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | Ao    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | WP    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 160 | GTP  | OH    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | UM    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | WB    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | QG    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | JL    | 501  | 159  | -       | 6/22/38/38 | 0/3/3/3 |
| 158 | GDP  | IZ    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | FN    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | MW    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | Ap    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | ZQ    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | EV    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | KF    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | HK    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | QD    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | ZR    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 156 | ATP  | 7e    | 4704 | -    | -       | 7/22/38/38 | 0/3/3/3 |
| 160 | GTP  | AL    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | IJ    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | HB    | 501  | -    | -       | 3/16/32/32 | 0/3/3/3 |
| 160 | GTP  | JE    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | OT    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | SE    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | KX    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | EA    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | WC    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | FH    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | RB    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | IP    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | VY    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | PU    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | QI    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | SO    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | LB    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | RF    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 158 | GDP  | FV    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | MZ    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | JB    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | Ab    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 156 | ATP  | 9f    | 4701 | -    | -       | 9/22/38/38 | 0/3/3/3 |
| 158 | GDP  | MI    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | TT    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | MU    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | GA    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | YC    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | OC    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | ZG    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | JK    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | KK    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | DJ    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | DS    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | SU    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | SQ    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | OU    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | UO    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | LZ    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | FS    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | ZC    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | UL    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | GO    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | XG    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | JX    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | SL    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | JV    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | VF    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | MN    | 502  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | NA    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | Ad    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | ZJ    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 158 | GDP  | DZ    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | BO    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | NG    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | RD    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | ZE    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | FF    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | CW    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | WI    | 602 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | NE    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | FJ    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | NM    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | Aa    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | HW    | 501 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | SS    | 602 | 159  | -       | 2/22/38/38 | 0/3/3/3 |
| 158 | GDP  | BC    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | BJ    | 602 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | ER    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | LG    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | TO    | 501 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | FK    | 501 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | CY    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | KM    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | LM    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | TH    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | ZP    | 501 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | NR    | 502 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | ON    | 501 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | XZ    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | CK    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | DW    | 602 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | EJ    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | TQ    | 602 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | NV    | 503 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | VD    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 158 | GDP  | AM    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 156 | ATP  | 7f    | 4702 | -    | -       | 7/22/38/38 | 0/3/3/3 |
| 160 | GTP  | FO    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | MD    | 502  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | MX    | 502  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | KL    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | TS    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | FD    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | TE    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | LH    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | ZH    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | BN    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | TD    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | CR    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | DD    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | CS    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | RR    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | NS    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | QV    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | BP    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | VU    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | ML    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | UR    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | UZ    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | CT    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | BM    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | CV    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | UC    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | EU    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | PI    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | OE    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | YX    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | AP    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | WT    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 158 | GDP  | MG    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | FY    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | AX    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | NY    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | TF    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | UB    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 156 | ATP  | 8f    | 4702 | -    | -       | 8/22/38/38 | 0/3/3/3 |
| 160 | GTP  | AJ    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | RW    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | EO    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | JG    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | PV    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | IH    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | BL    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | FQ    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | KC    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 157 | ADP  | 8e    | 4701 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 158 | GDP  | LW    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | GV    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | QF    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | SG    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | HV    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | GI    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | GM    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | MQ    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 156 | ATP  | 8e    | 4703 | -    | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | LD    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | WR    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | EW    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | GR    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | VS    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | WL    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | HN    | 501  | -    | -       | 3/16/32/32 | 0/3/3/3 |
| 160 | GTP  | PE    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 158 | GDP  | ZW    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | CN    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | II    | 501  | 159  | -       | 3/22/38/38 | 0/3/3/3 |
| 160 | GTP  | QQ    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | IQ    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | BW    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | WH    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | XN    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | Aj    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | DE    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | LC    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | VN    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | WK    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | OX    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | BS    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | CI    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | NH    | 502  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | KR    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | JH    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | NN    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | CM    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | OQ    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | LL    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 156 | ATP  | 9e    | 5004 | -    | -       | 9/22/38/38 | 0/3/3/3 |
| 160 | GTP  | ZZ    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | NP    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | WG    | 501  | 159  | -       | 2/22/38/38 | 0/3/3/3 |
| 158 | GDP  | ZI    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | VQ    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | TW    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | TA    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | FM    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | JA    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | SZ    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 160 | GTP  | RC    | 501 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | PO    | 602 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | RT    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | OD    | 602 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | FG    | 501 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | XR    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | TU    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | OW    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | AG    | 501 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 160 | GTP  | BV    | 602 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | XV    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | UE    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | GC    | 602 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | TJ    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | NI    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | IO    | 501 | 159  | -       | 3/22/38/38 | 0/3/3/3 |
| 160 | GTP  | JR    | 602 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | KW    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | RK    | 602 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | IB    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | XF    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | YE    | 602 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | QT    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | ZF    | 602 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | BA    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | GF    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | PL    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | XA    | 501 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | Ag    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | HY    | 501 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | Am    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | Ai    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | QR    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | KB    | 501 | 159  | -       | 5/22/38/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 158 | GDP  | ZA    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | RE    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | XI    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | DL    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | JY    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | RG    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | RM    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 156 | ATP  | 7a    | 4704 | -    | -       | 6/22/38/38 | 0/3/3/3 |
| 160 | GTP  | DB    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | CL    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | XP    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | SP    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 157 | ADP  | 7e    | 4701 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 160 | GTP  | YJ    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | XJ    | 501  | -    | -       | 3/16/32/32 | 0/3/3/3 |
| 160 | GTP  | PK    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | Ae    | 501  | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 156 | ATP  | 8e    | 4704 | -    | -       | 9/22/38/38 | 0/3/3/3 |
| 158 | GDP  | OM    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | RU    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | XB    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | YQ    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | XW    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | LY    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | VO    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | HL    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | PZ    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | WJ    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | ES    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 157 | ADP  | 9f    | 4702 | -    | -       | 6/16/32/32 | 0/3/3/3 |
| 158 | GDP  | HZ    | 501  | -    | -       | 3/16/32/32 | 0/3/3/3 |
| 158 | GDP  | AW    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | EG    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | DO    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 160 | GTP  | EC    | 501 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | PF    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | EI    | 501 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | PX    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | TN    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | KA    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | VX    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | ZY    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | CF    | 501 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | YY    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | EE    | 501 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | KO    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | HF    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | YM    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | BR    | 501 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | FC    | 501 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | UF    | 501 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | GS    | 602 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | TX    | 602 | 159  | -       | 4/22/38/38 | 0/3/3/3 |
| 160 | GTP  | JP    | 602 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | QU    | 602 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | OJ    | 602 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | RY    | 602 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | SC    | 602 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | YN    | 501 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | Af    | 501 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | IV    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | JU    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | Al    | 602 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | DN    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | OL    | 602 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | UX    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | LS    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | JD    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 158 | GDP  | NU    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | DF    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | WE    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | WW    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | RL    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | DX    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | VC    | 501  | 159  | -       | 2/22/38/38 | 0/3/3/3 |
| 160 | GTP  | OP    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | DV    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | PH    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | TP    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | ZV    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | PR    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | OV    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | MB    | 502  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | FW    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | EB    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | EY    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | NT    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | RX    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | IY    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | WU    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | IL    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | EZ    | 602  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | AQ    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | NZ    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | BK    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | IS    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | AI    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | LU    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | UN    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | NC    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 156 | ATP  | 9e    | 5001 | -    | -       | 8/22/38/38 | 0/3/3/3 |
| 160 | GTP  | KV    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 160 | GTP  | HI    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | IK    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | QY    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | YS    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | HM    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | NB    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | XD    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | BZ    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | TC    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | HG    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | ZN    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | GU    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 156 | ATP  | 7e    | 4702 | -    | -       | 5/22/38/38 | 0/3/3/3 |
| 156 | ATP  | 9e    | 5003 | -    | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | YF    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | YU    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | An    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | DC    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | GK    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | EX    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | ZB    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | DU    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | CQ    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | AT    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | ZX    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | VZ    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | VJ    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | QH    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | ZT    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | CD    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | XT    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | VL    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | MT    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | AS    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 160 | GTP  | IM    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | KZ    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | BX    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | PP    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | OY    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | ZL    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | PT    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | RH    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | XU    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | AK    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | NL    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | MA    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | JC    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | NQ    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | US    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | CZ    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | DR    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | YD    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | JZ    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | MH    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | ME    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | HR    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | YW    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | NX    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | PD    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | XQ    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | BI    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | DH    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | GX    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | WV    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | Ak    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 157 | ADP  | 9e    | 5002 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 158 | GDP  | SD    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | EM    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 160 | GTP  | GE    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | RQ    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 156 | ATP  | 9f    | 4704 | -    | -       | 8/22/38/38 | 0/3/3/3 |
| 158 | GDP  | MC    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | SJ    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | VB    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | VG    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | XC    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | HD    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | KS    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | KD    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | PQ    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | FT    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | GH    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | QA    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | YL    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | HQ    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | ND    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 156 | ATP  | 7a    | 4702 | -    | -       | 9/22/38/38 | 0/3/3/3 |
| 158 | GDP  | KY    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | QN    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | RO    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | AU    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | QW    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 157 | ADP  | 7b    | 4704 | -    | -       | 7/16/32/32 | 0/3/3/3 |
| 158 | GDP  | JM    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | ID    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | RJ    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | AF    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | RP    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | MJ    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | AY    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | YO    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | YR    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 158 | GDP  | GD    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | XE    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | PG    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | LN    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | VM    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | AZ    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | OS    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 156 | ATP  | 7b    | 4701 | -    | -       | 4/22/38/38 | 0/3/3/3 |
| 158 | GDP  | SV    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | LV    | 502  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | LE    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | AV    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | CP    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | GW    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | YP    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | AD    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | IT    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | ZM    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | CA    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | XO    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | JQ    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | QM    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | RZ    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | UG    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | WZ    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | JW    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | XL    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 156 | ATP  | 7b    | 4702 | -    | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | MY    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | YZ    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | ET    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | UD    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | CB    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | VW    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 158 | GDP  | VH    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | MR    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | KU    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | WO    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | XY    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | KG    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | SW    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | MO    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | UJ    | 501  | 159  | -       | 4/22/38/38 | 0/3/3/3 |
| 160 | GTP  | AR    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | BD    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | SA    | 501  | 159  | -       | 4/22/38/38 | 0/3/3/3 |
| 160 | GTP  | WS    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | OO    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | KQ    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | EK    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 156 | ATP  | 7f    | 4704 | -    | -       | 4/22/38/38 | 0/3/3/3 |
| 160 | GTP  | JT    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | QO    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | ZK    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | RA    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | IA    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | EQ    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | XK    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | IF    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | VP    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | EH    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 156 | ATP  | 7e    | 4703 | -    | -       | 9/22/38/38 | 0/3/3/3 |
| 158 | GDP  | GB    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | HP    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | GT    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | TK    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | CH    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | UK    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 158 | GDP  | EL    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | WN    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 157 | ADP  | 7a    | 4703 | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 160 | GTP  | YA    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | QK    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | WQ    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | IN    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | SI    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | QX    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | DA    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | SN    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | GZ    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | QE    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | IR    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | DT    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | OB    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | HC    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | PN    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | QZ    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | TG    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | FP    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | FR    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | VK    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | SK    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | HH    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | DG    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | WF    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | VA    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | BU    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | CU    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | UQ    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 156 | ATP  | 8f    | 4704 | -    | -       | 8/22/38/38 | 0/3/3/3 |
| 160 | GTP  | OR    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | QS    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 158 | GDP  | QJ    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | Ac    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | KJ    | 602 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | YH    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | KT    | 501 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | JJ    | 501 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | OF    | 501 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | RI    | 501 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | UU    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | GP    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | PW    | 501 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | FX    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | WD    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | YK    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | SF    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | YT    | 602 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | GG    | 501 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | XH    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | TL    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | KP    | 602 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | UA    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | BT    | 602 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | ZU    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | BH    | 602 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | NF    | 502 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | NK    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | BY    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | TR    | 501 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | HX    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | SB    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | HT    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | SR    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | SM    | 501 | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | SH    | 501 | -    | -       | 2/16/32/32 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 158 | GDP  | AA    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | HO    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | UI    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | HU    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | FI    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 156 | ATP  | 8e    | 4702 | -    | -       | 9/22/38/38 | 0/3/3/3 |
| 158 | GDP  | CC    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | XS    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | HE    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | VE    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | TV    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | TZ    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | LI    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | SX    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | BF    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | DI    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | DM    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | DY    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | WX    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | HA    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | YB    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | OZ    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | IG    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | HJ    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | MK    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | KN    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | EF    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | DK    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | FL    | 602  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | OI    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | BB    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | LR    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | PM    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | TI    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 156 | ATP  | 7a    | 4701 | -    | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | WA    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | JO    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | LF    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | UH    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 156 | ATP  | 8f    | 4703 | -    | -       | 6/22/38/38 | 0/3/3/3 |
| 160 | GTP  | VI    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | AH    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | BG    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | GL    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | UP    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | OA    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | WY    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | DP    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | RV    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | YV    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | QB    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | ST    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | MF    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 156 | ATP  | 7f    | 4703 | -    | -       | 9/22/38/38 | 0/3/3/3 |
| 160 | GTP  | UW    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 156 | ATP  | 9f    | 4703 | -    | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | GQ    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | AO    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | CO    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | GJ    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | OK    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | MM    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | RS    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | JS    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | JI    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | EN    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | ZO    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | DQ    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 156 | ATP  | 7b    | 4703 | -    | -       | 9/22/38/38 | 0/3/3/3 |
| 158 | GDP  | PA    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | IW    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | NO    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | PC    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | FA    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | CJ    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | LJ    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | IU    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | HS    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | LA    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | IX    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | VR    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | XX    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | LQ    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | AE    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | IE    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | TY    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | NJ    | 503  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | UY    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | AN    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | KE    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | Ah    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 157 | ADP  | 7f    | 4701 | -    | -       | 8/16/32/32 | 0/3/3/3 |
| 160 | GTP  | SY    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | LO    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | CX    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | KI    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | TM    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | OG    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | AC    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | QC    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | JF    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | ED    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 158 | GDP  | VT    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | BQ    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | JN    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | RN    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 157 | ADP  | 8f    | 4701 | -    | -       | 7/16/32/32 | 0/3/3/3 |
| 158 | GDP  | PJ    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | QL    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | TB    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | LX    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | YG    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | VV    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | LK    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | LT    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | KH    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | QP    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 160 | GTP  | PS    | 501  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 160 | GTP  | AB    | 602  | 159  | -       | 5/22/38/38 | 0/3/3/3 |
| 158 | GDP  | GN    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 158 | GDP  | FB    | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |

The worst 5 of 231 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 157 | 9e    | 5002 | ADP  | C5-C4 | 4.58 | 1.47        | 1.39     |
| 157 | 7e    | 4701 | ADP  | C5-C4 | 4.55 | 1.47        | 1.39     |
| 157 | 8e    | 4701 | ADP  | C5-C4 | 4.54 | 1.47        | 1.39     |
| 157 | 7a    | 4703 | ADP  | C5-C4 | 4.46 | 1.47        | 1.39     |
| 157 | 8f    | 4701 | ADP  | C5-C4 | 4.45 | 1.47        | 1.39     |

The worst 5 of 2246 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 158 | FH    | 501 | GDP  | C5-C4-N3 | -6.51 | 118.03      | 128.39   |
| 158 | ED    | 501 | GDP  | C5-C4-N3 | -6.34 | 118.30      | 128.39   |
| 158 | AC    | 501 | GDP  | C5-C4-N3 | -6.28 | 118.40      | 128.39   |
| 158 | FZ    | 501 | GDP  | C5-C4-N3 | -6.27 | 118.40      | 128.39   |
| 158 | AO    | 501 | GDP  | C5-C4-N3 | -6.27 | 118.42      | 128.39   |

There are no chirality outliers.

5 of 2595 torsion outliers are listed below:

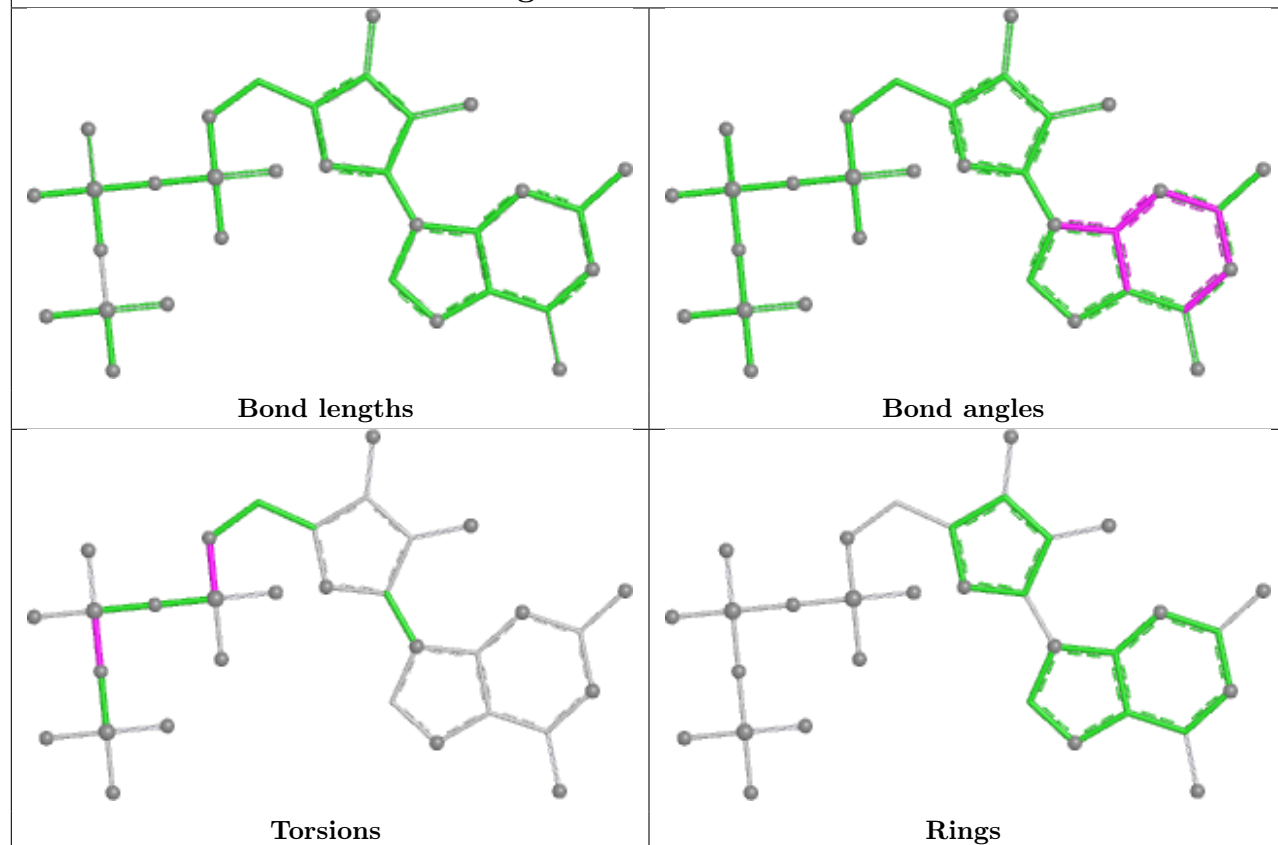
| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 156 | 7a    | 4701 | ATP  | C5'-O5'-PA-O3A |
| 156 | 7a    | 4701 | ATP  | C4'-C5'-O5'-PA |
| 156 | 7a    | 4702 | ATP  | PB-O3B-PG-O2G  |
| 156 | 7a    | 4702 | ATP  | C5'-O5'-PA-O2A |
| 156 | 7a    | 4702 | ATP  | C5'-O5'-PA-O3A |

There are no ring outliers.

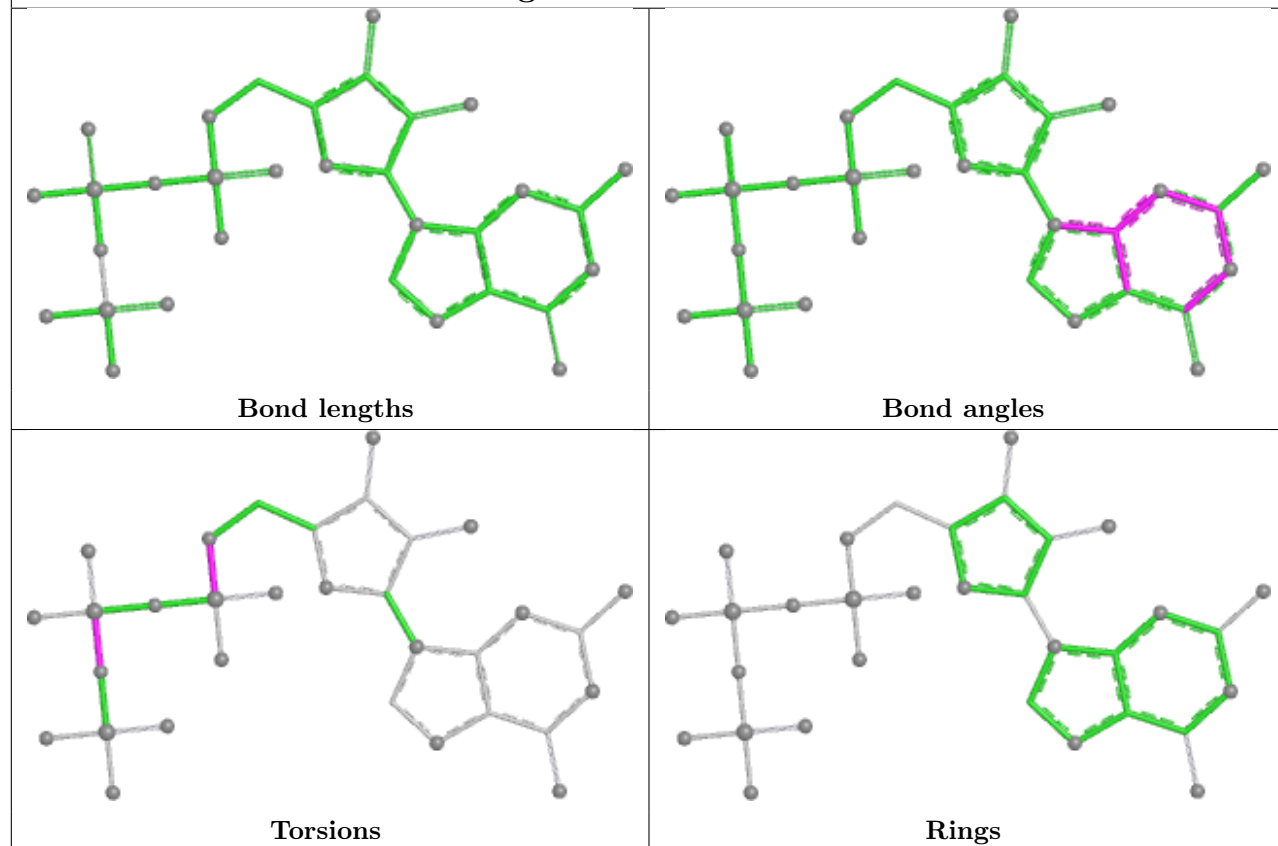
No monomer is involved in short contacts.

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.

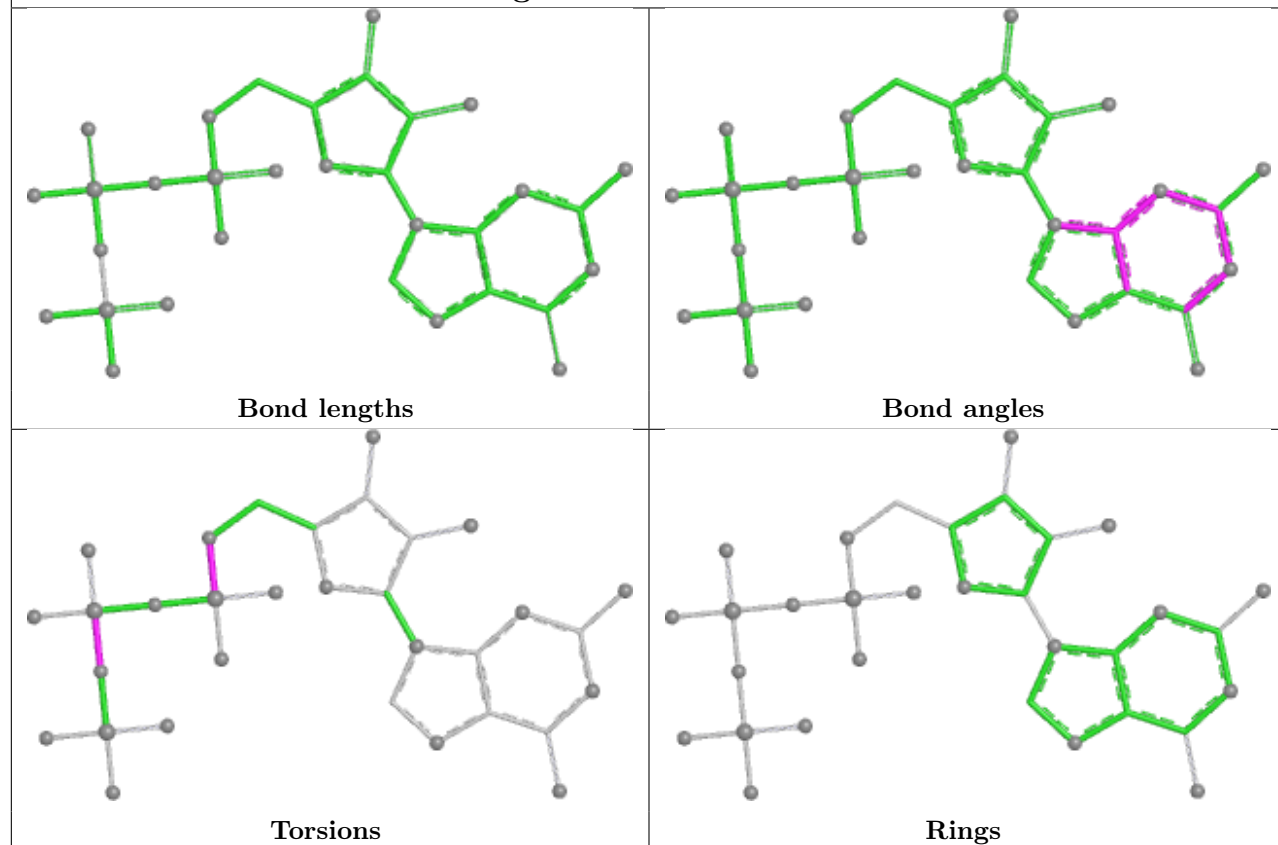
## Ligand GTP UT 501



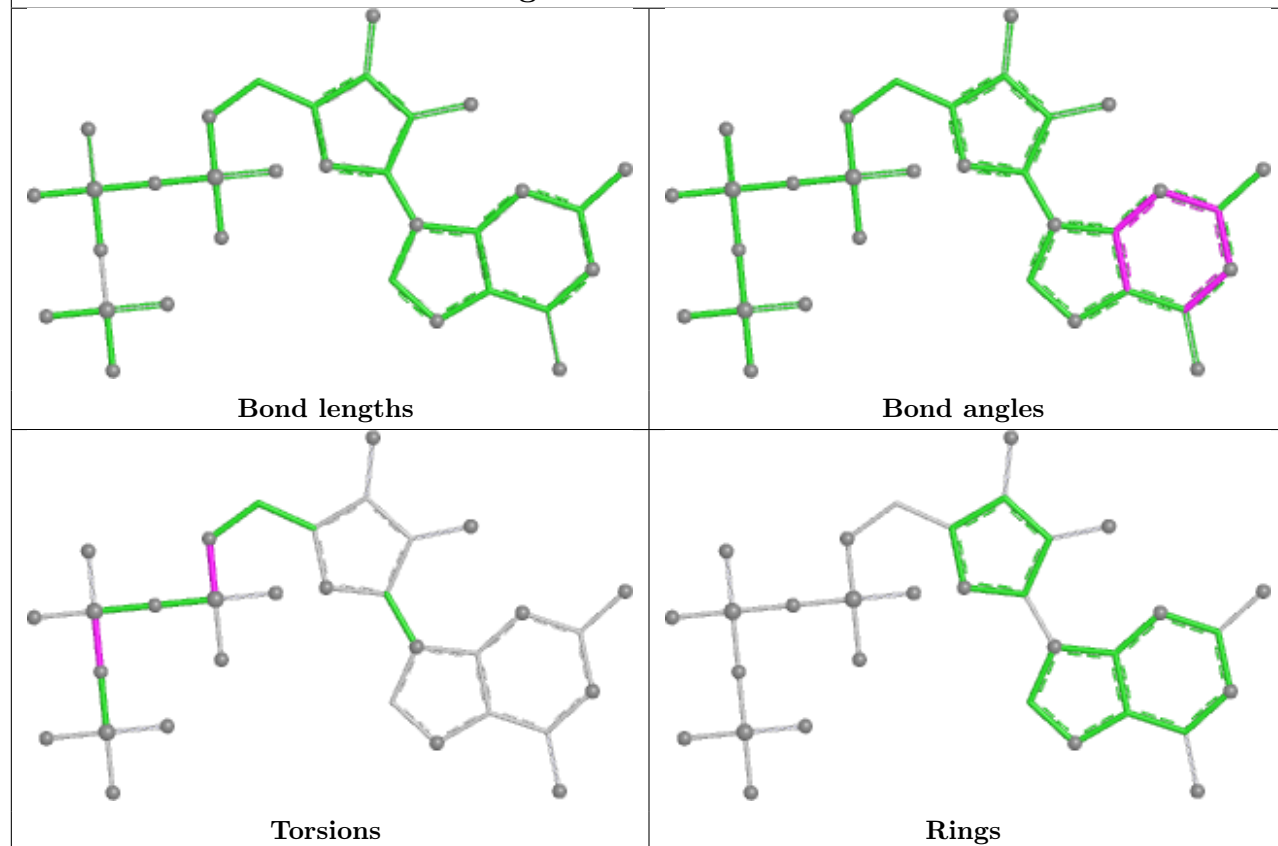
## Ligand GTP PY 602

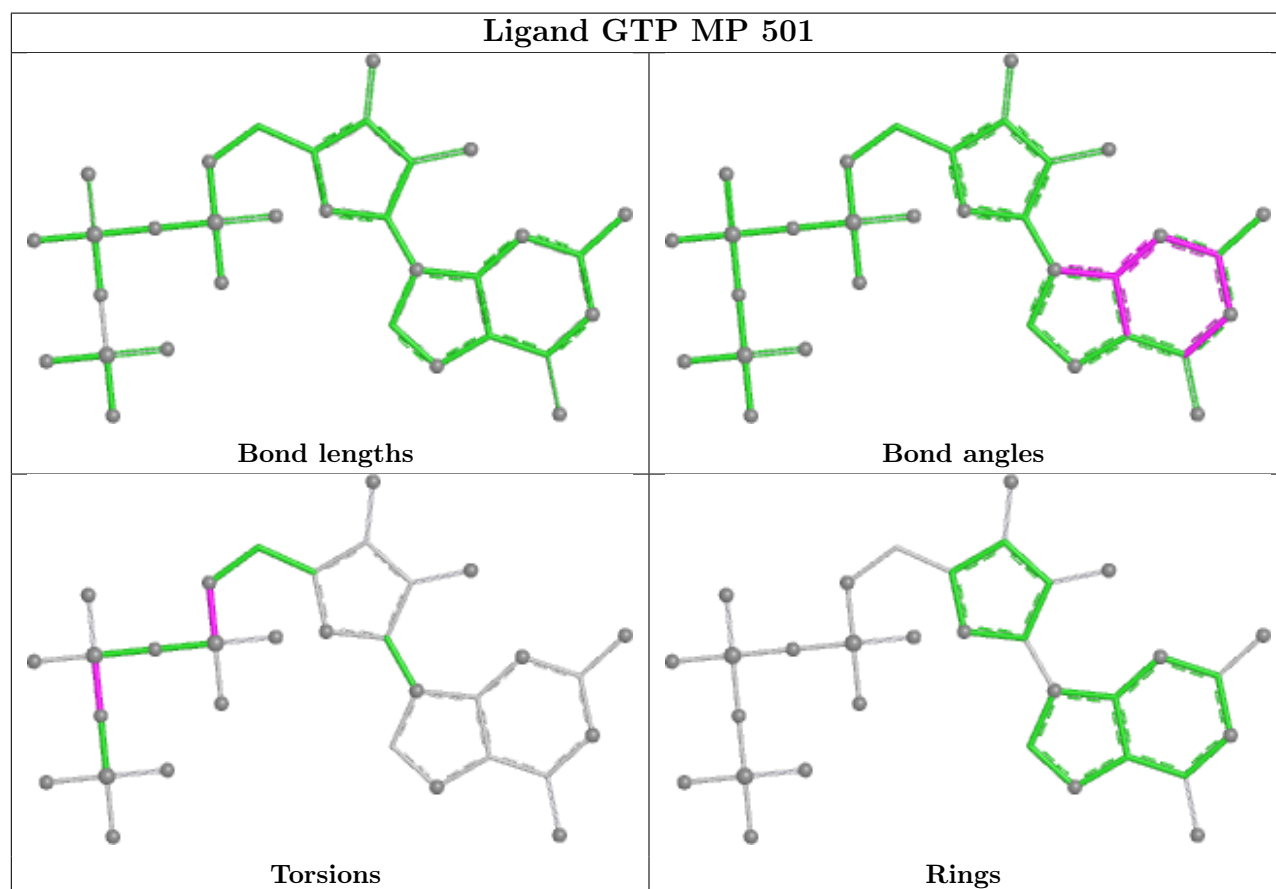
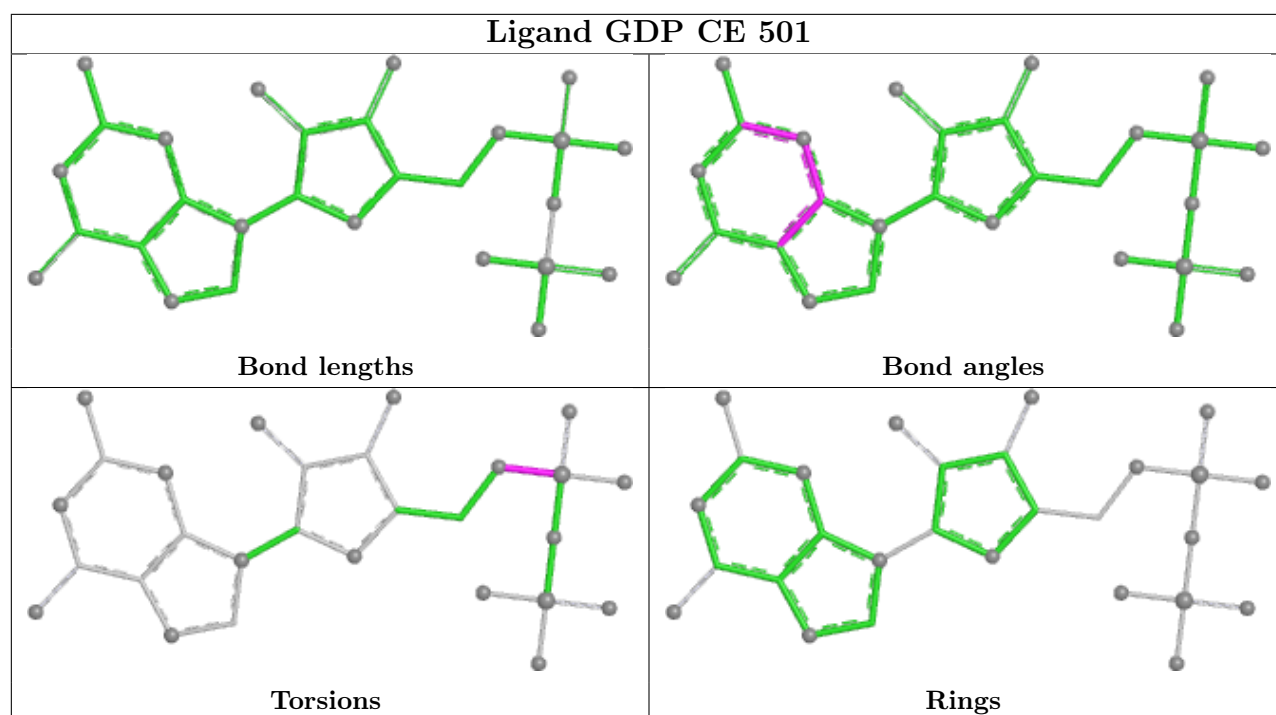


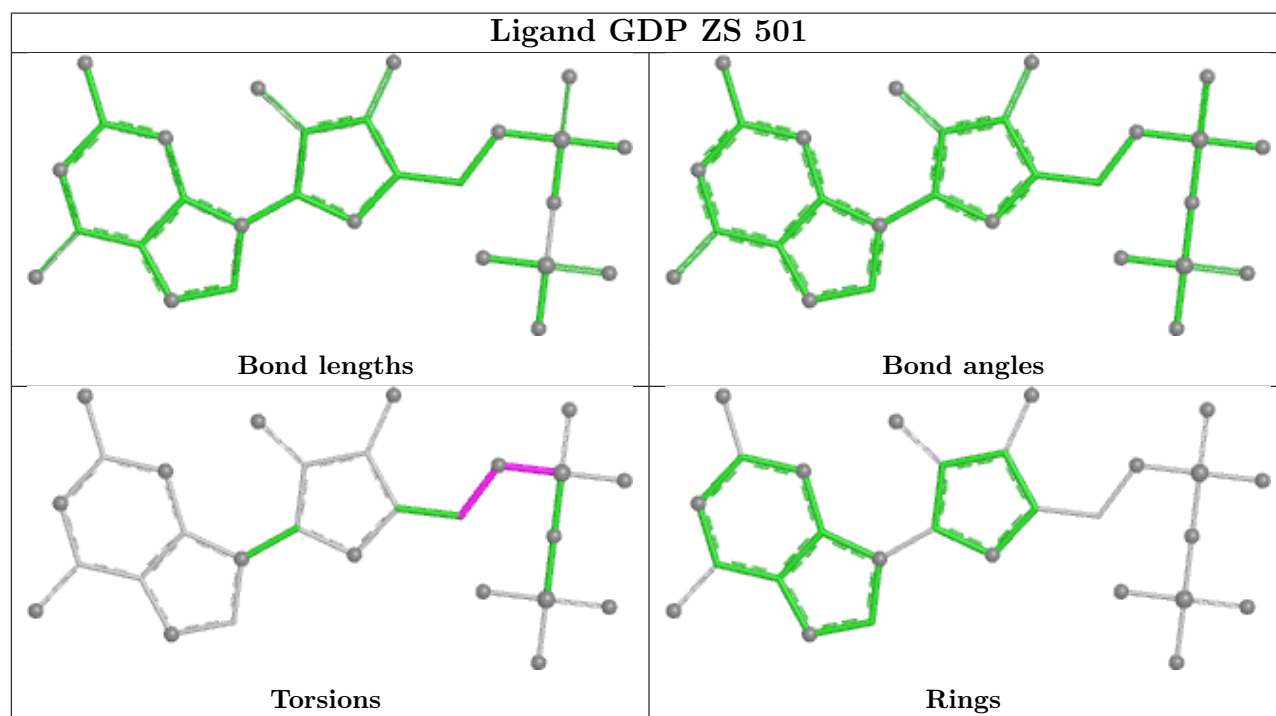
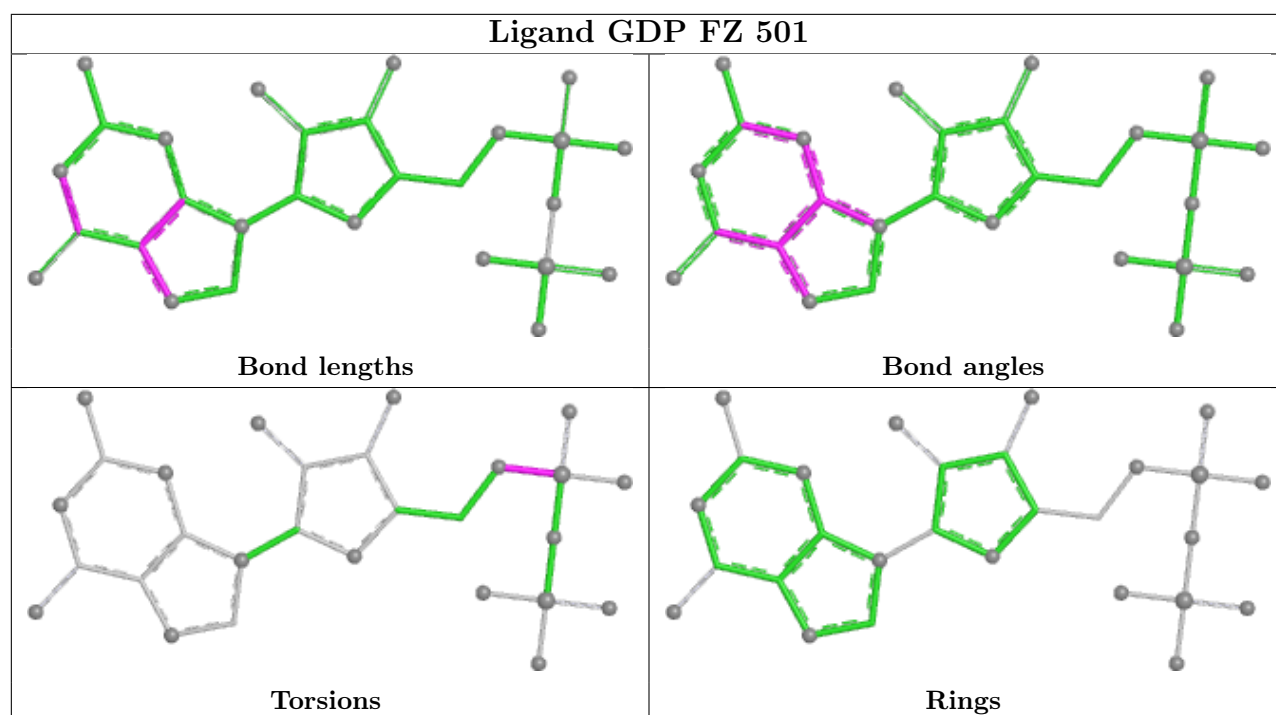
## Ligand GTP MV 502



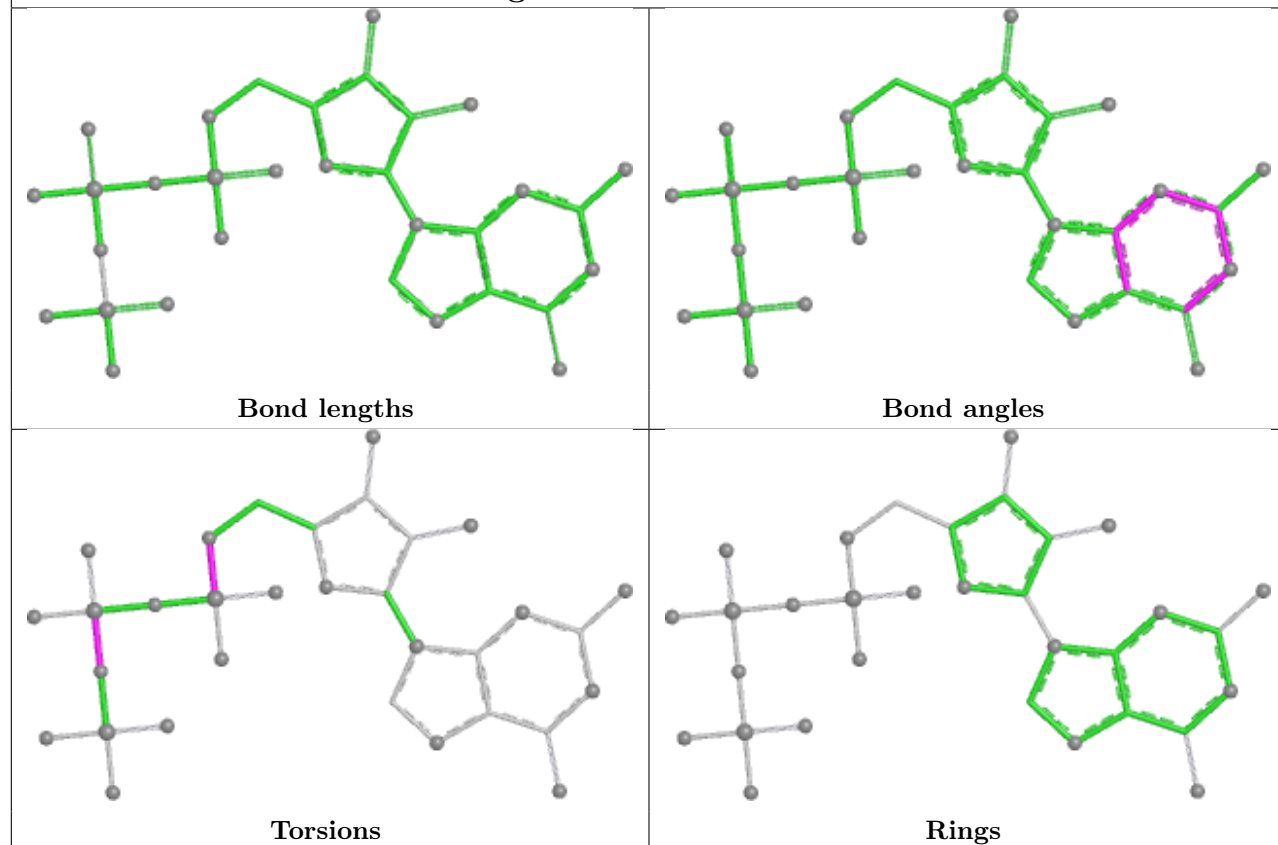
## Ligand GTP ZD 501



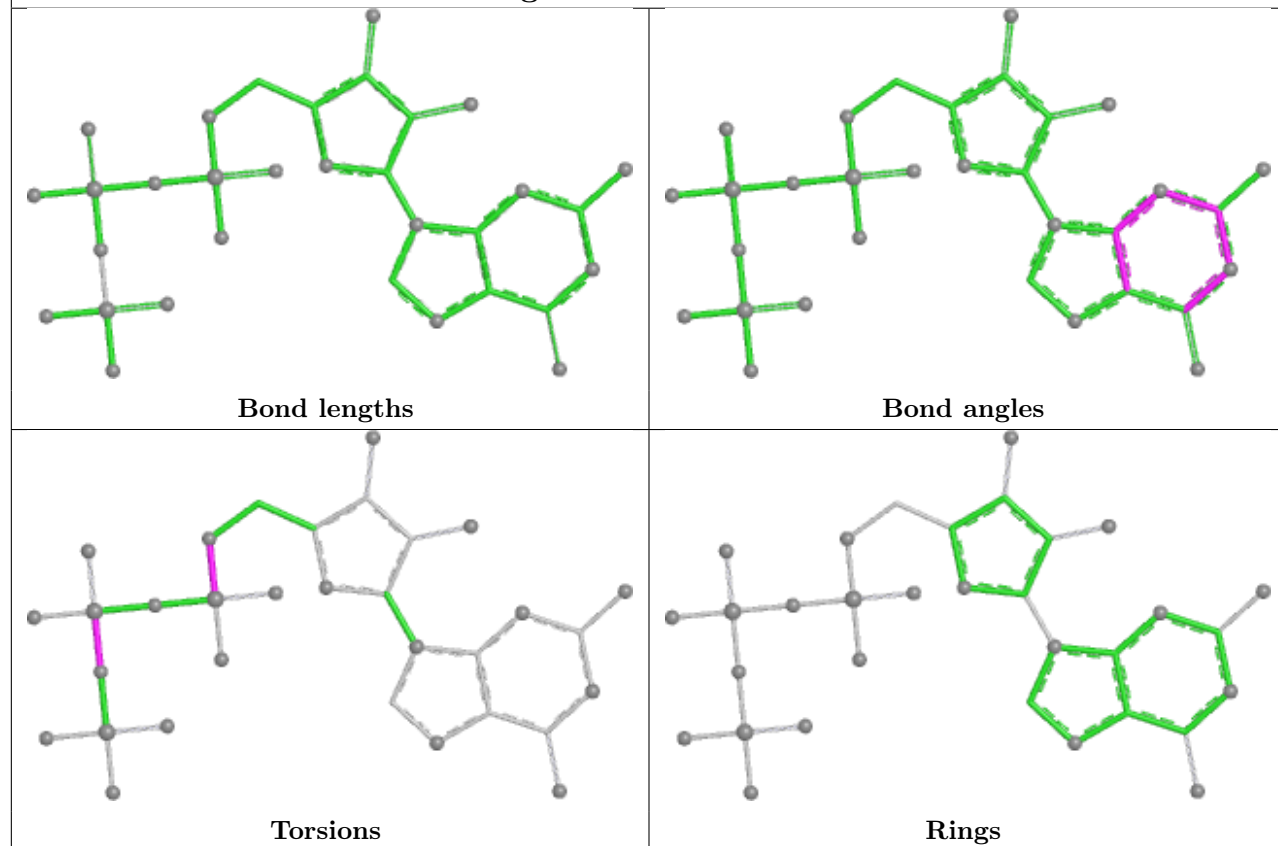




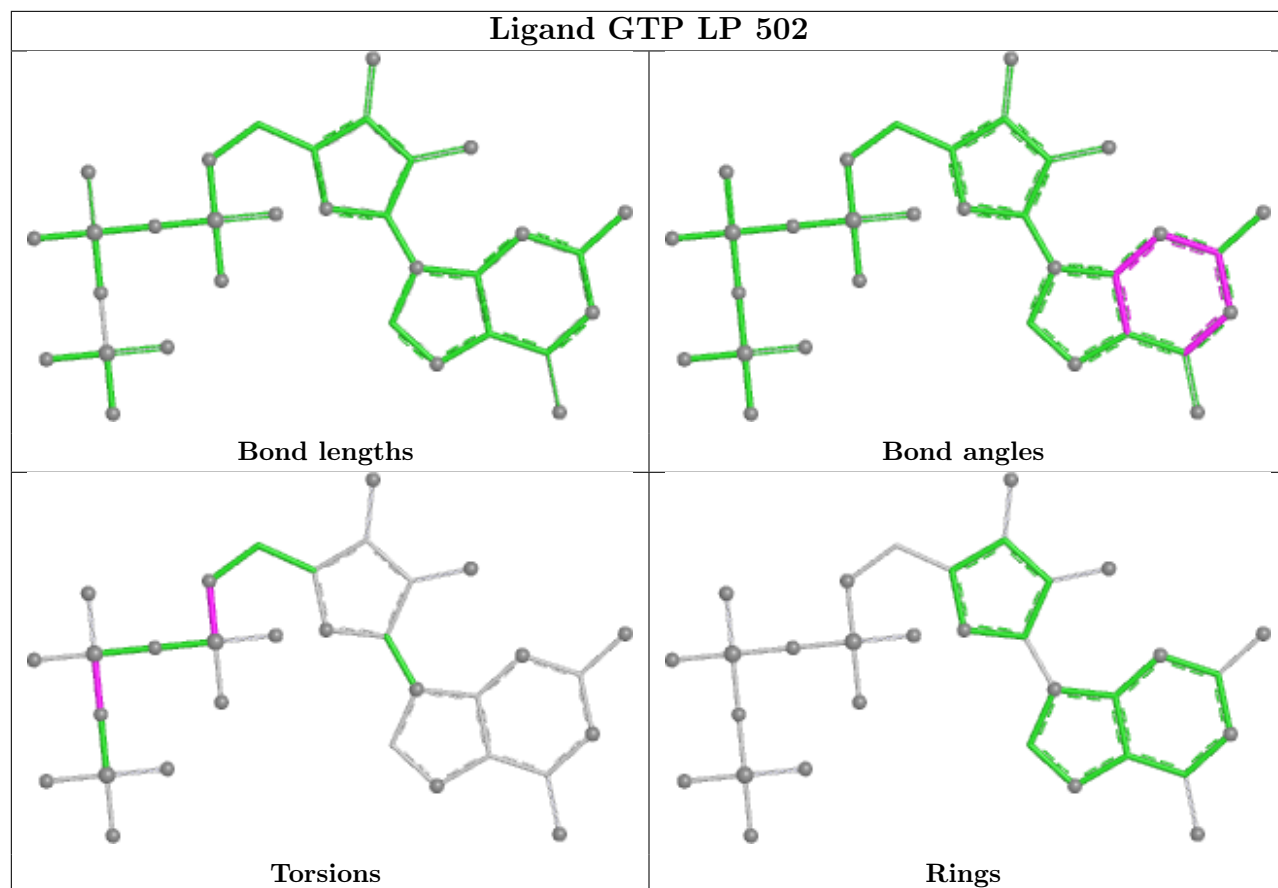
## Ligand GTP WM 602



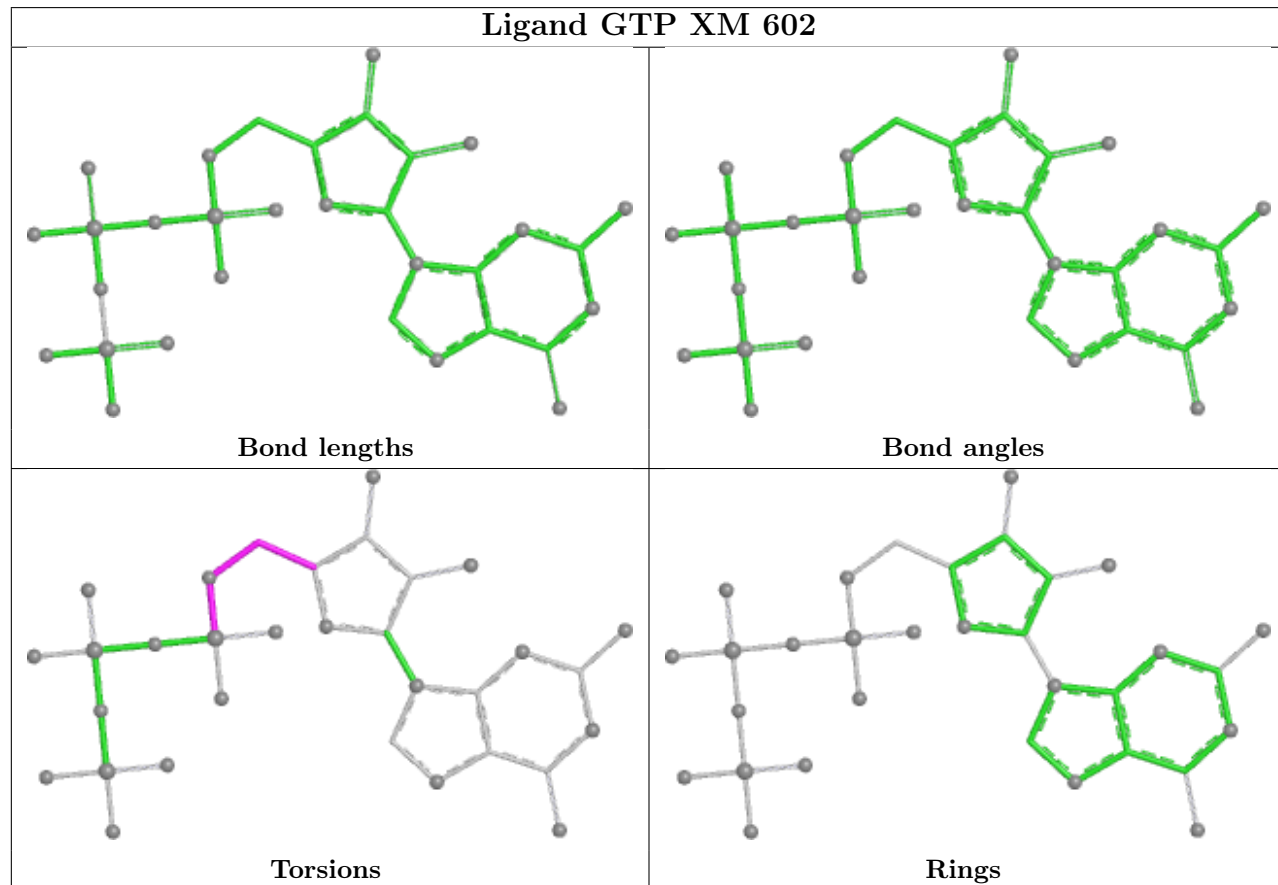
## Ligand GTP FE 501



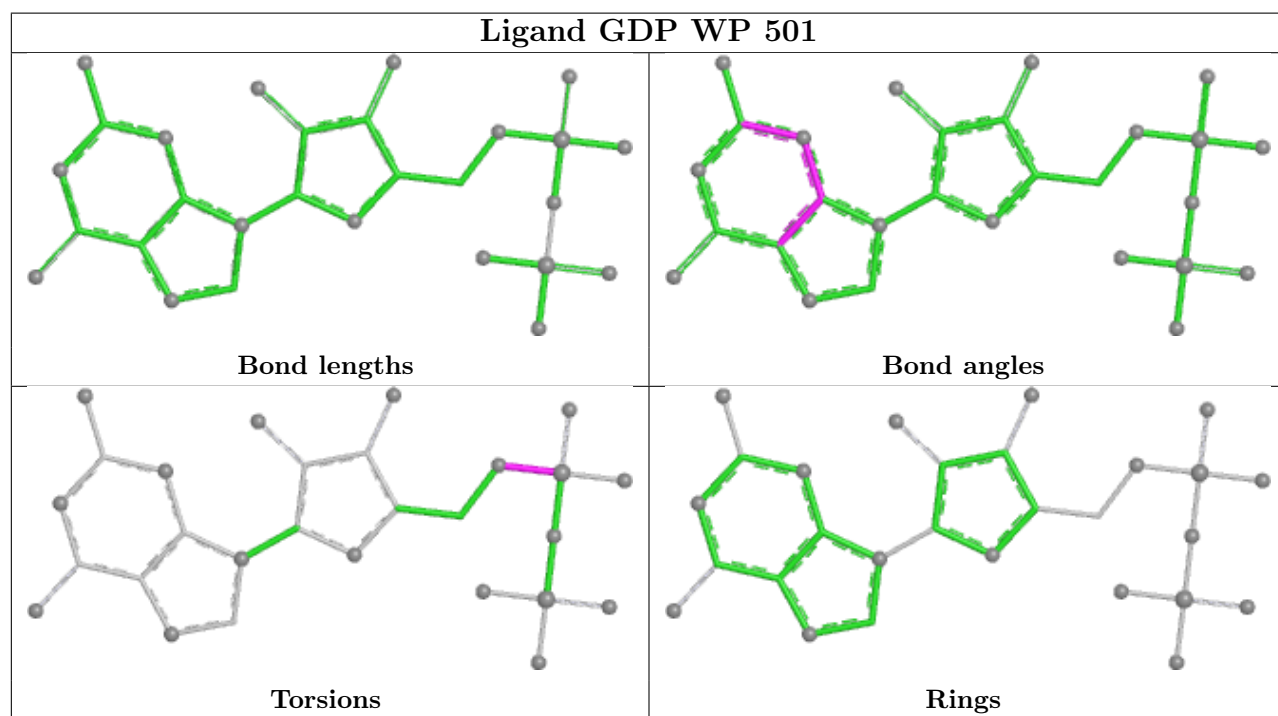
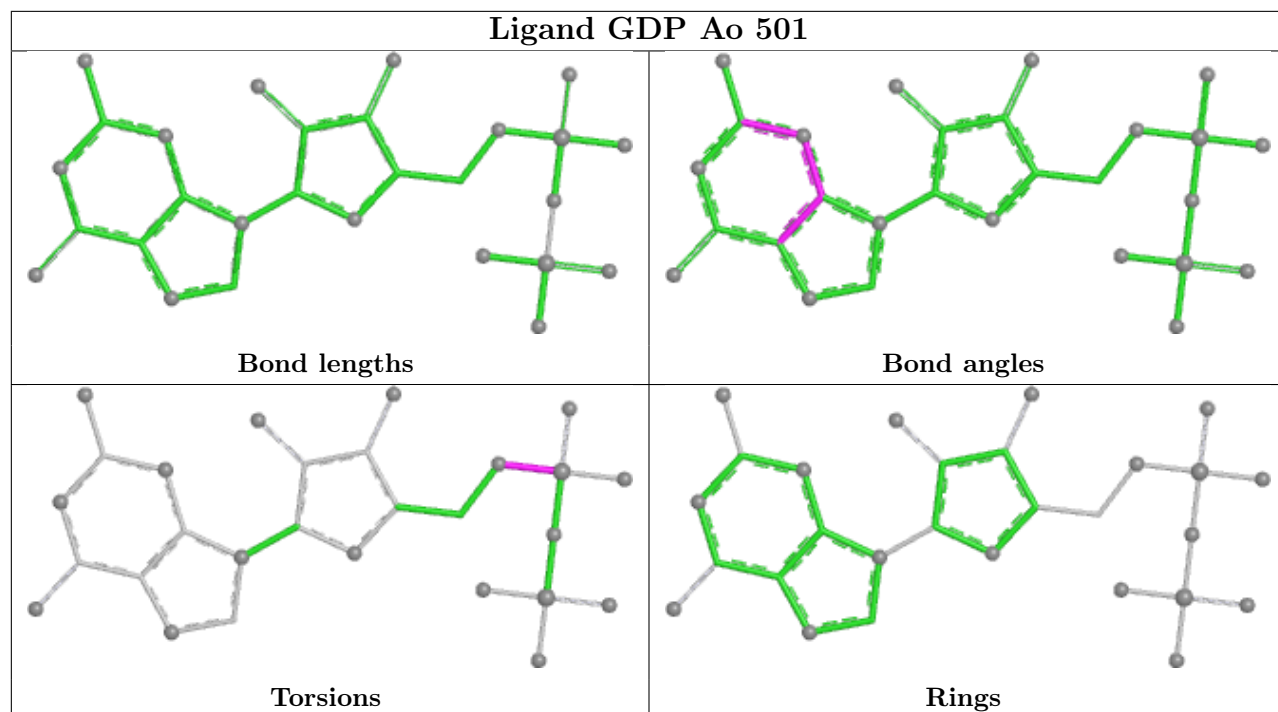
## Ligand GTP LP 502

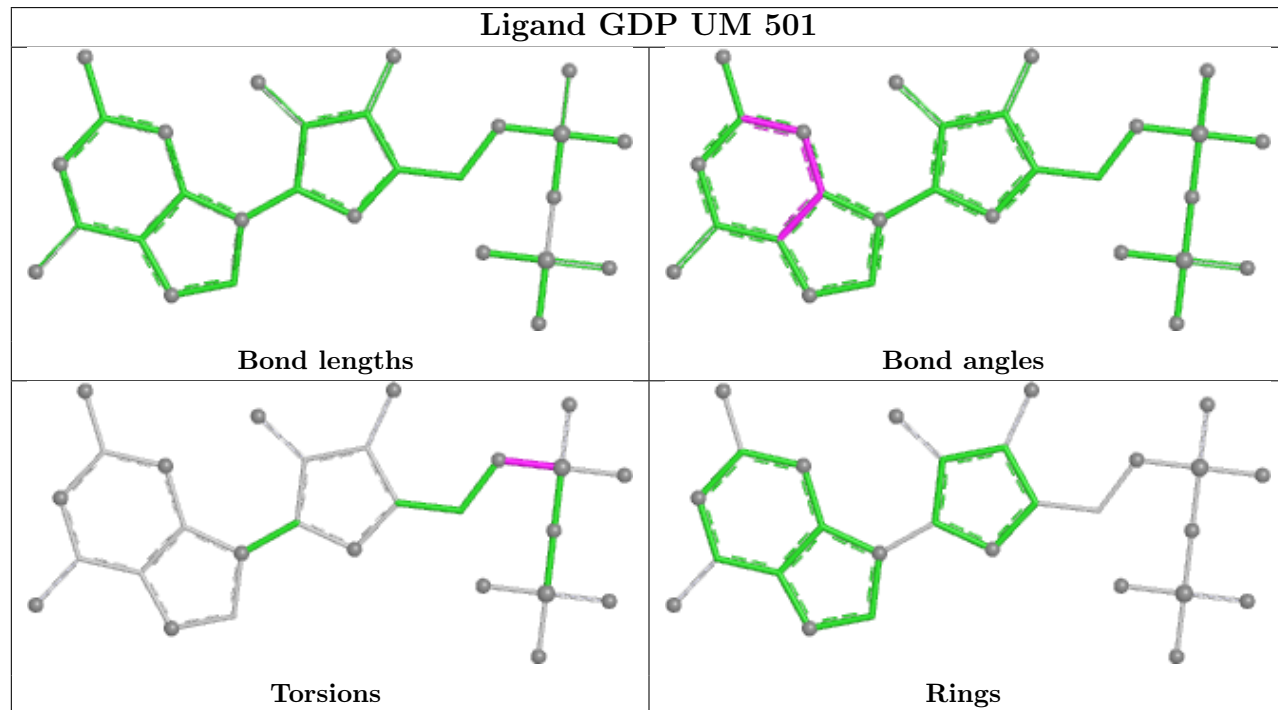
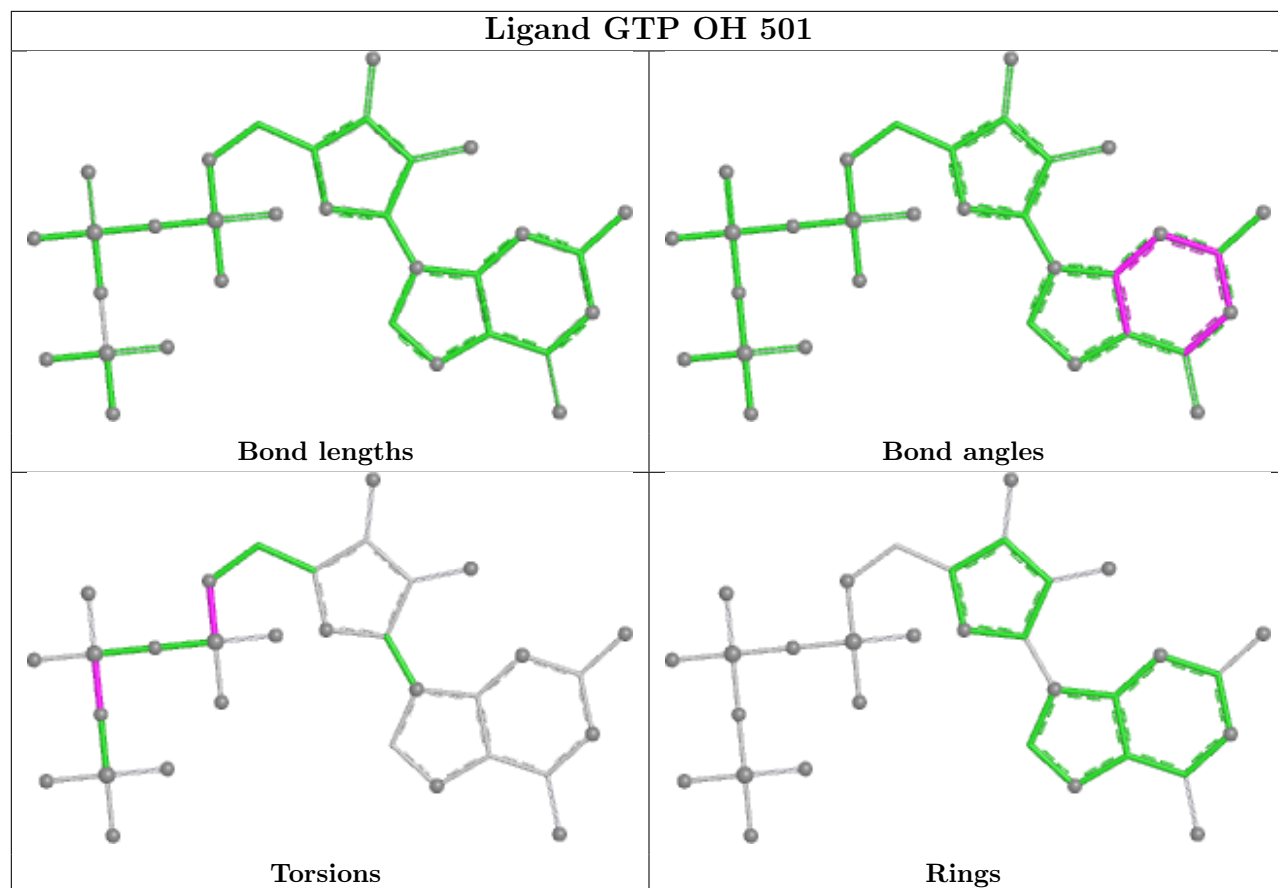


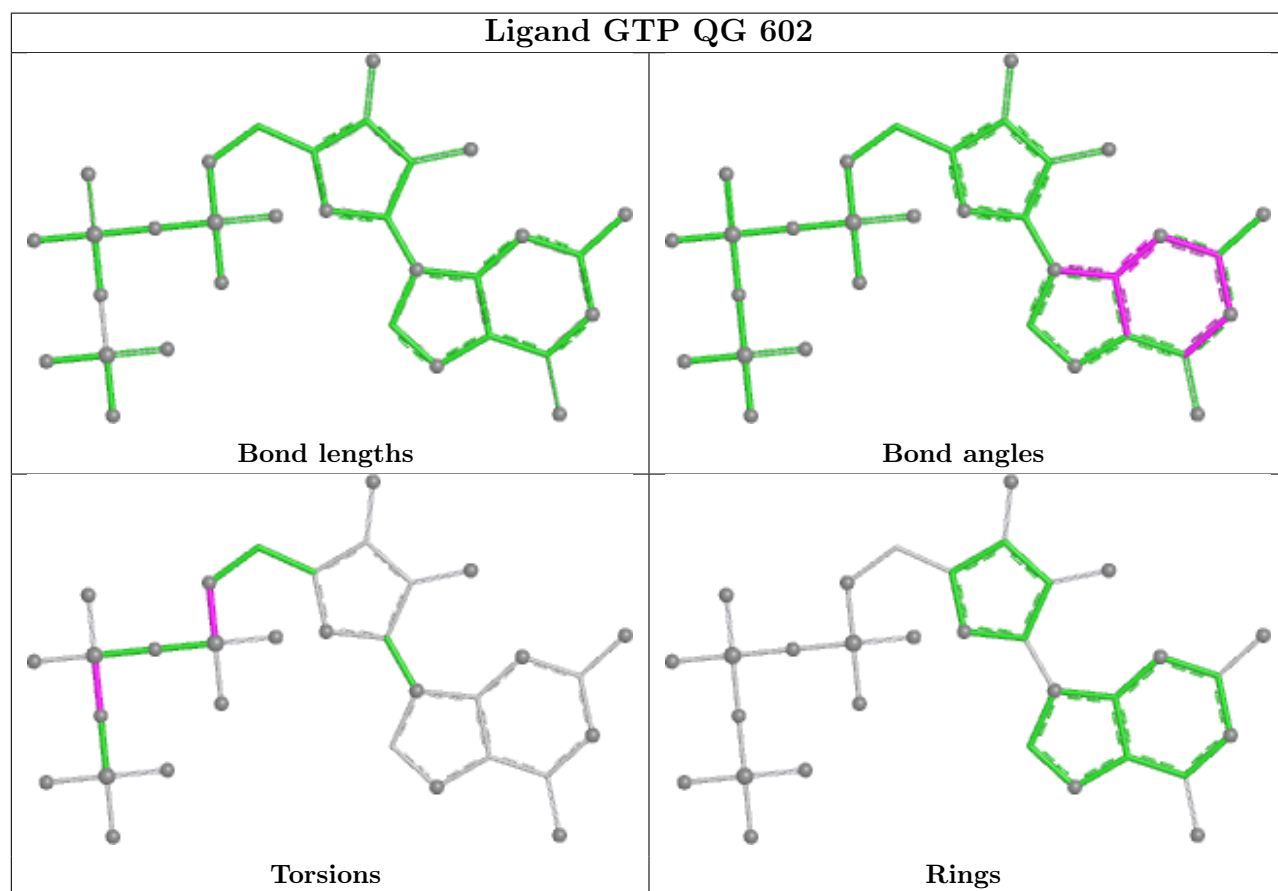
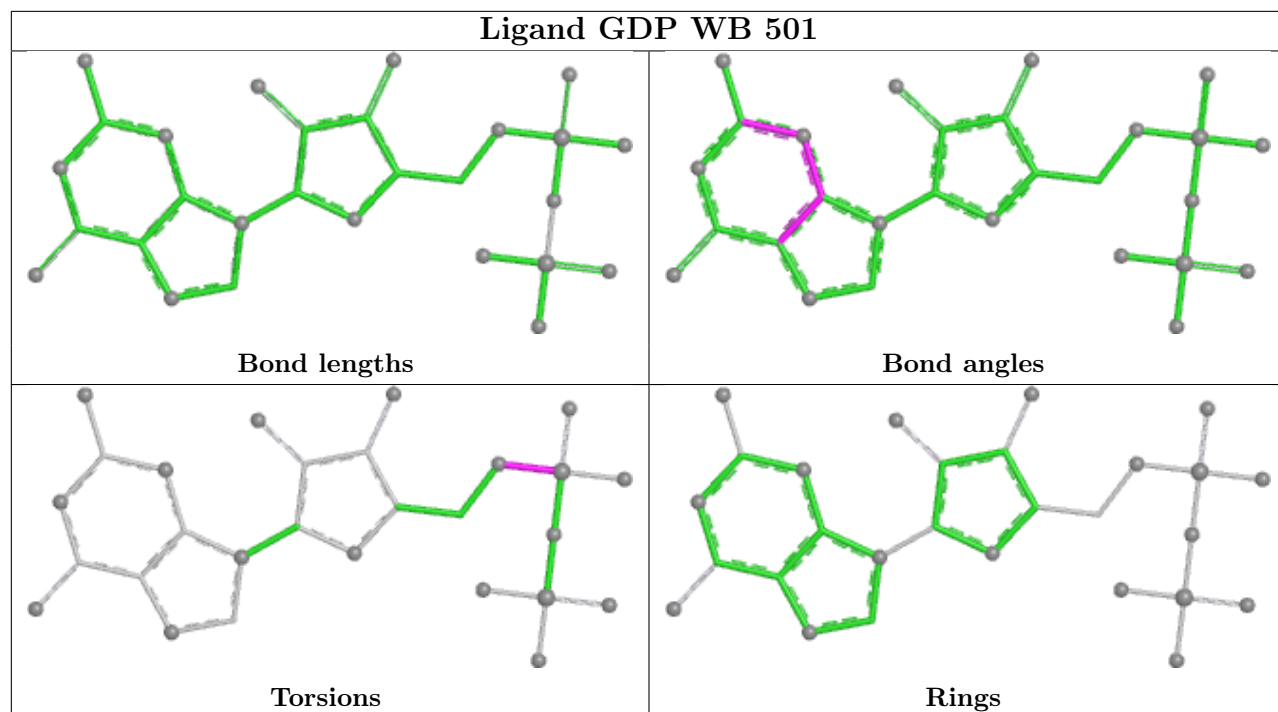
## Ligand GTP XM 602

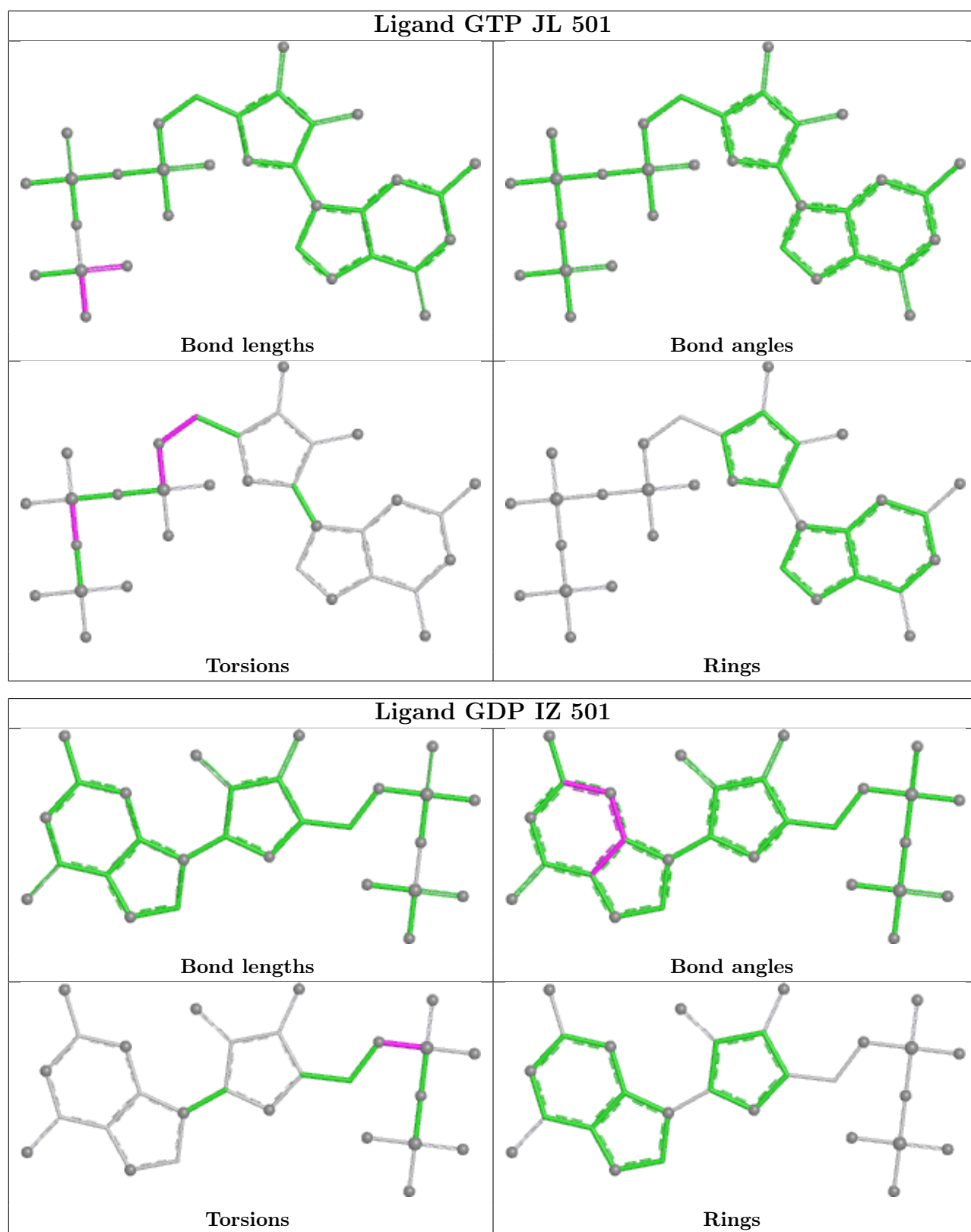


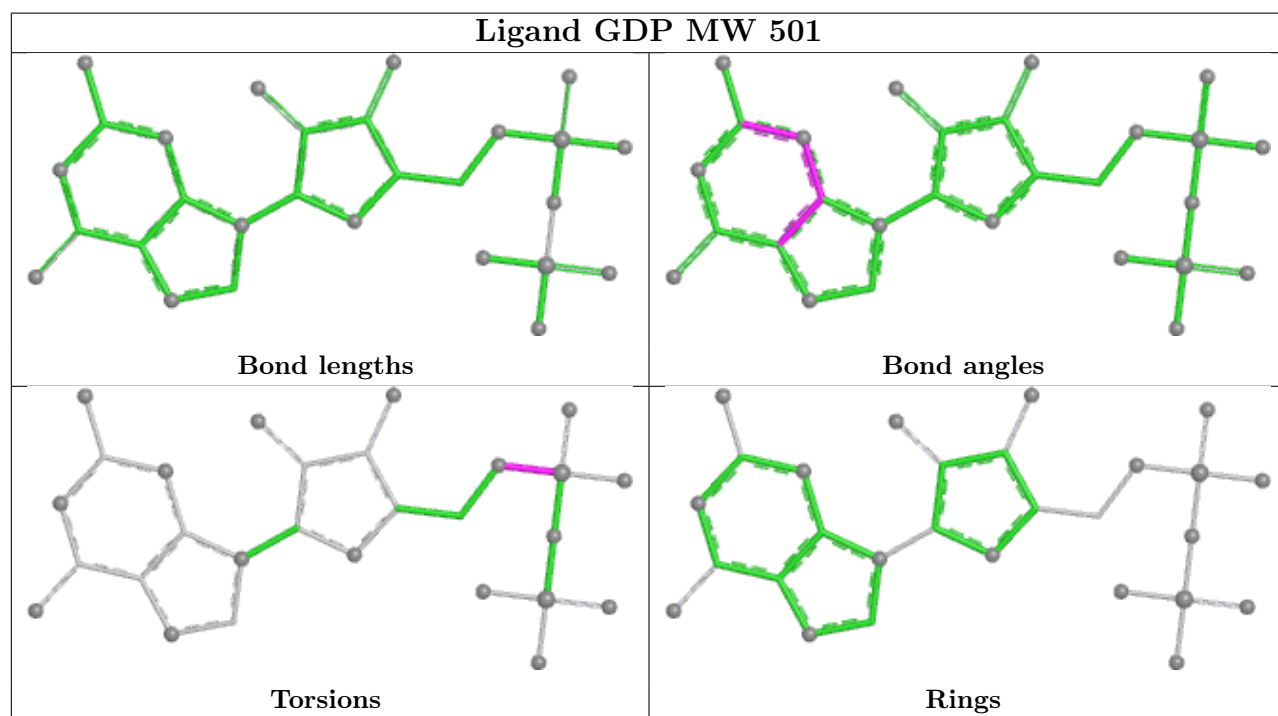
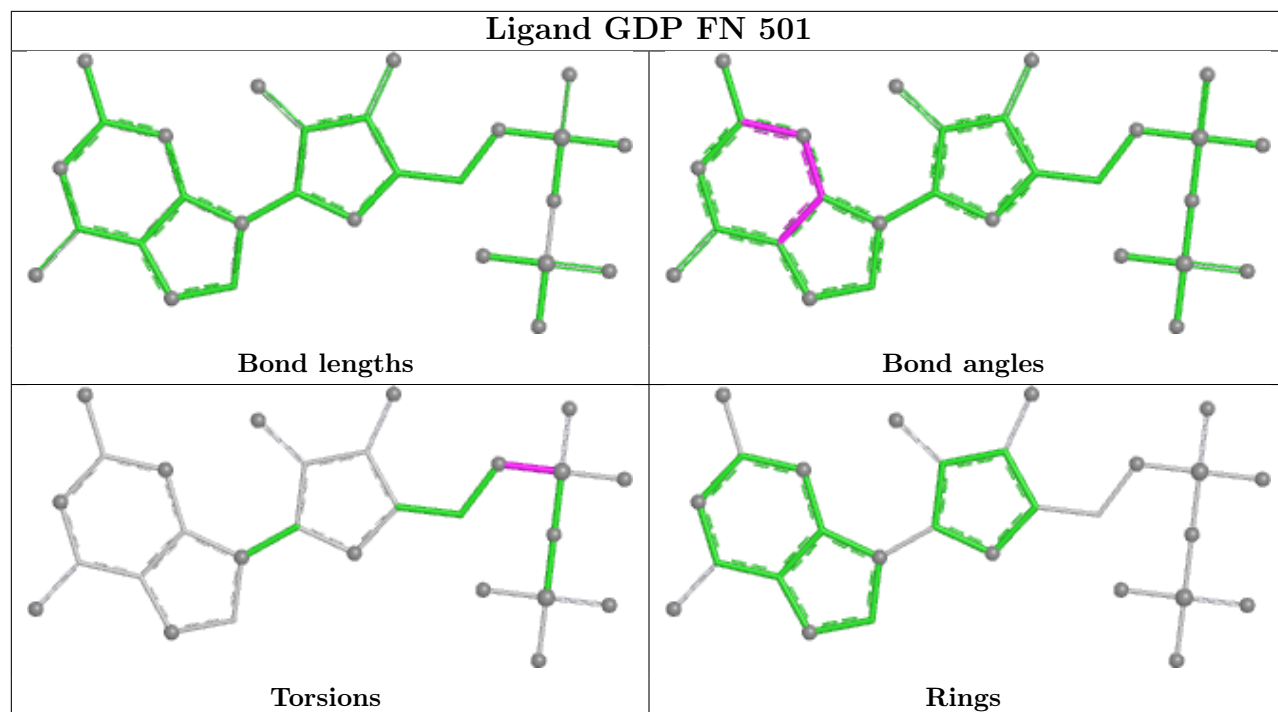


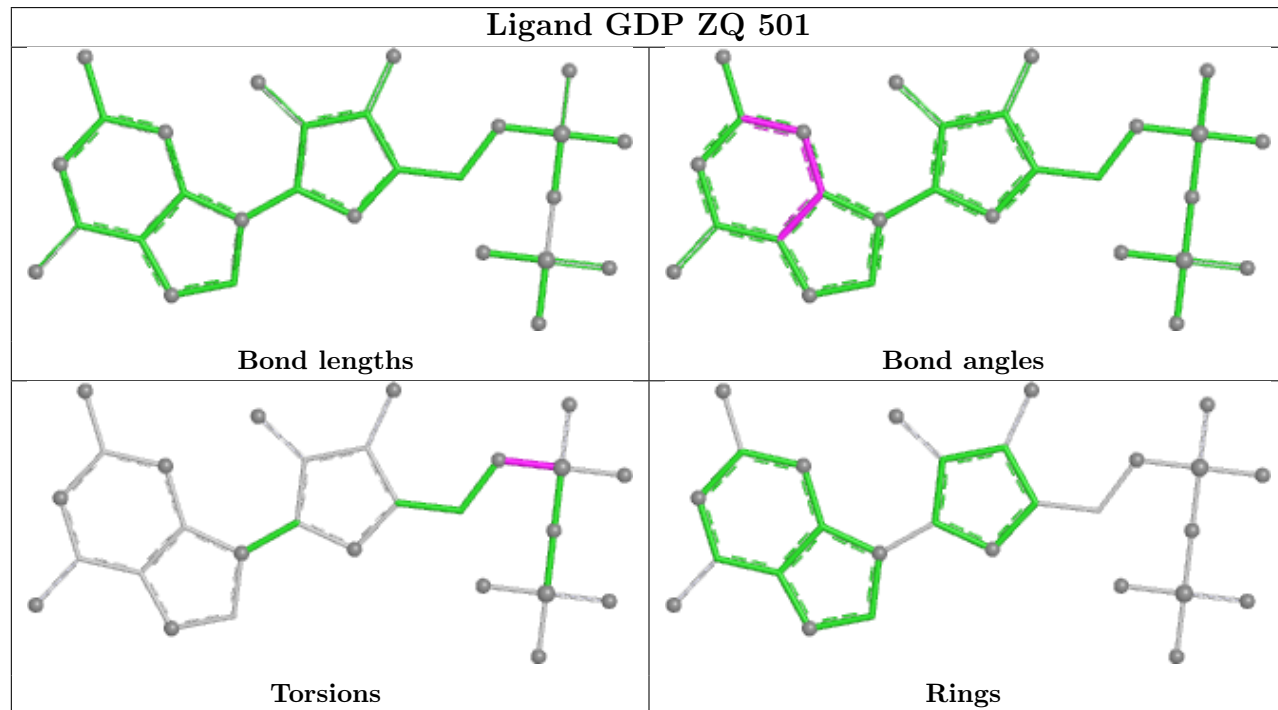
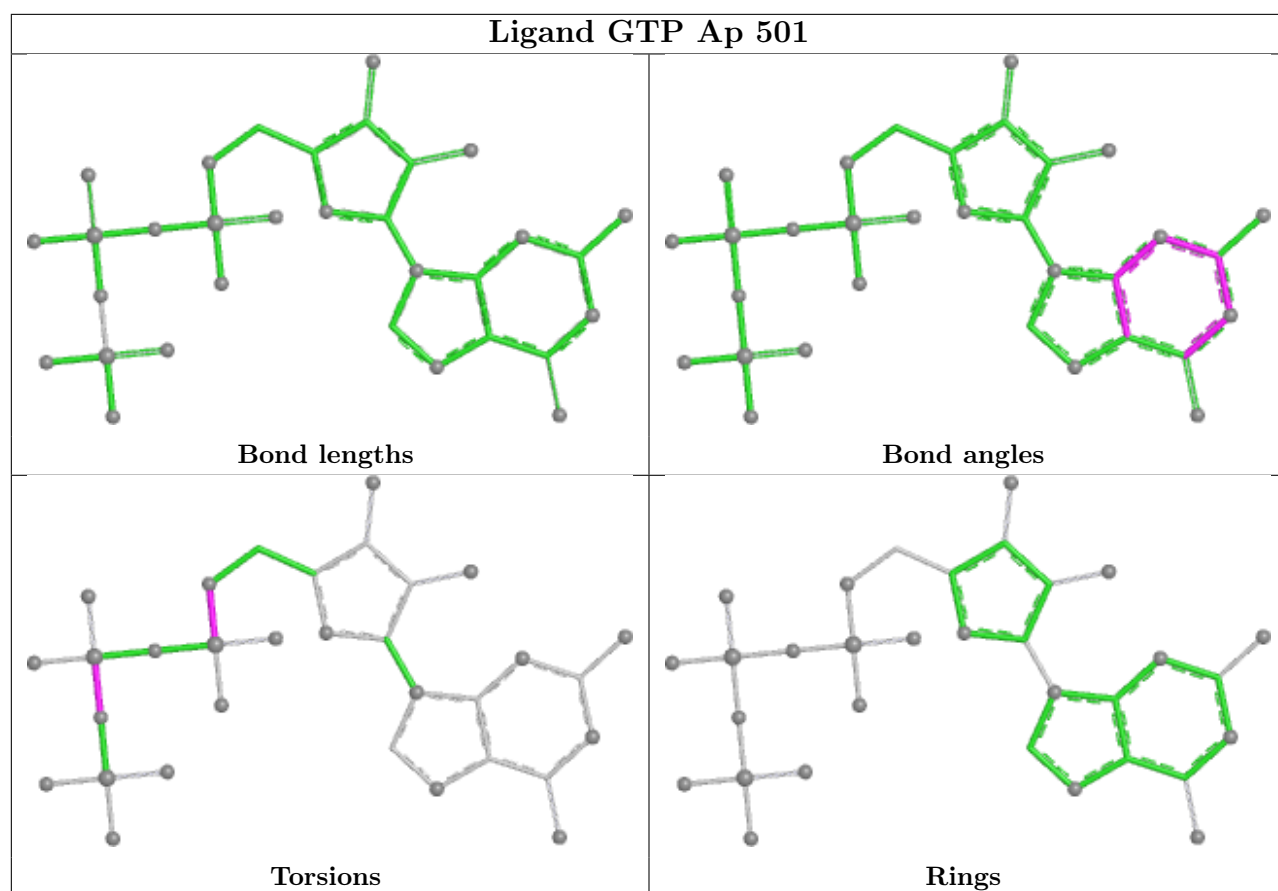


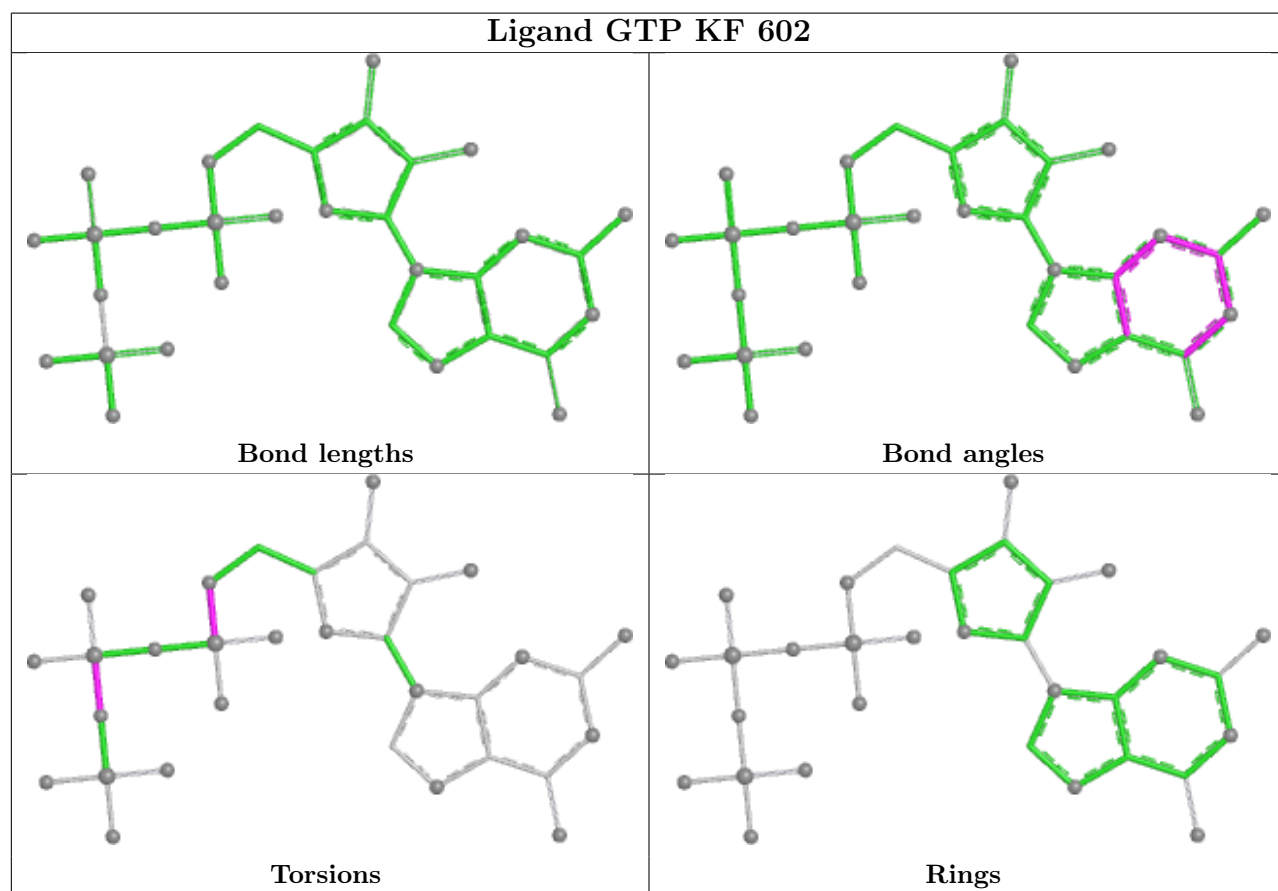
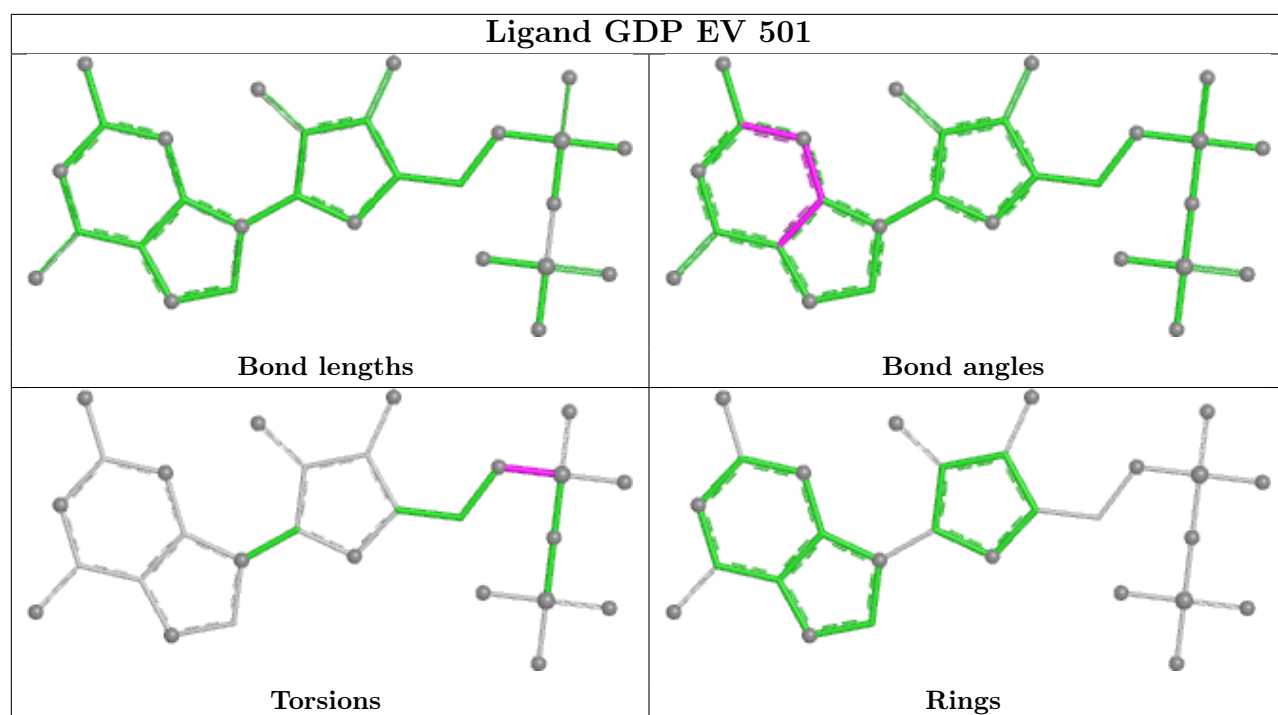


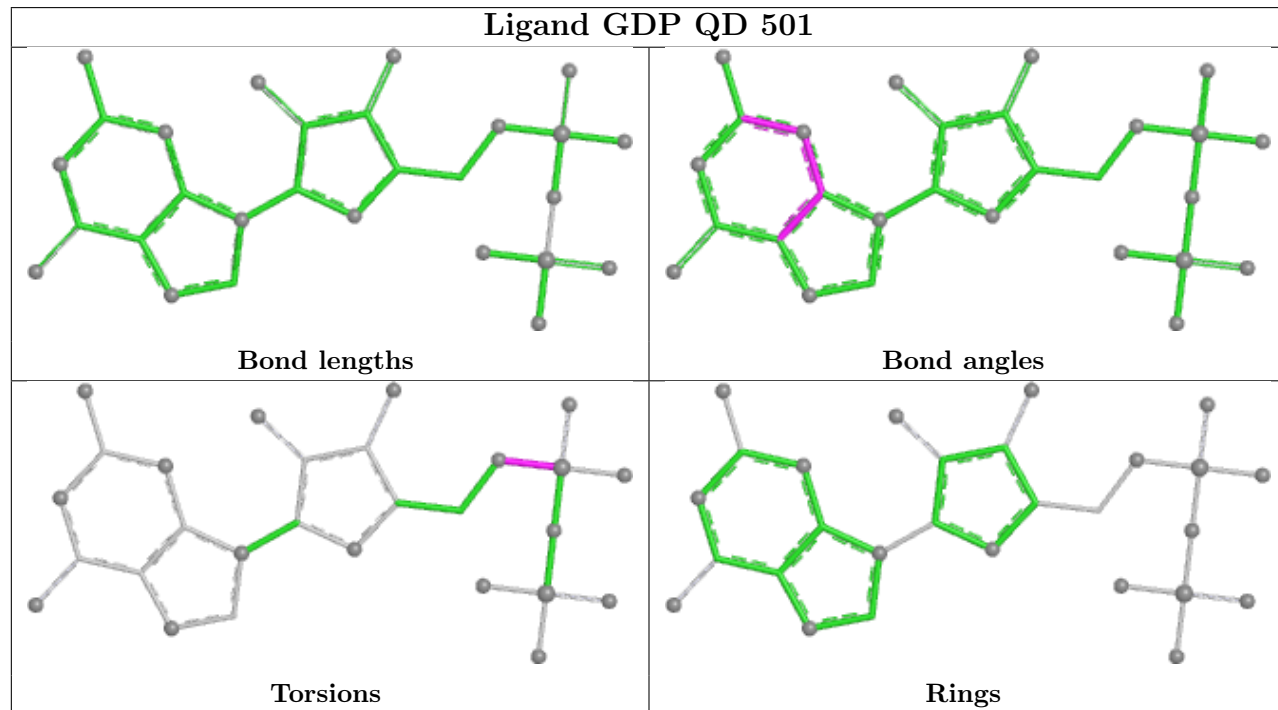
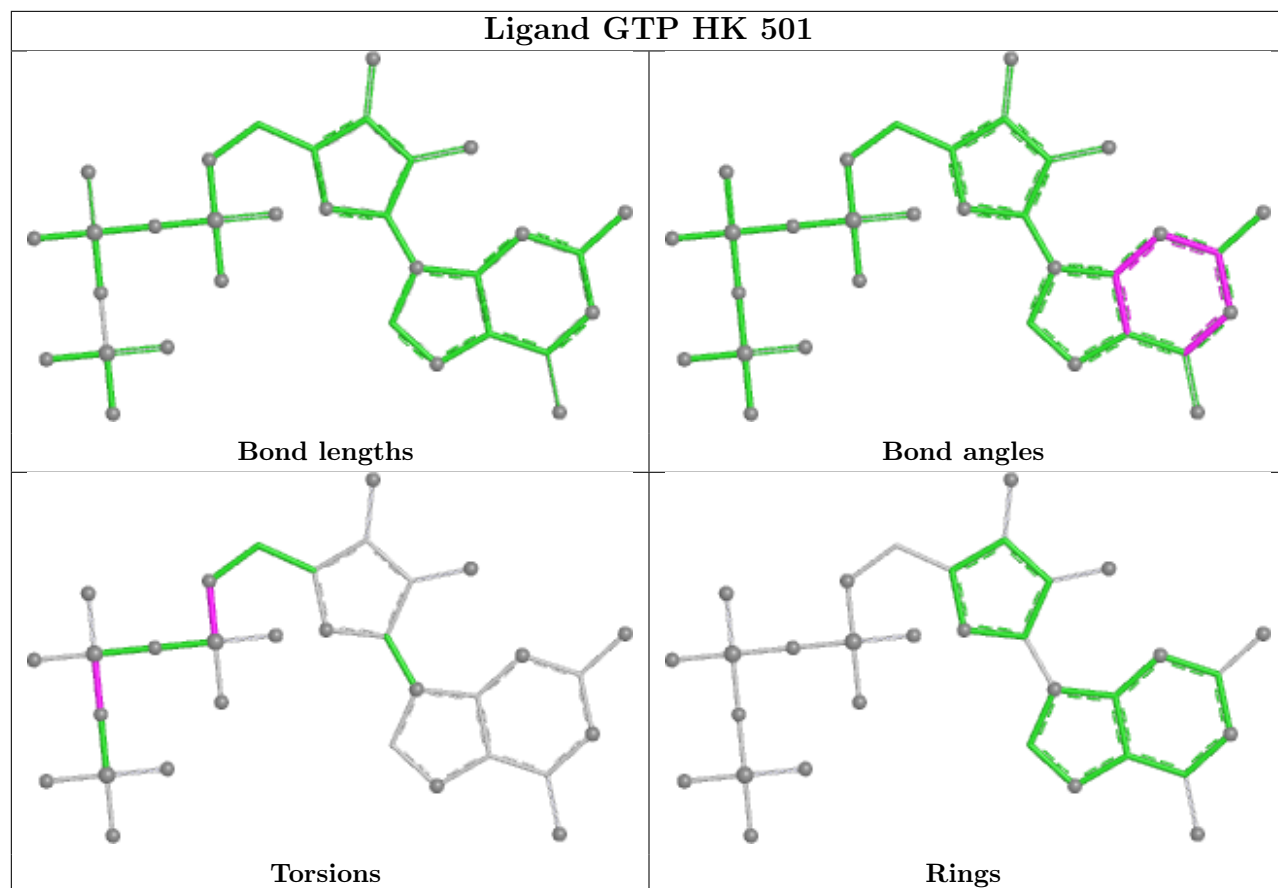




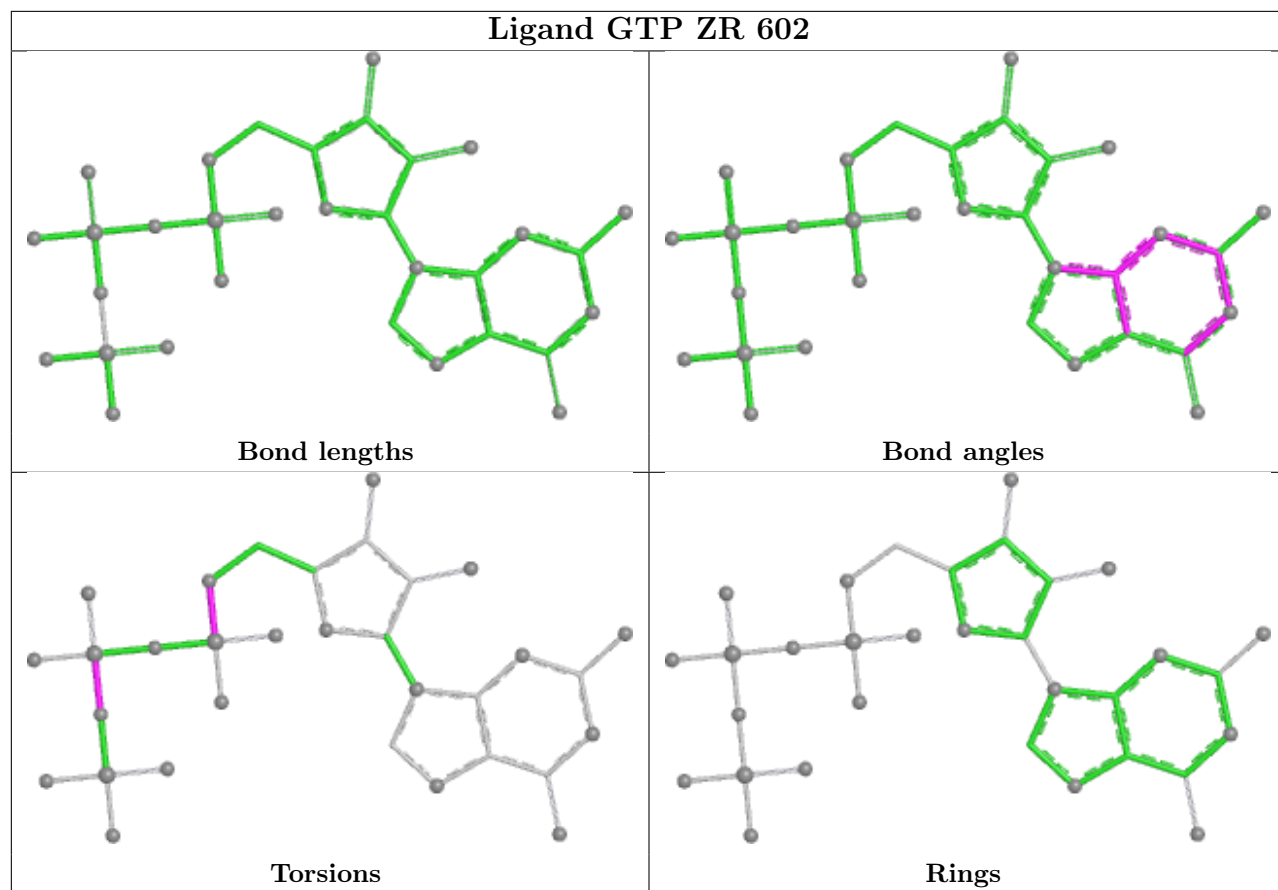


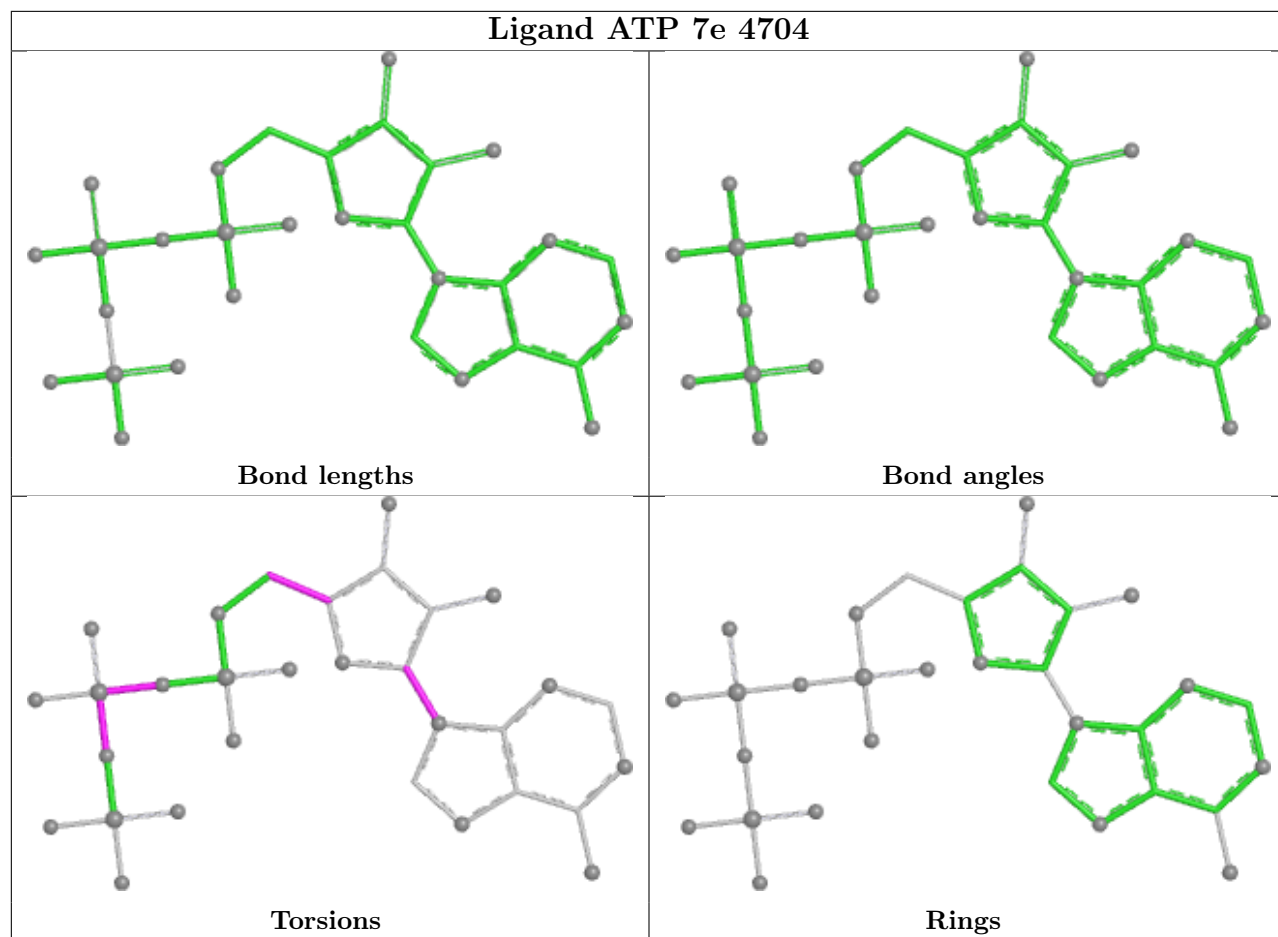




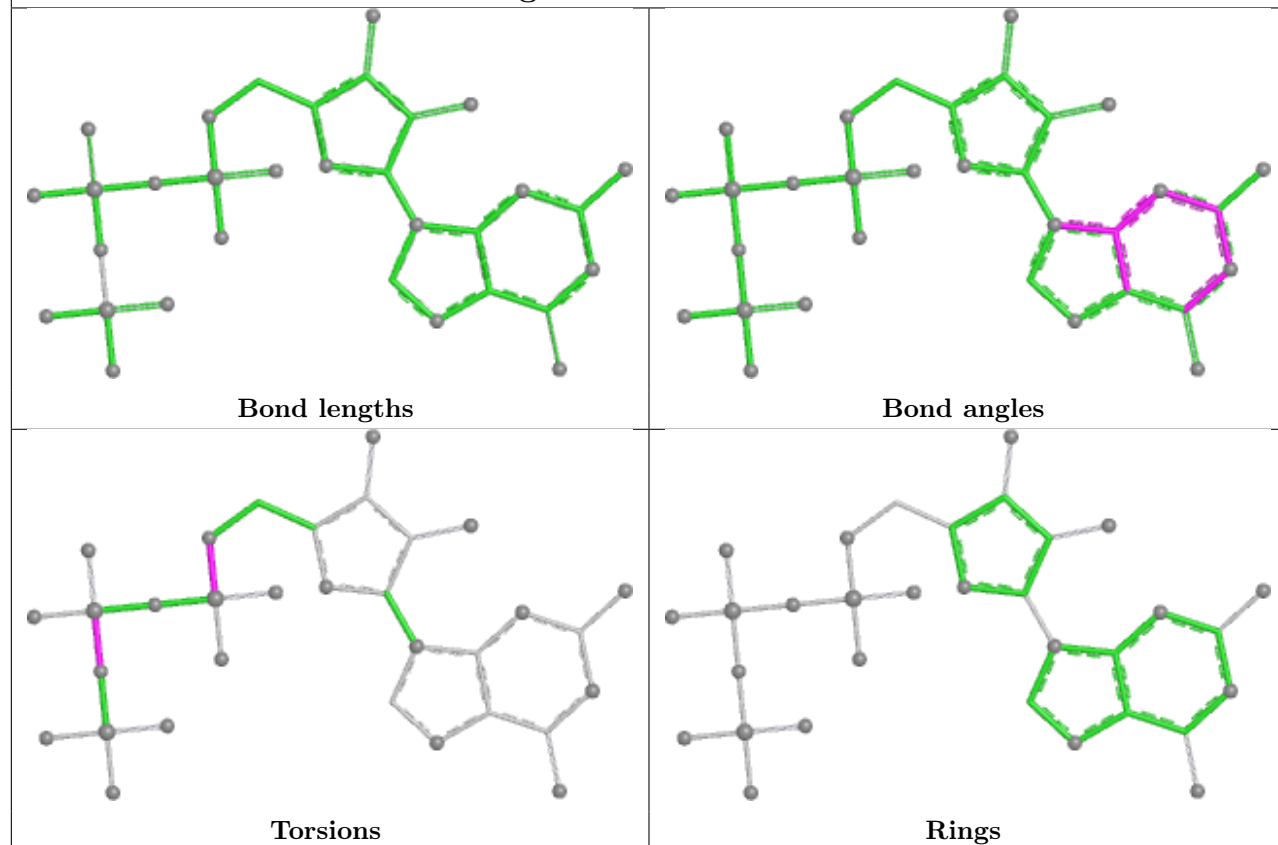




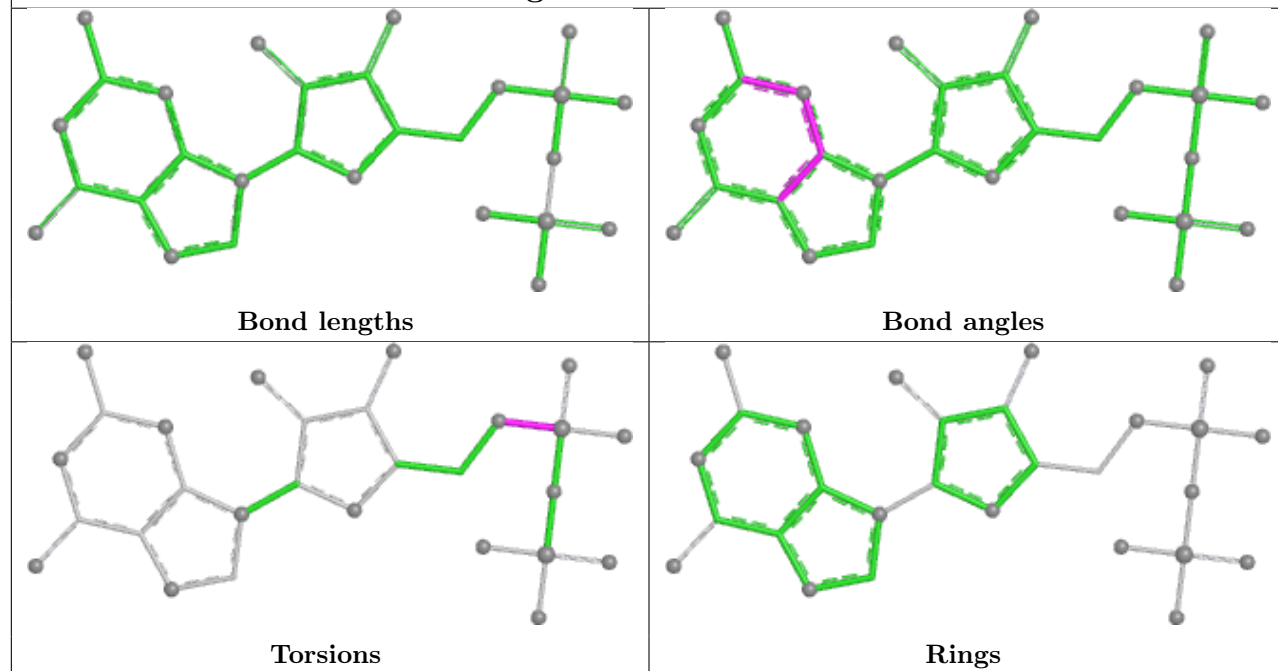


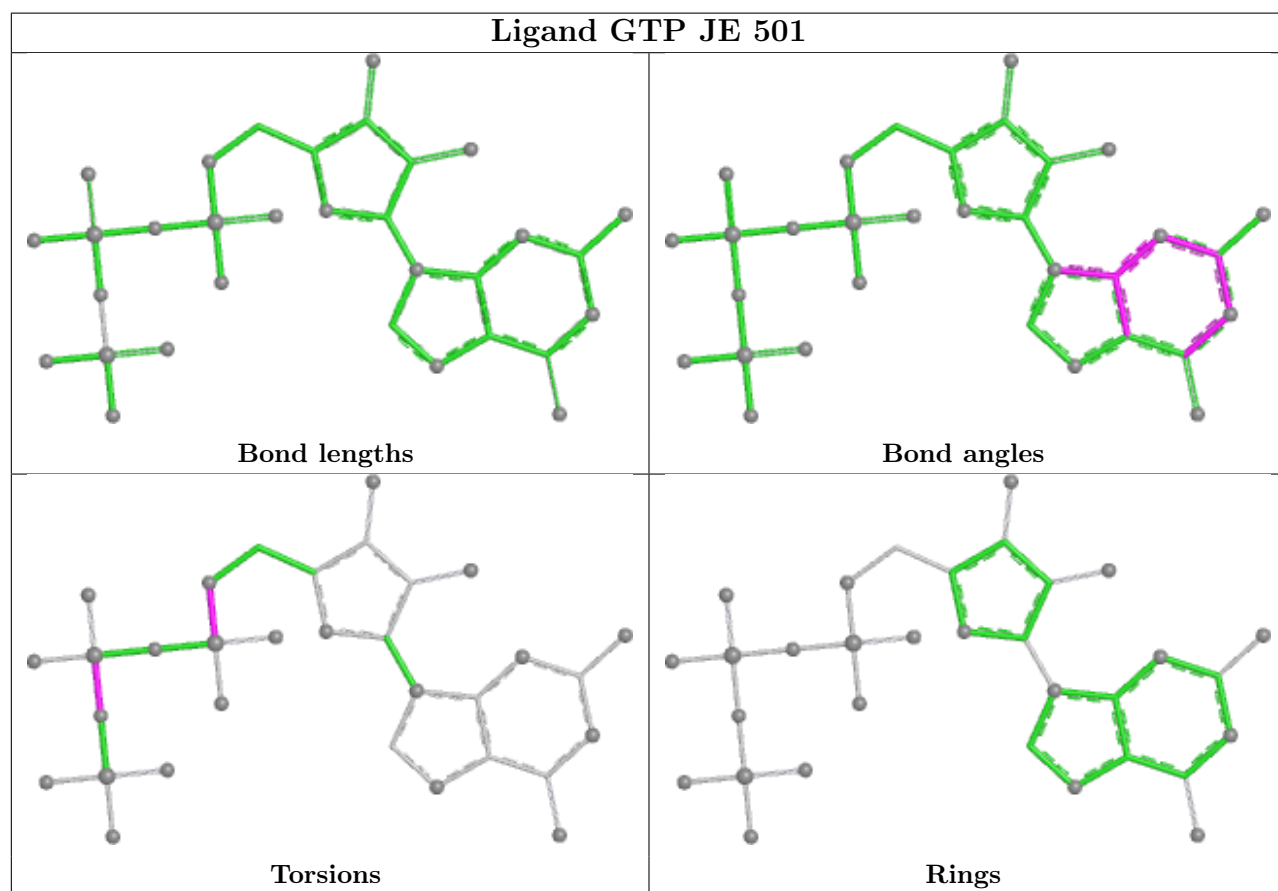
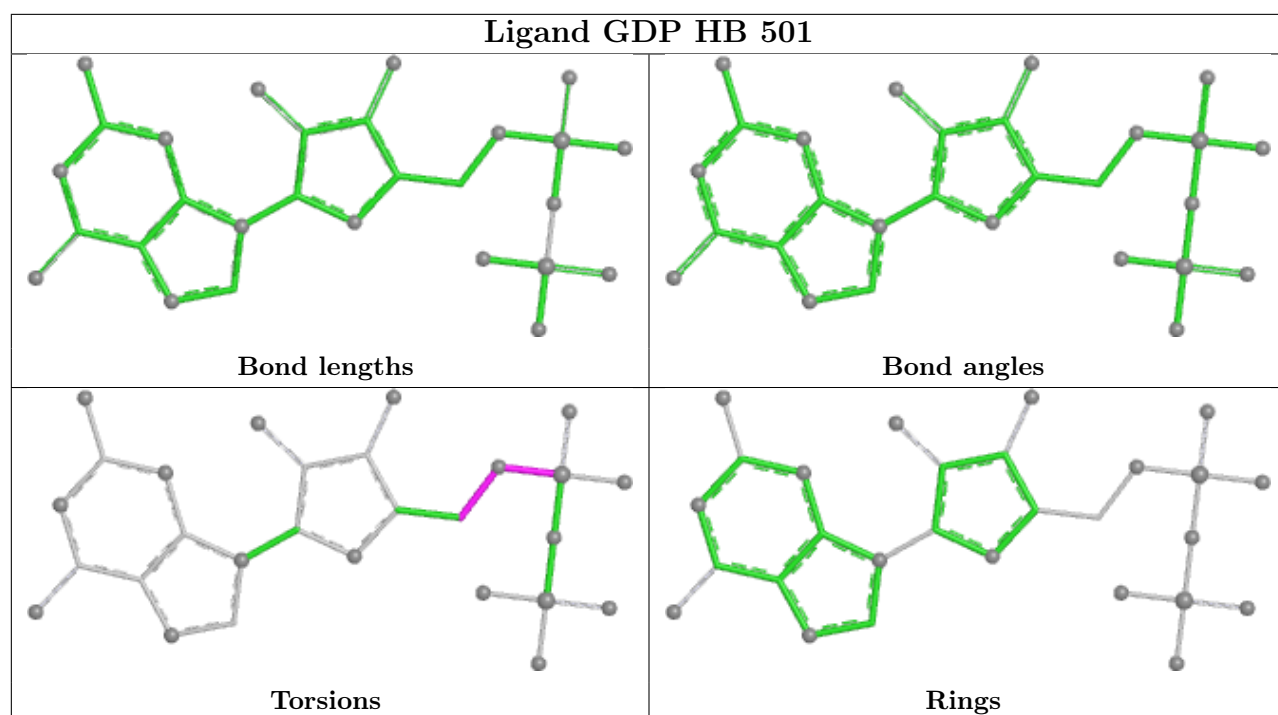


## Ligand GTP AL 602

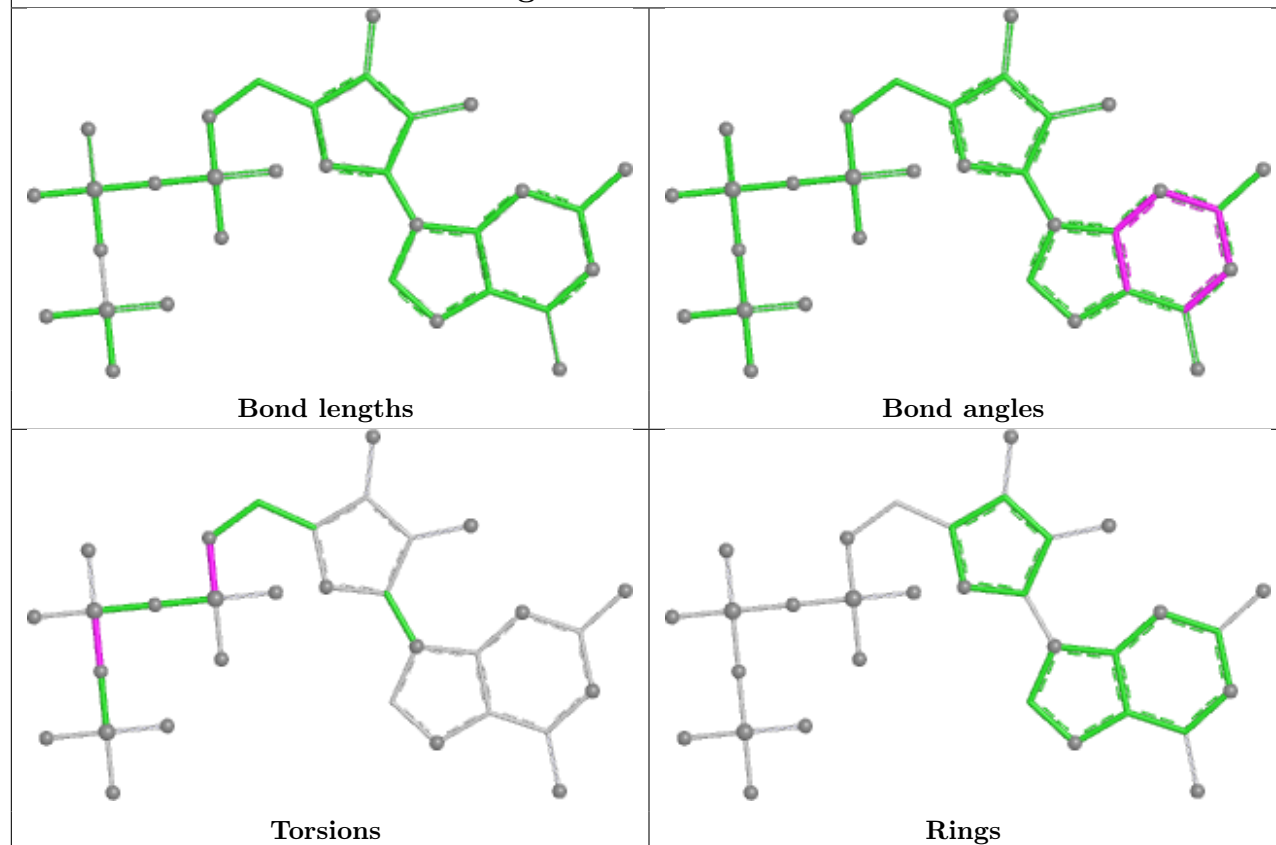


## Ligand GDP IJ 501

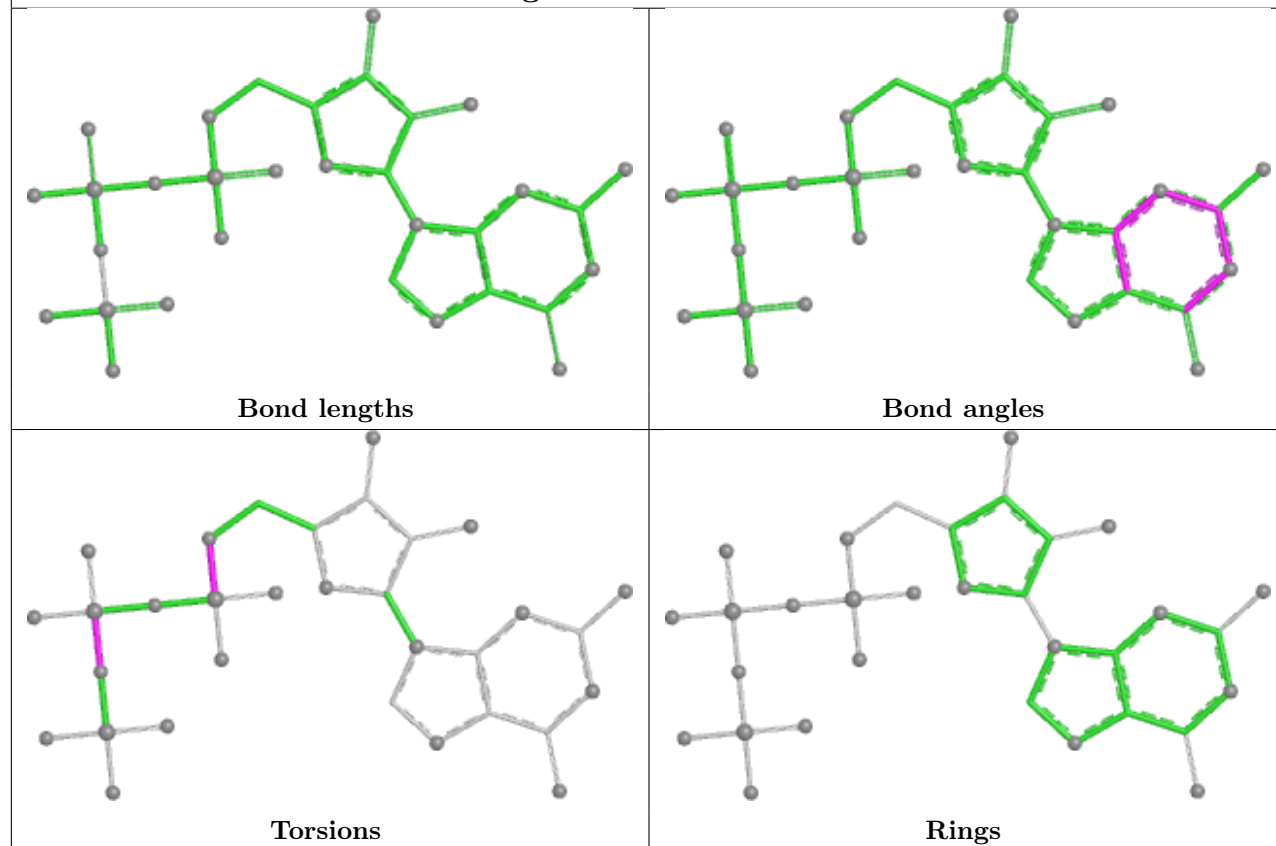




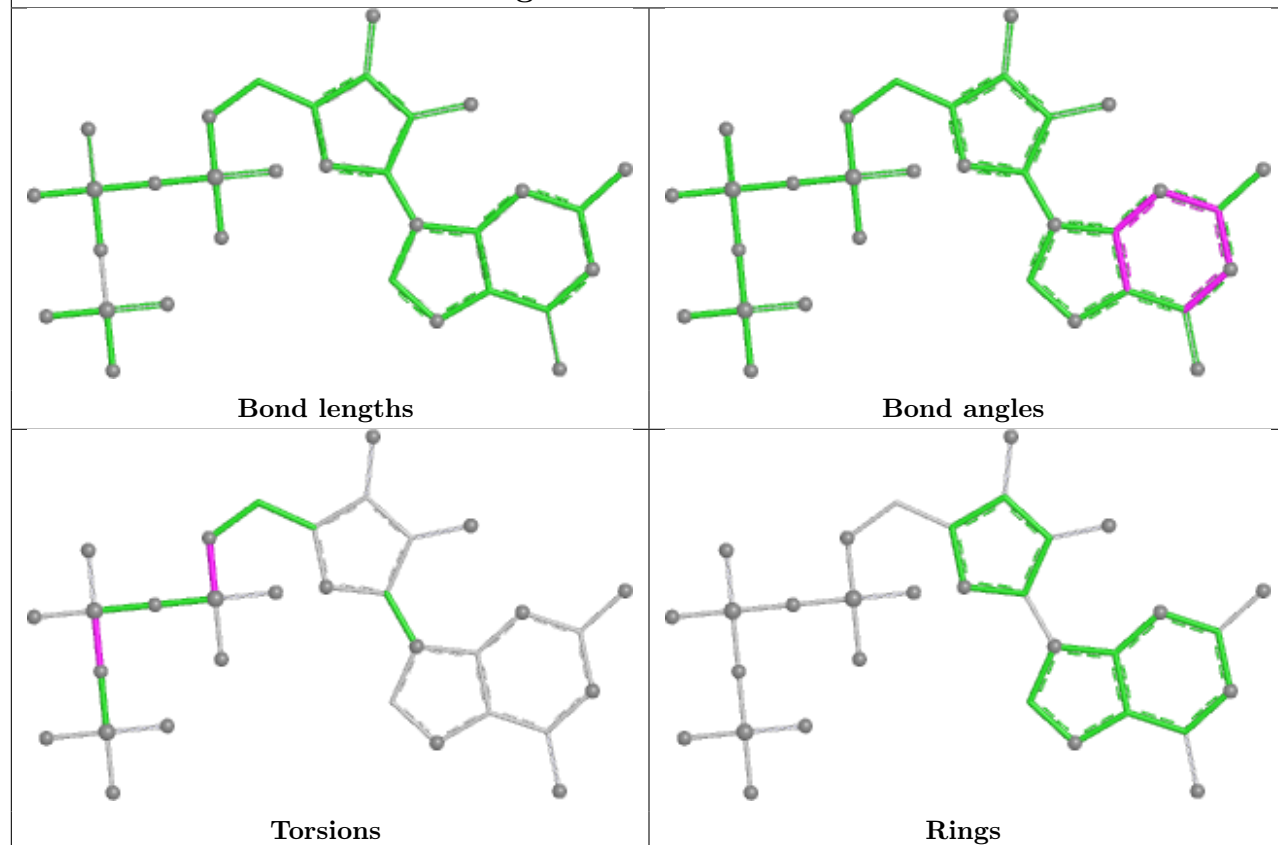
## Ligand GTP OT 602



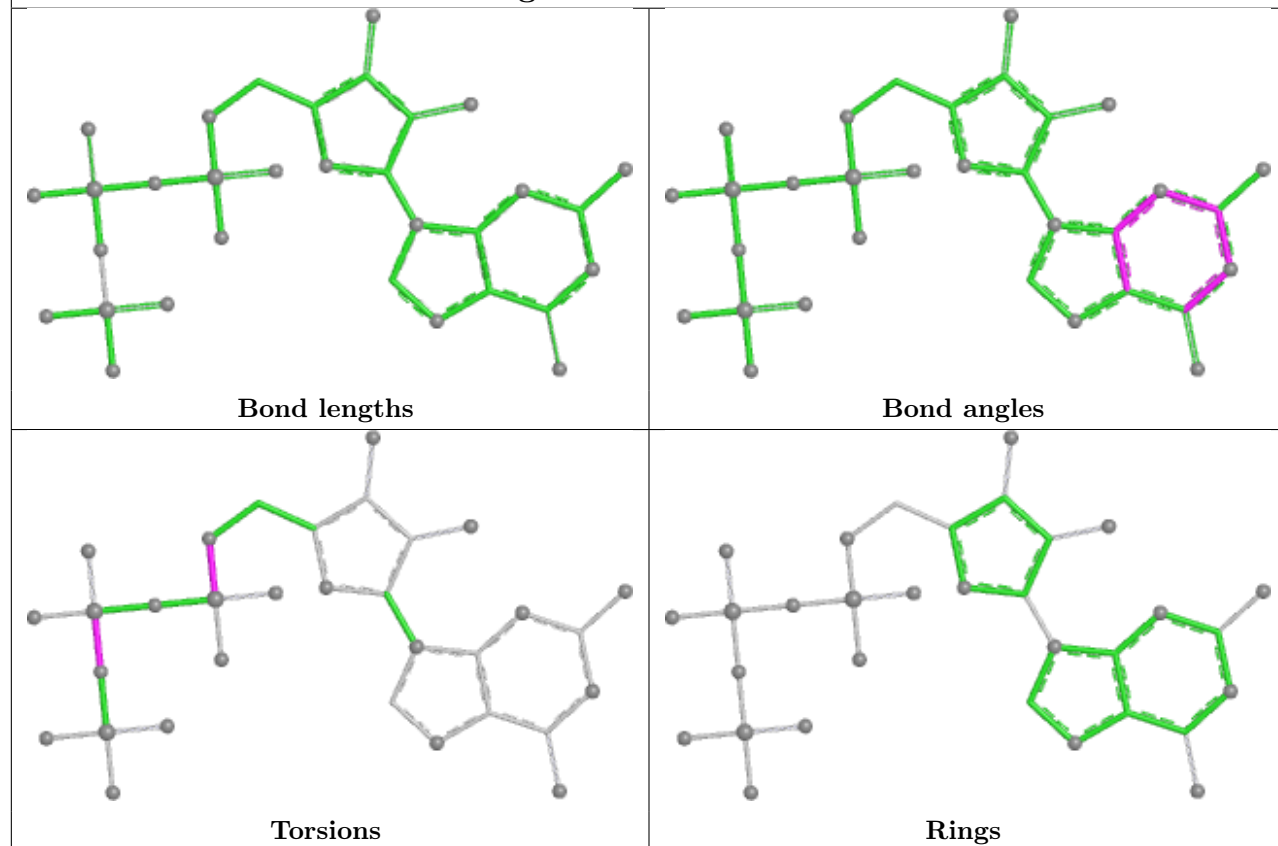
## Ligand GTP SE 501



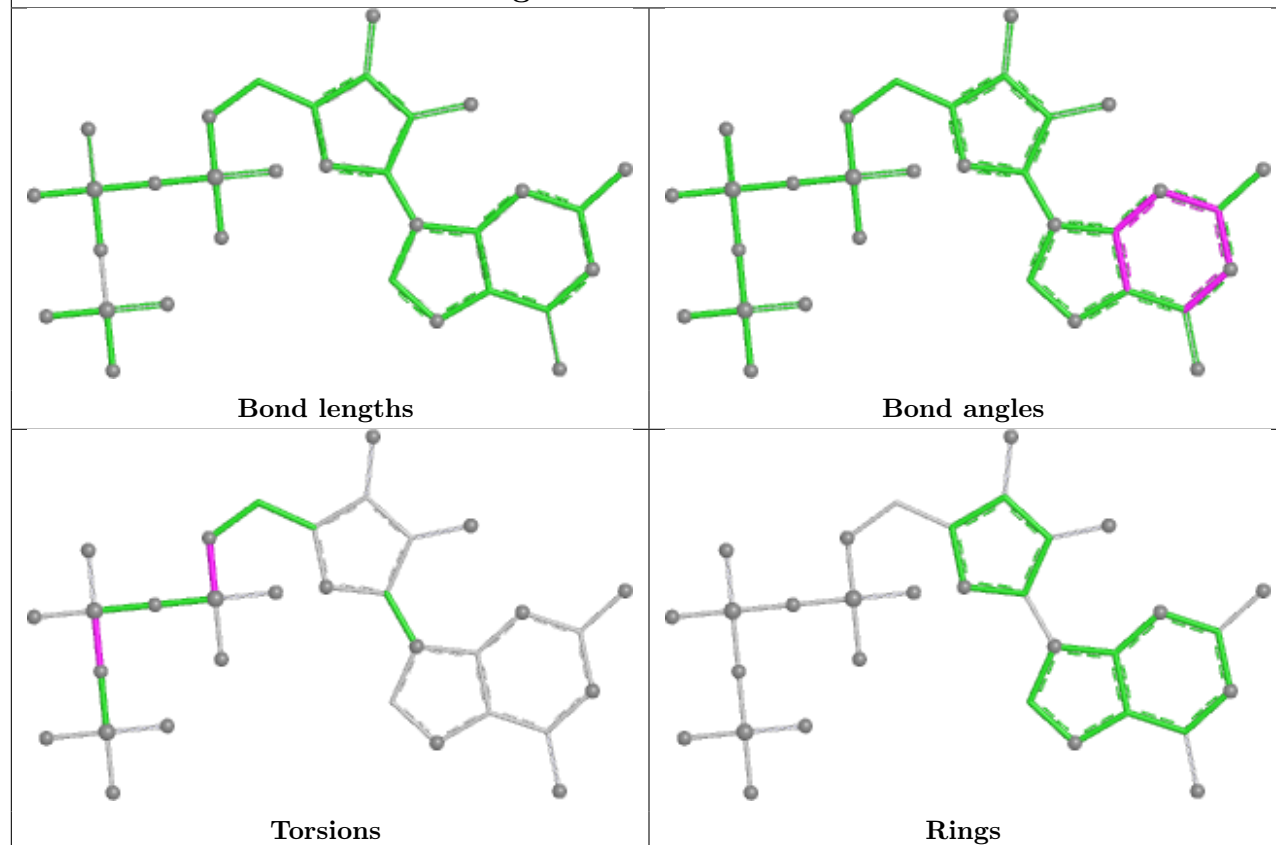
## Ligand GTP KX 501



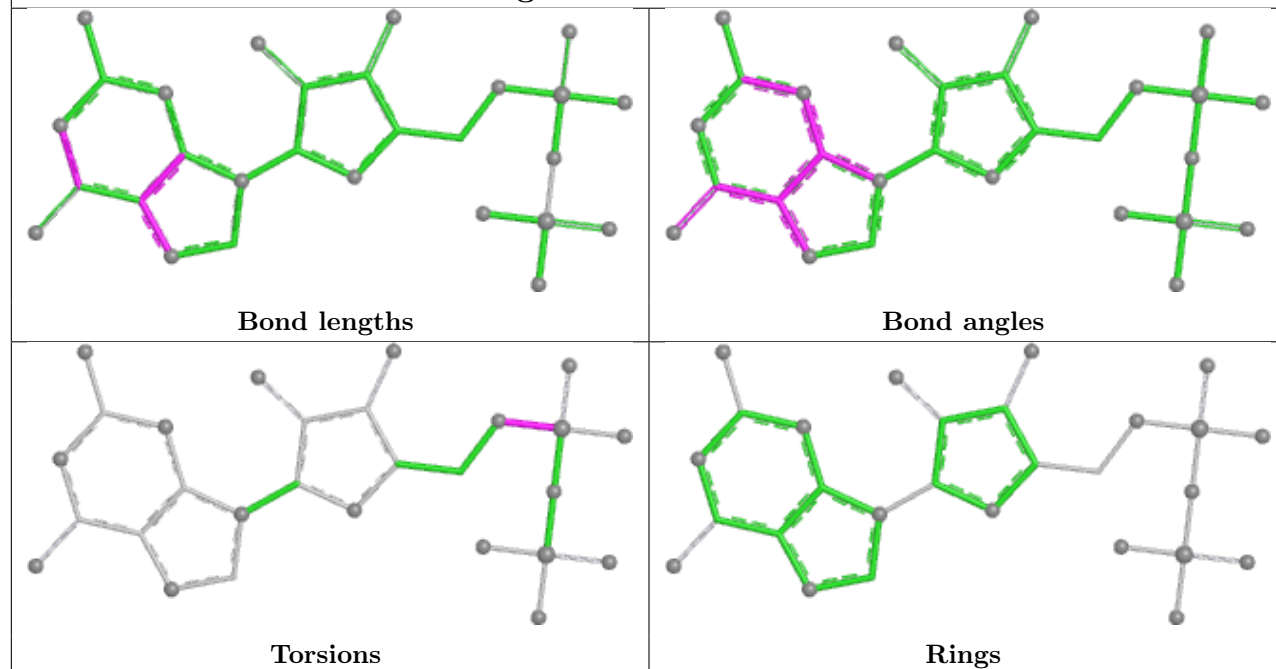
## Ligand GTP EA 501

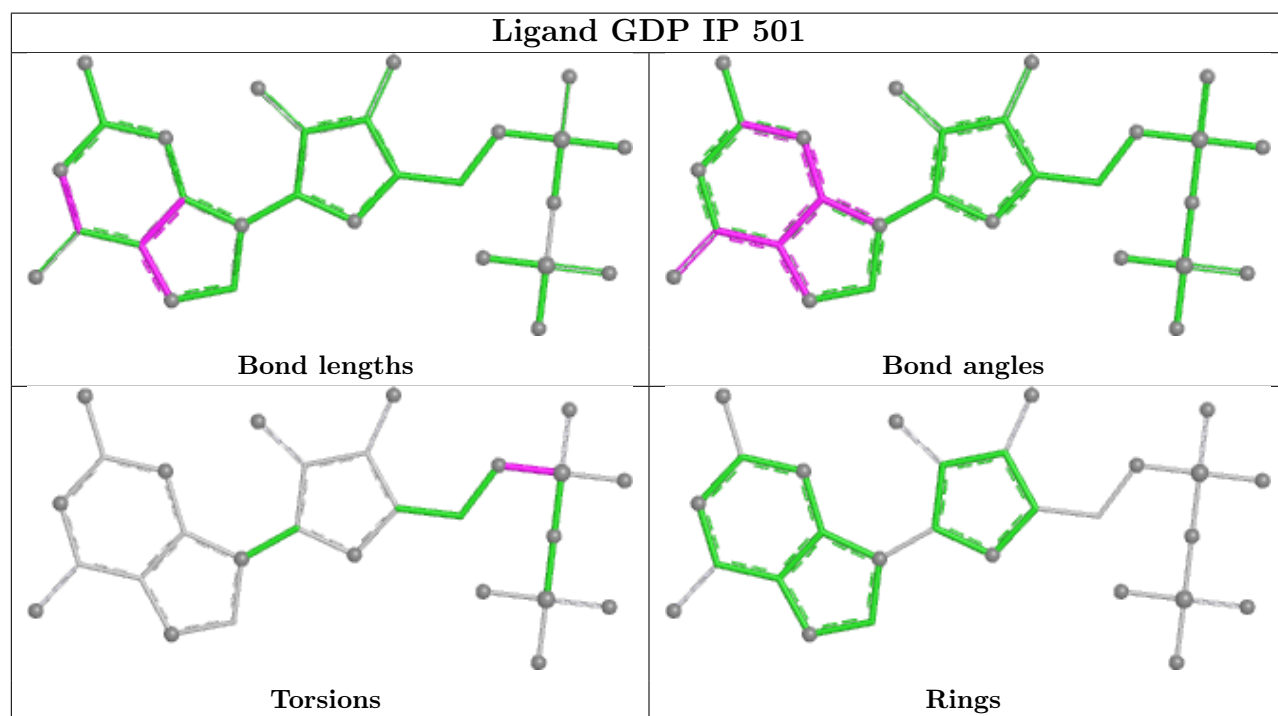
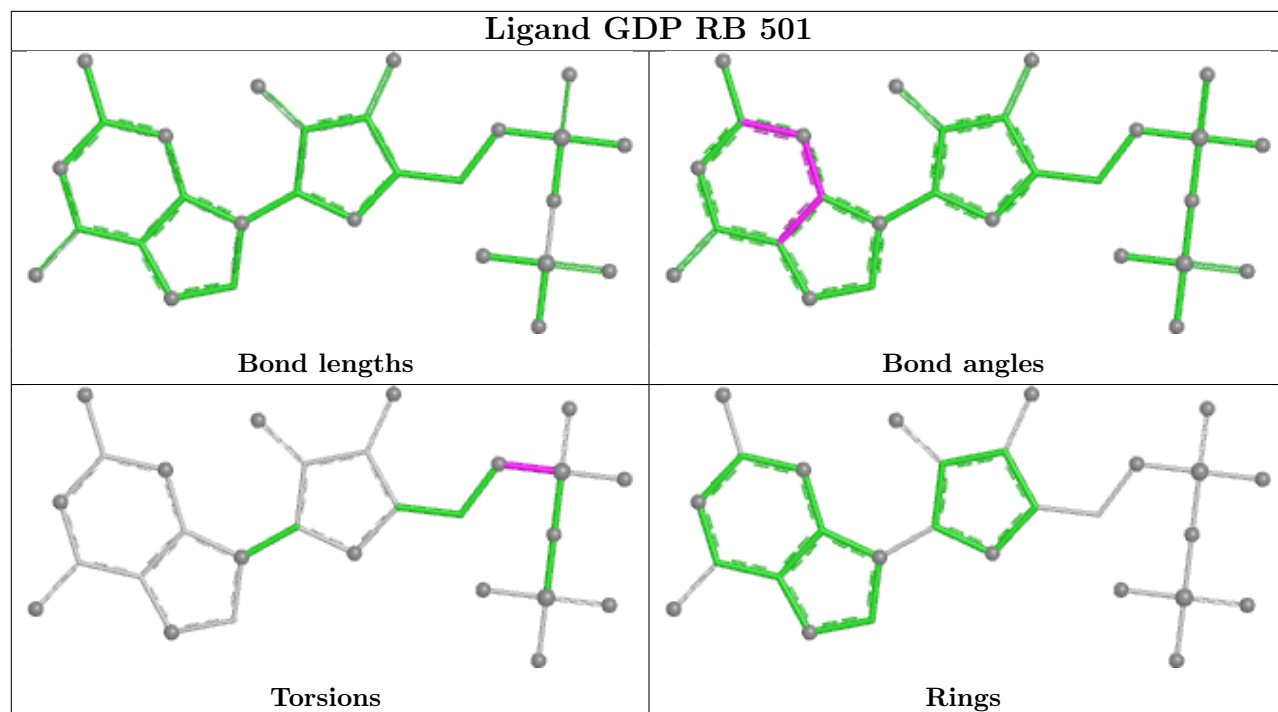


## Ligand GTP WC 501



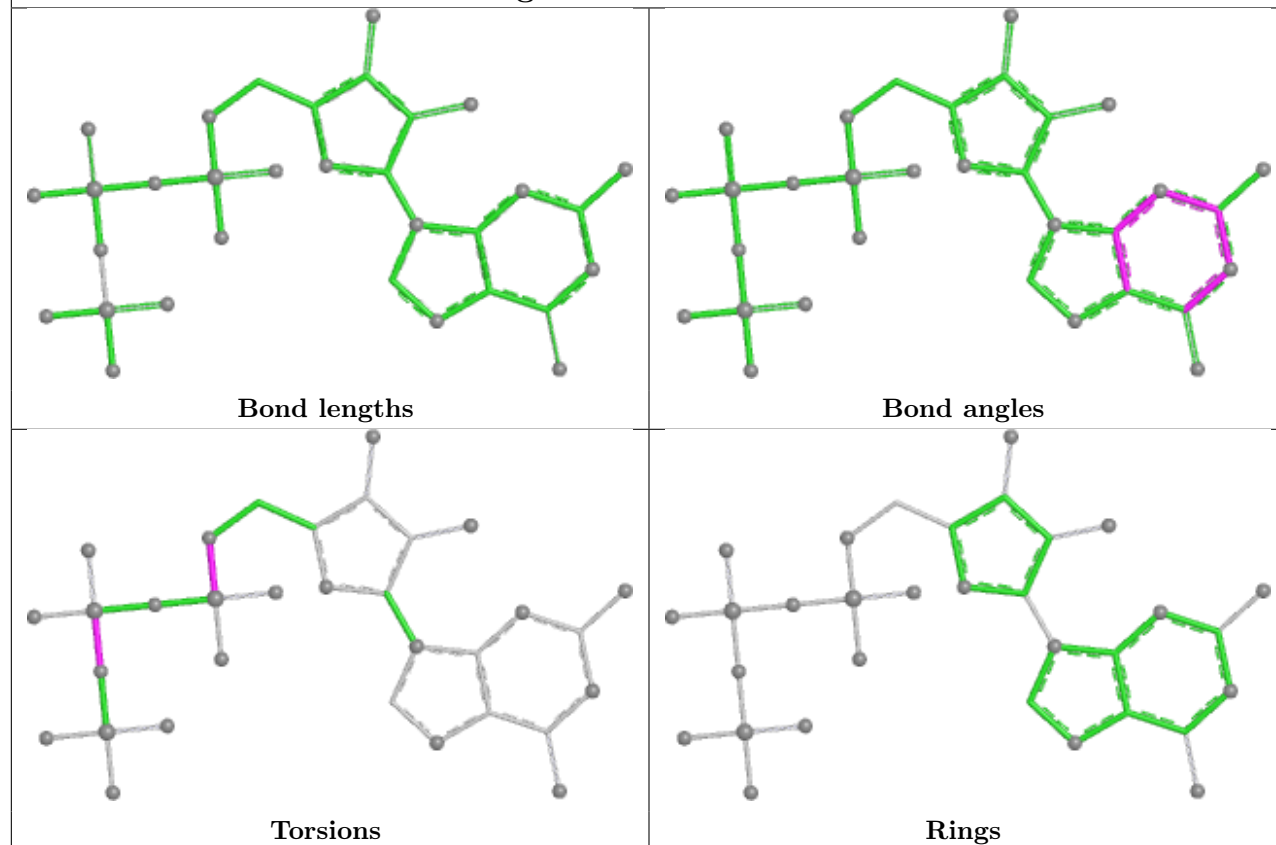
## Ligand GDP FH 501



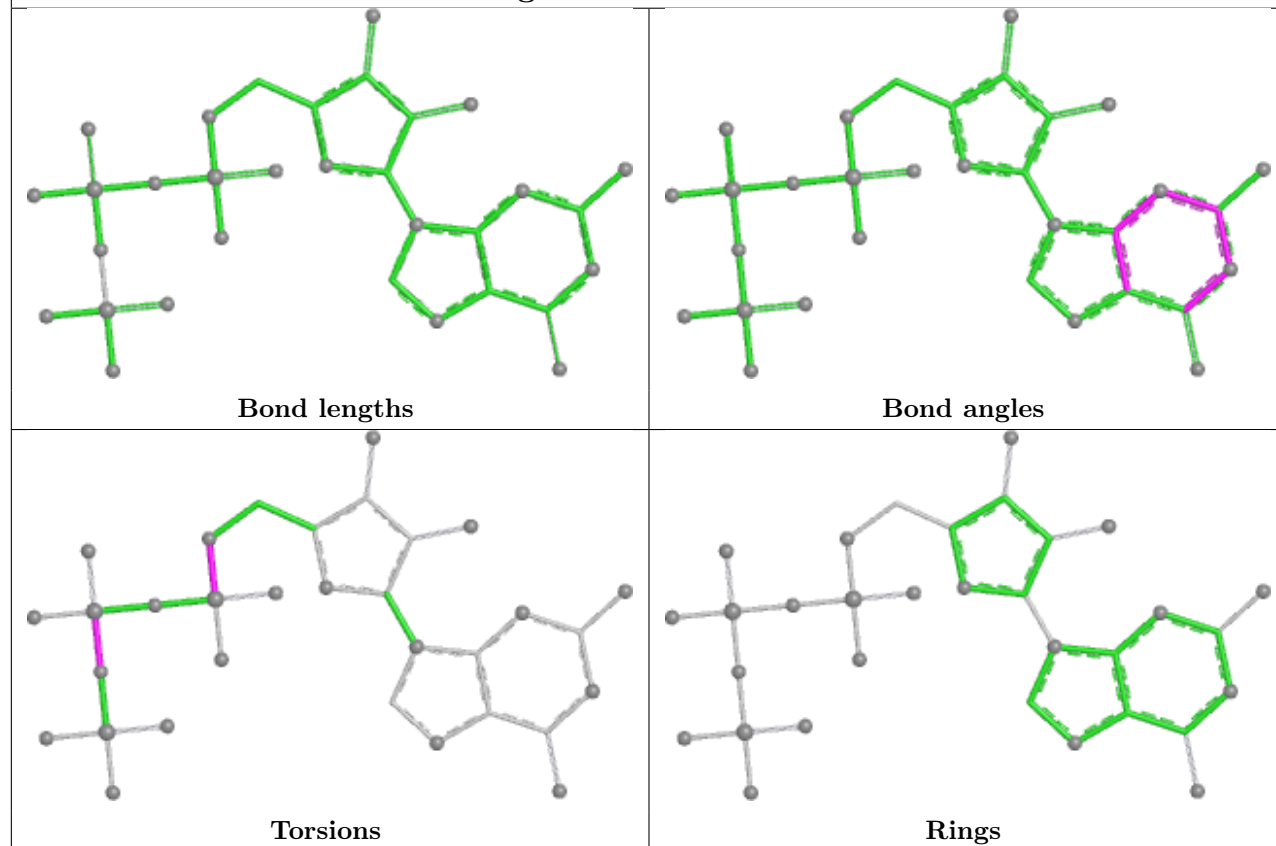


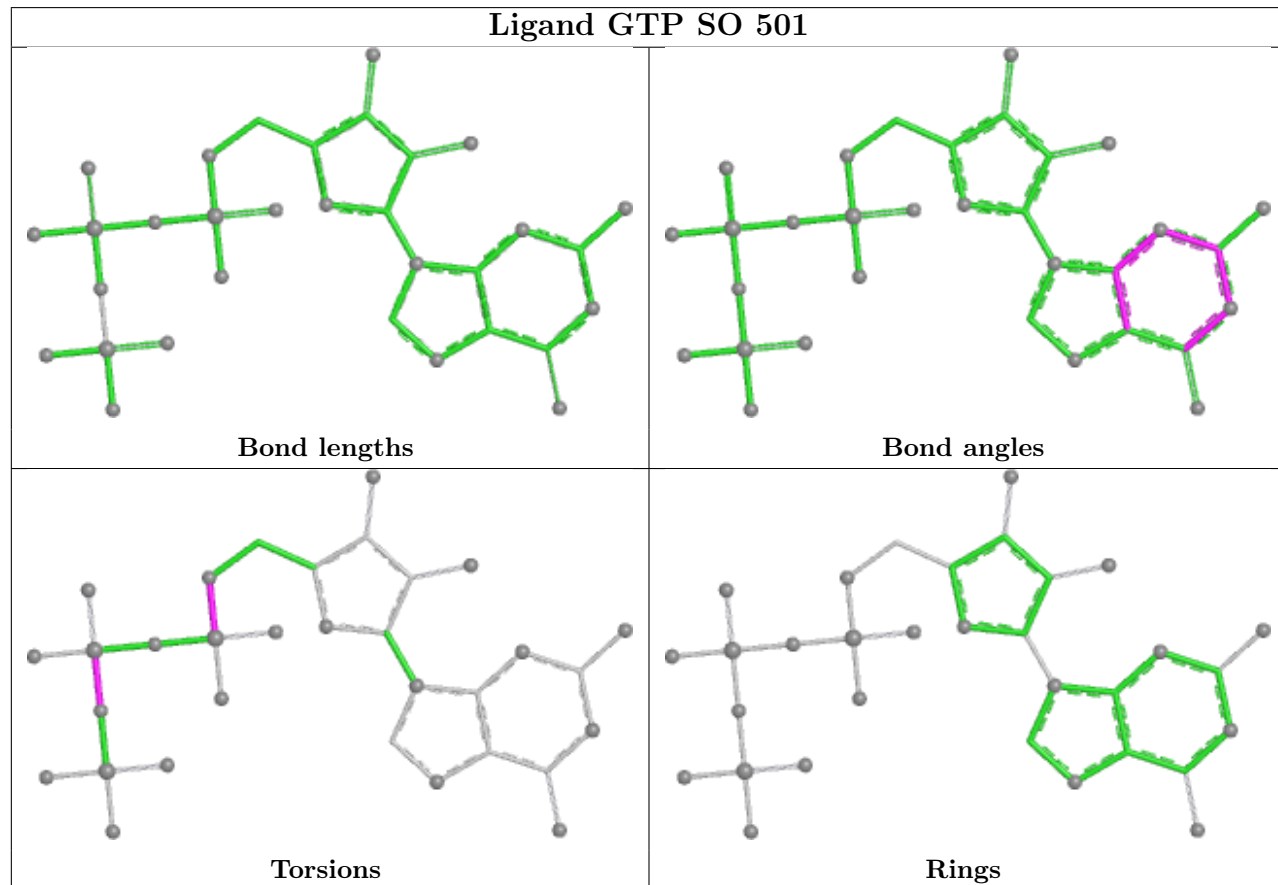
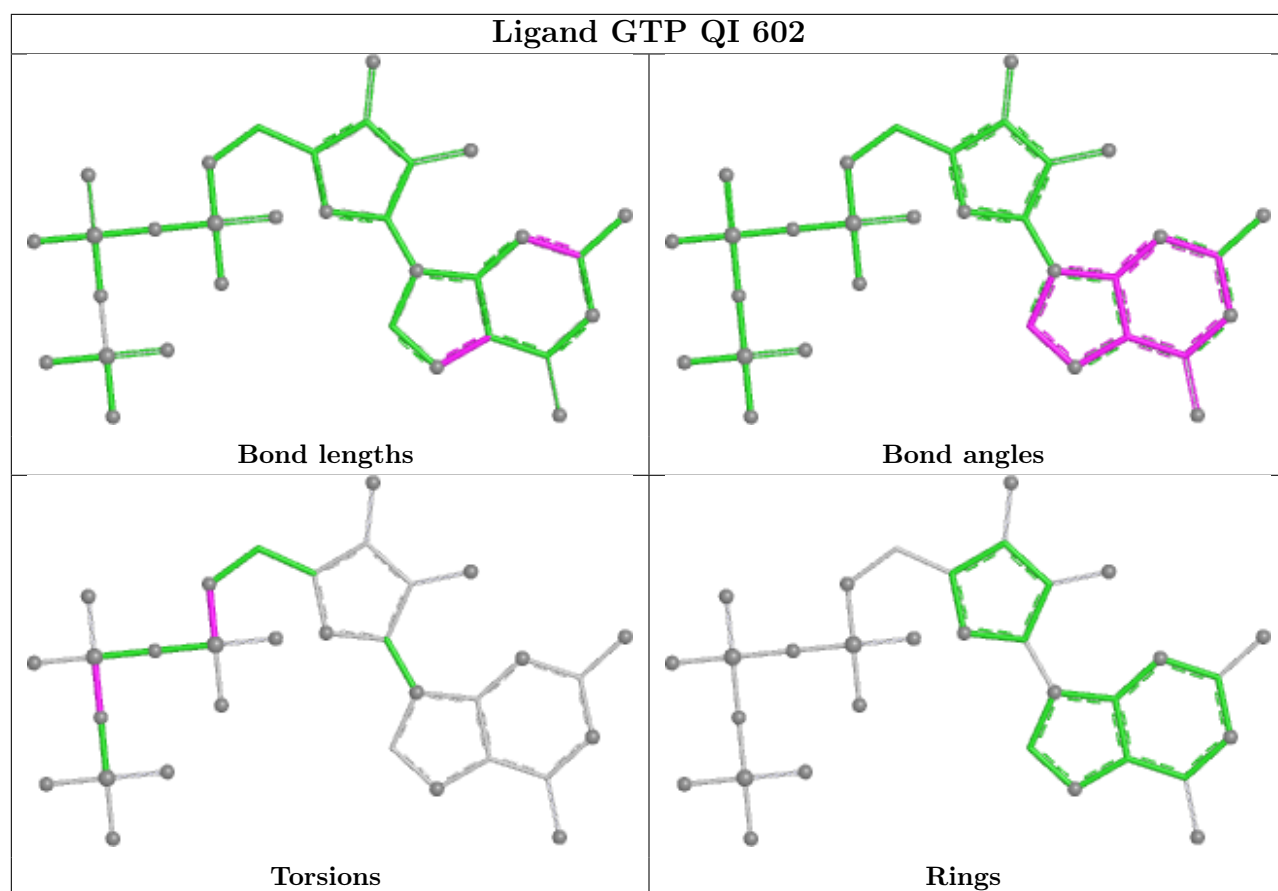


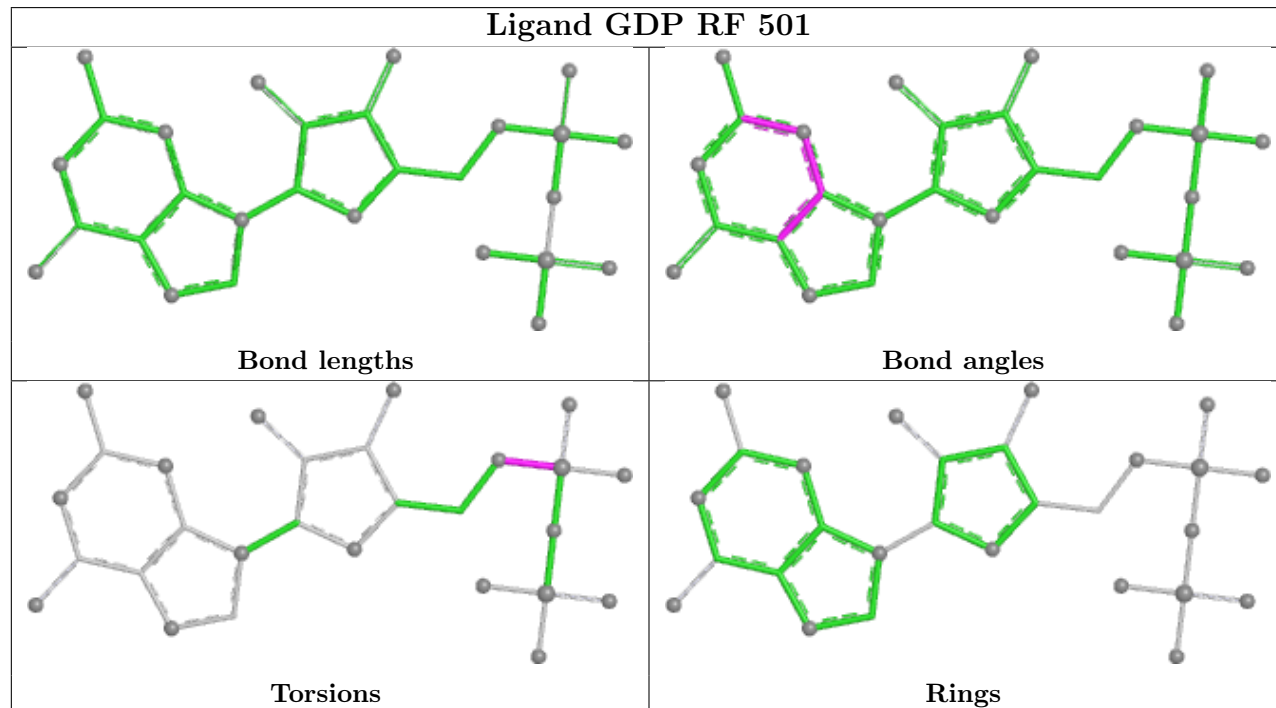
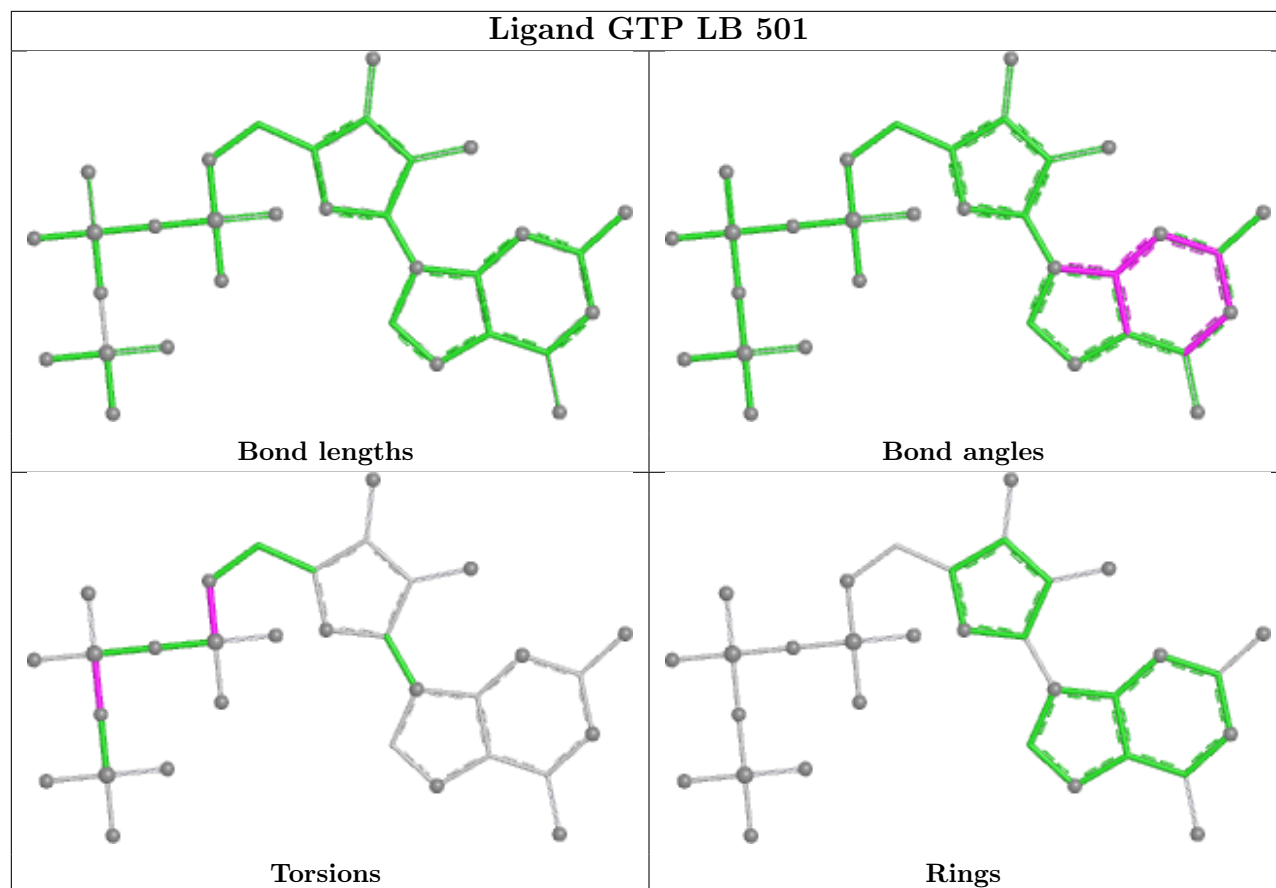
## Ligand GTP VY 501

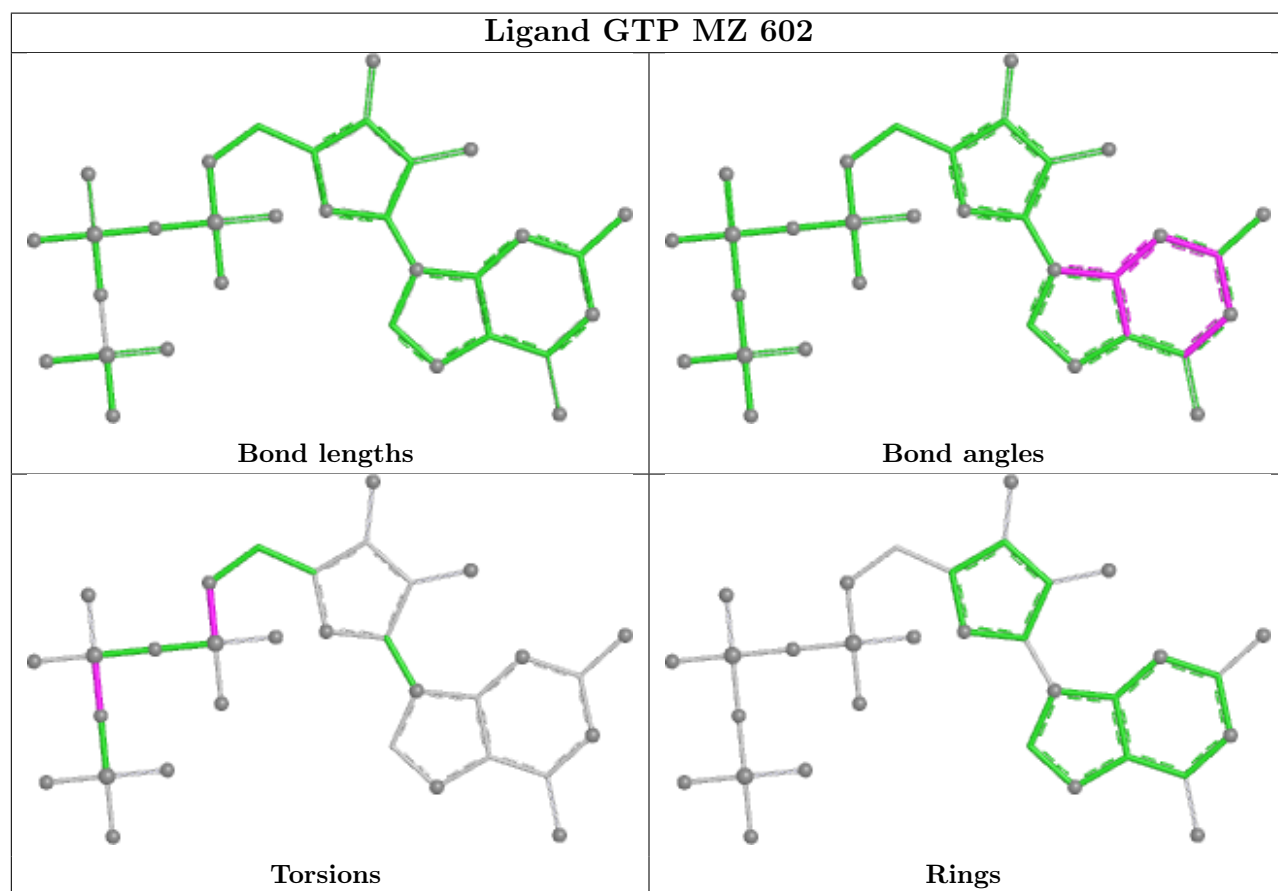
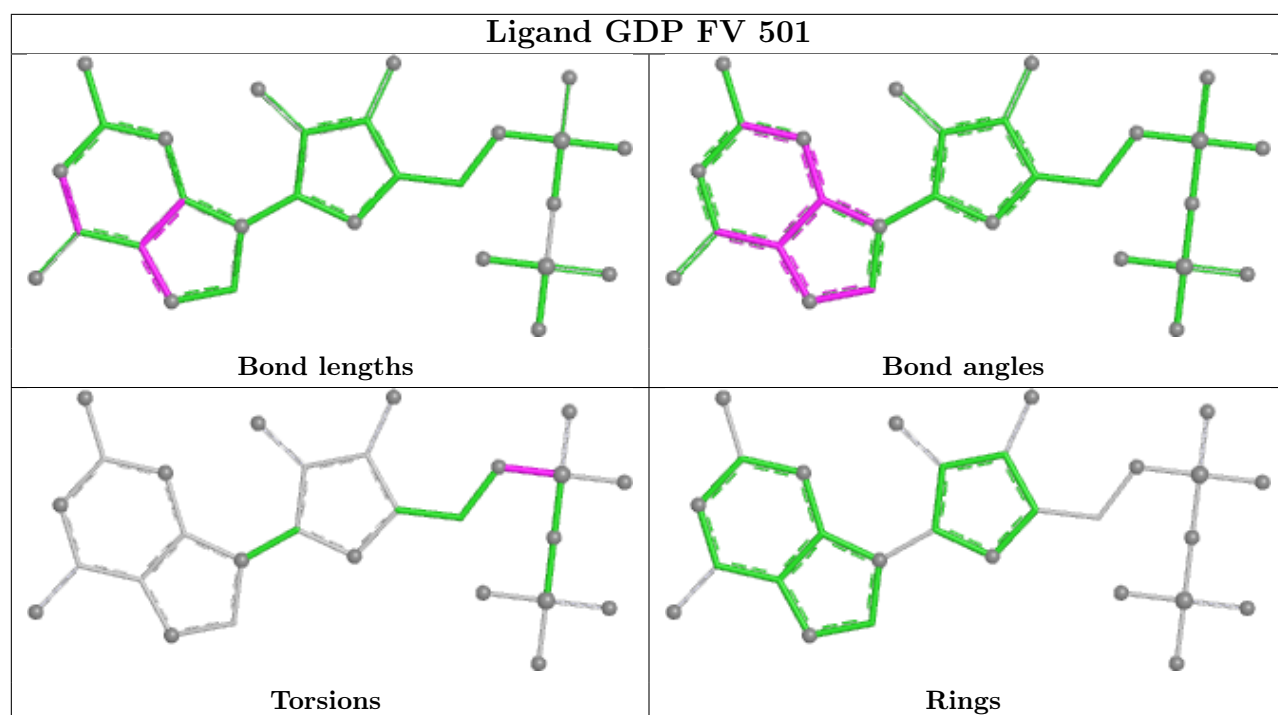


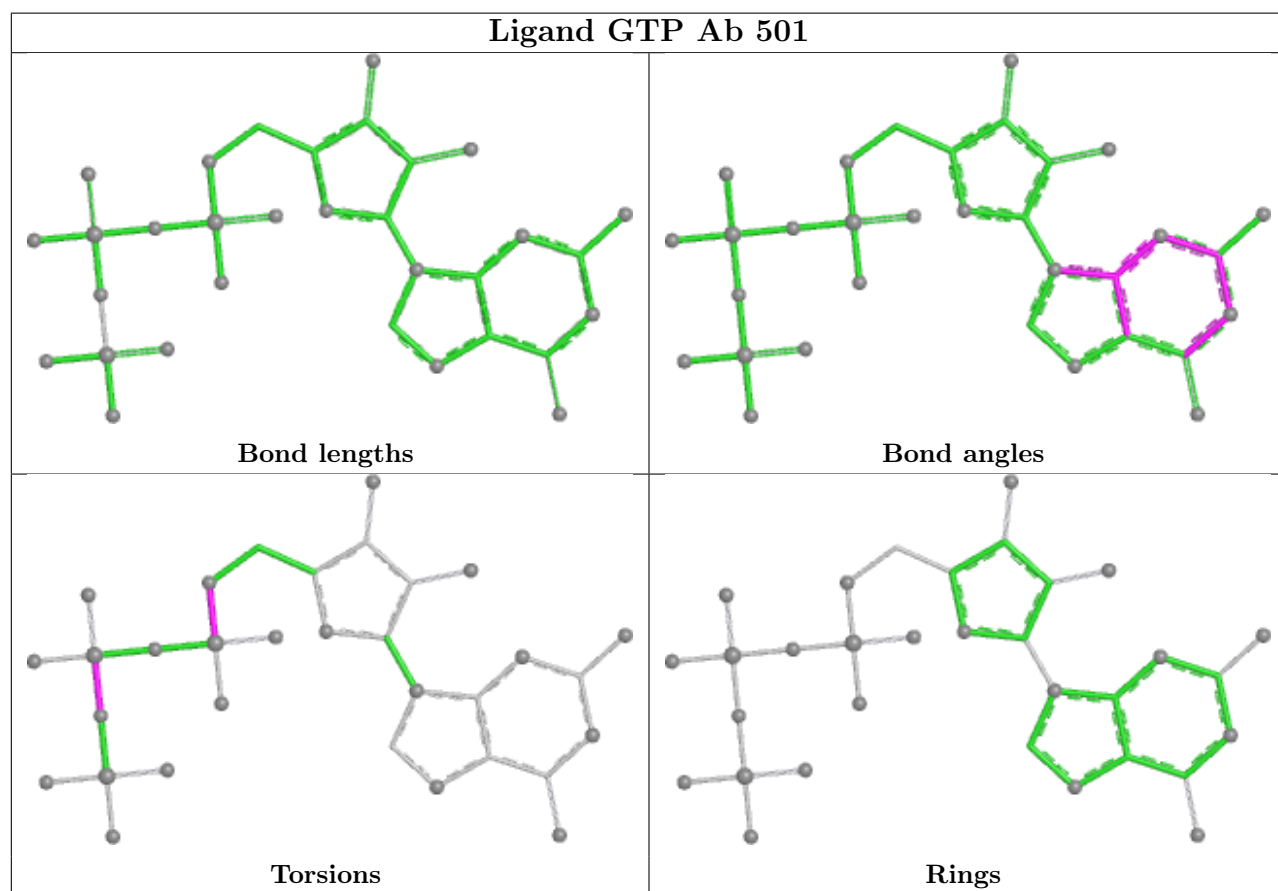
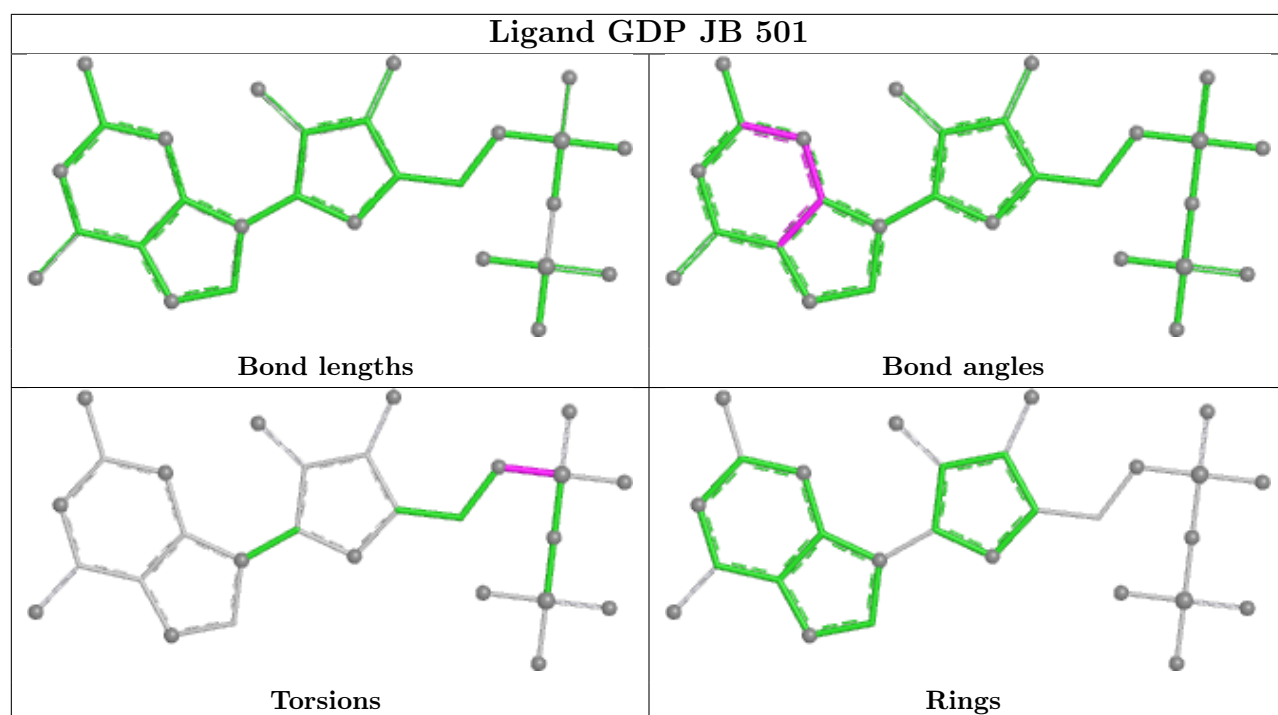
## Ligand GTP PU 602



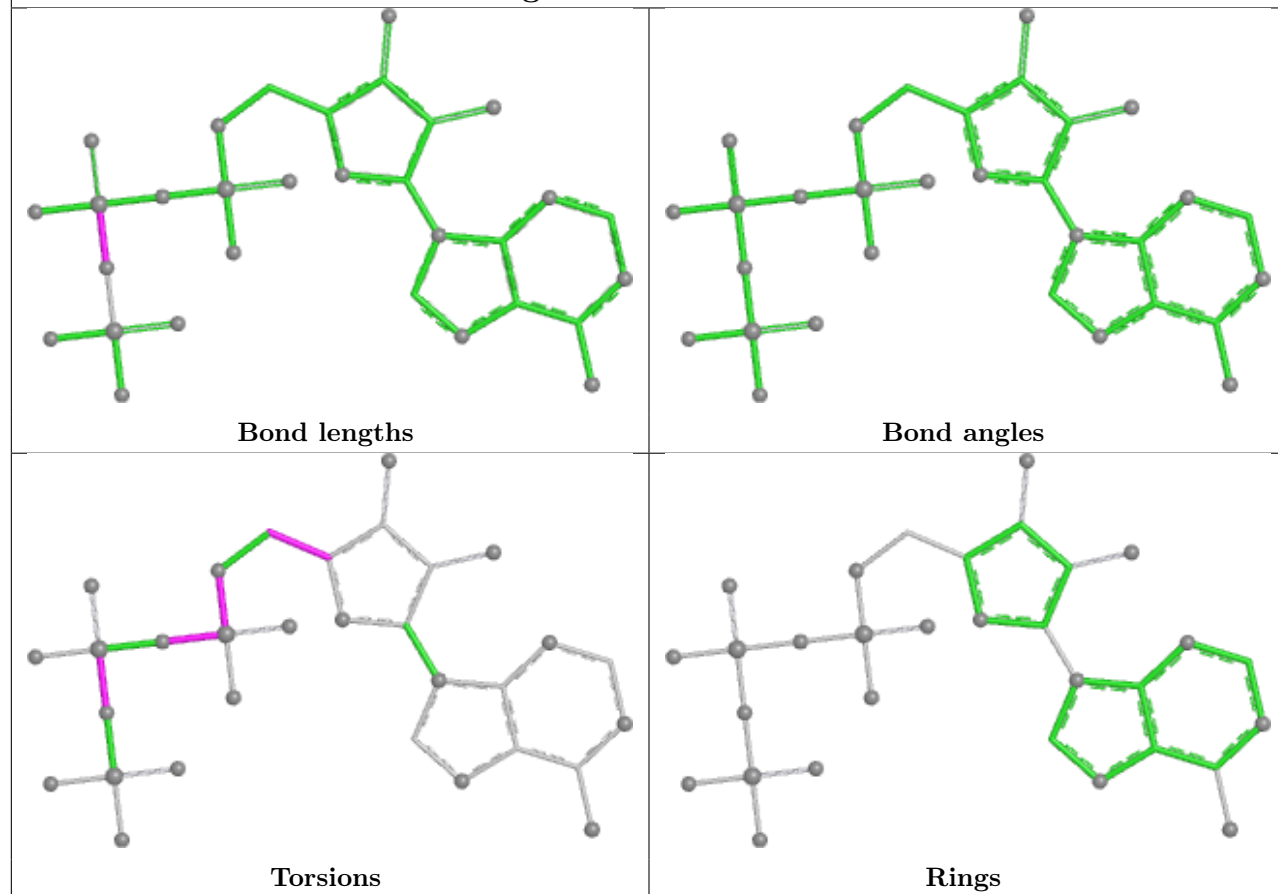




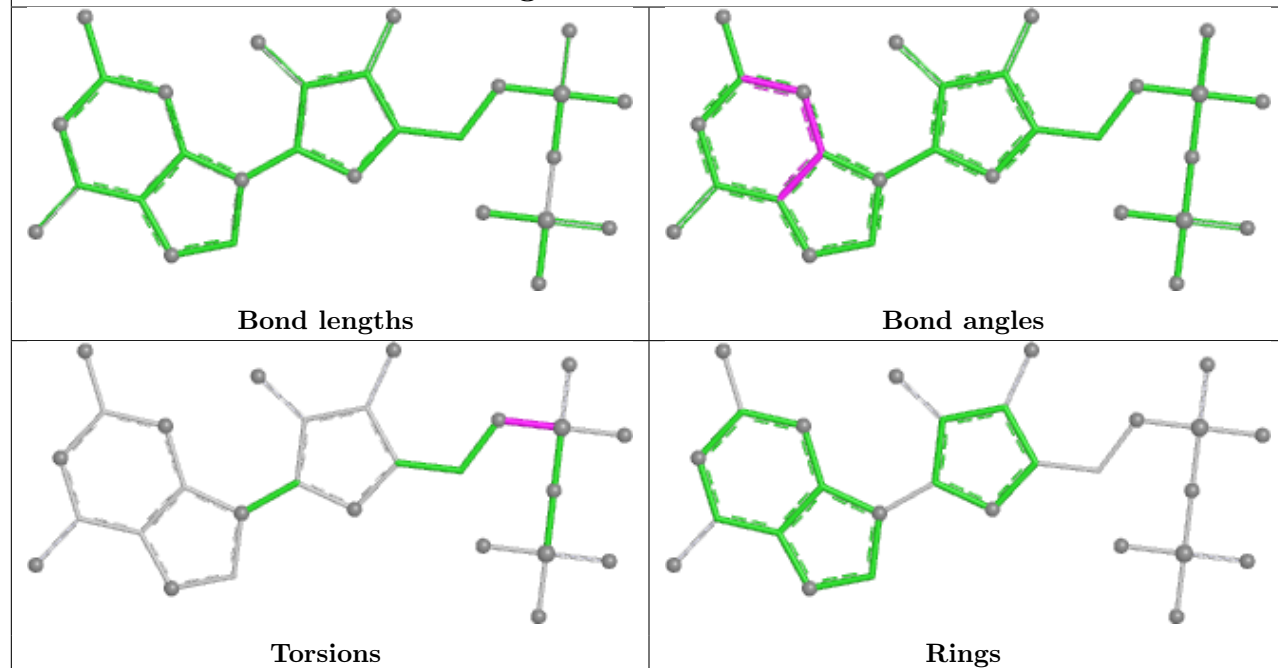


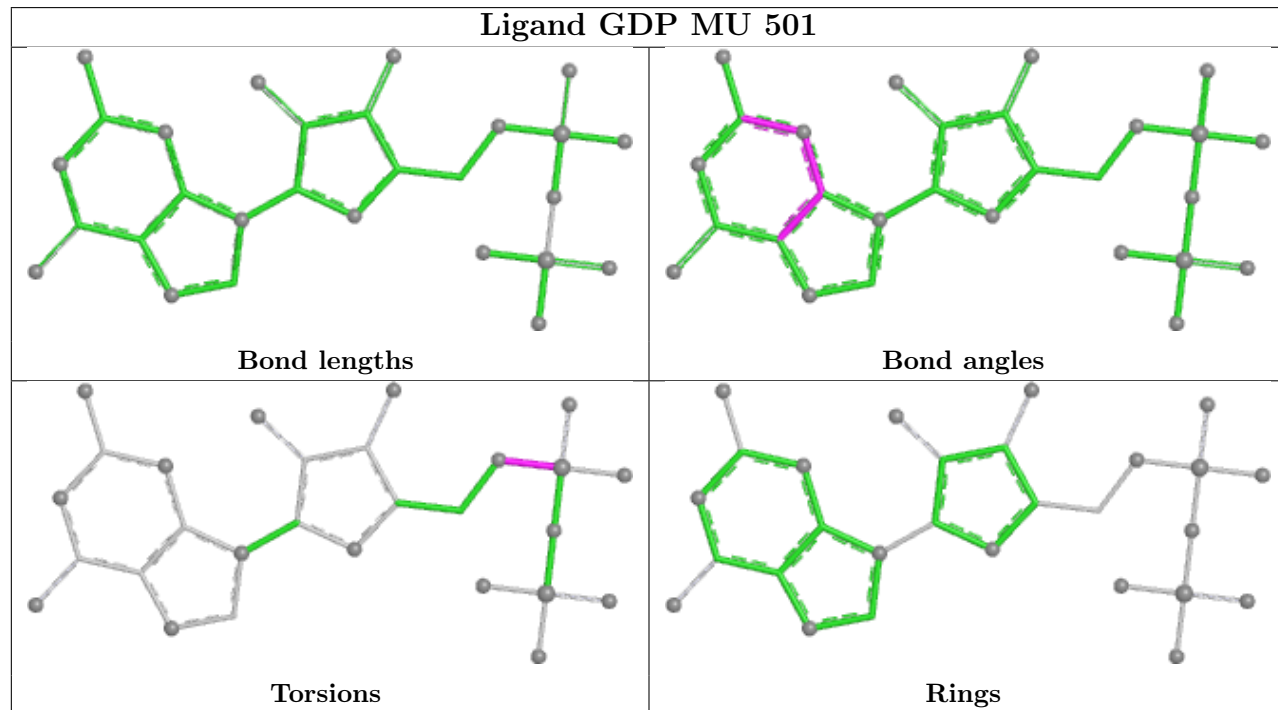
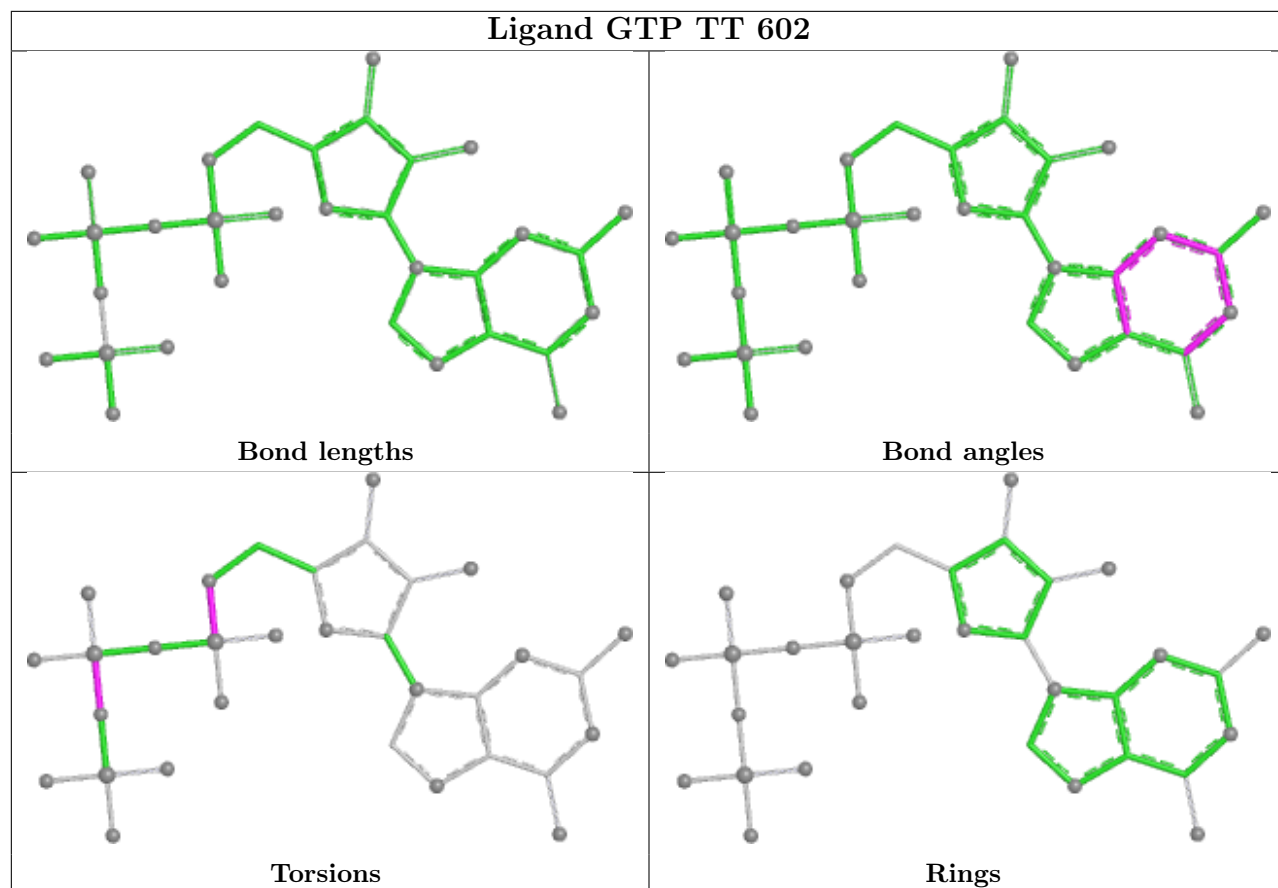


## Ligand ATP 9f 4701

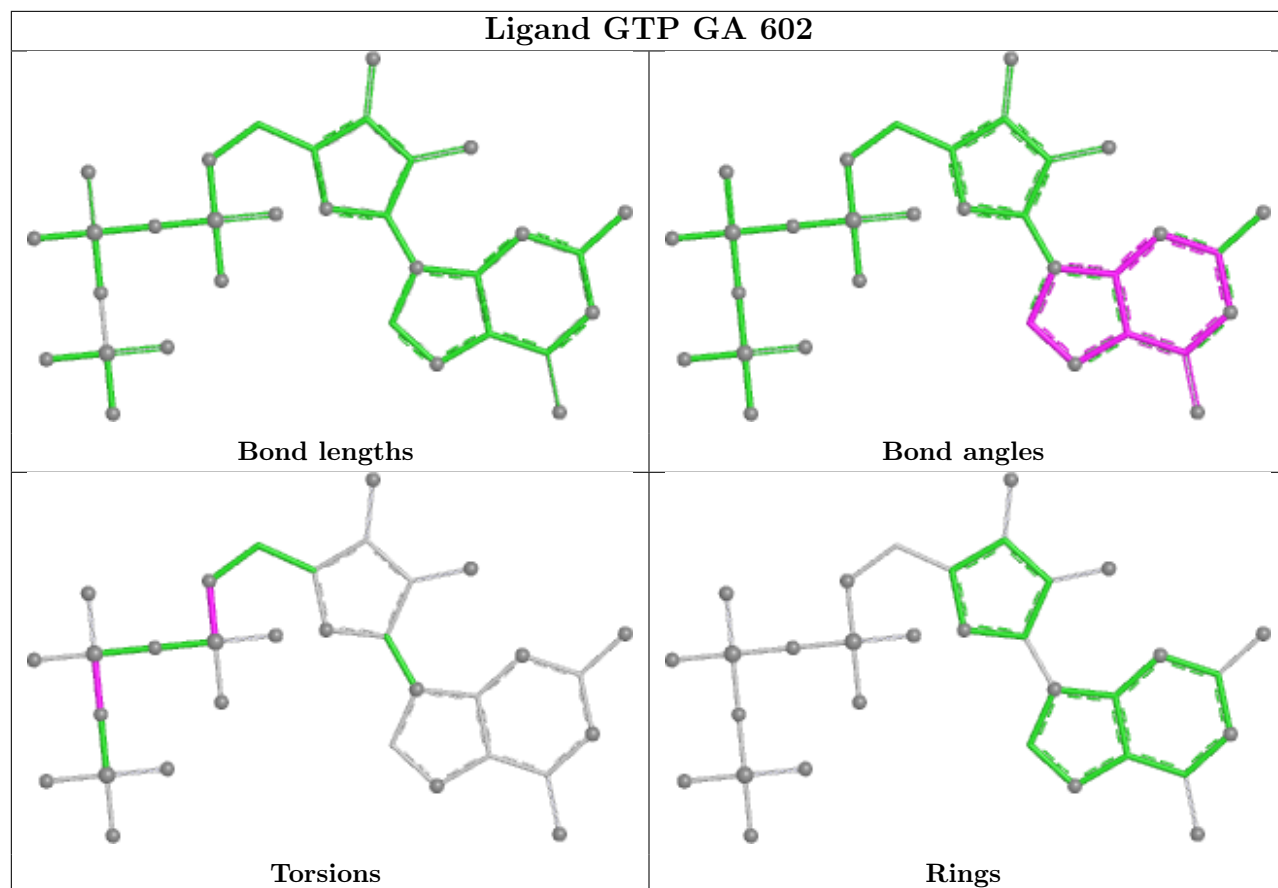


## Ligand GDP MI 501

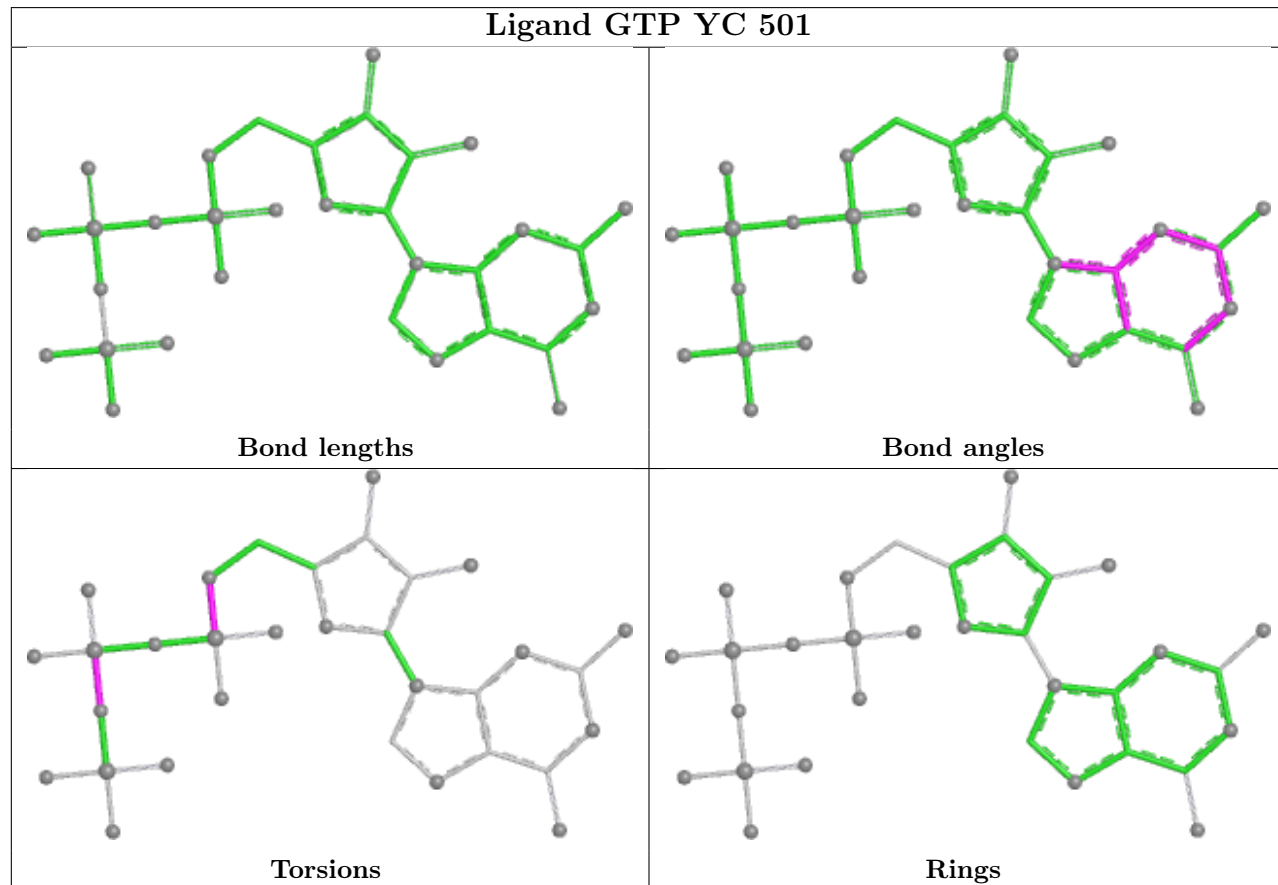




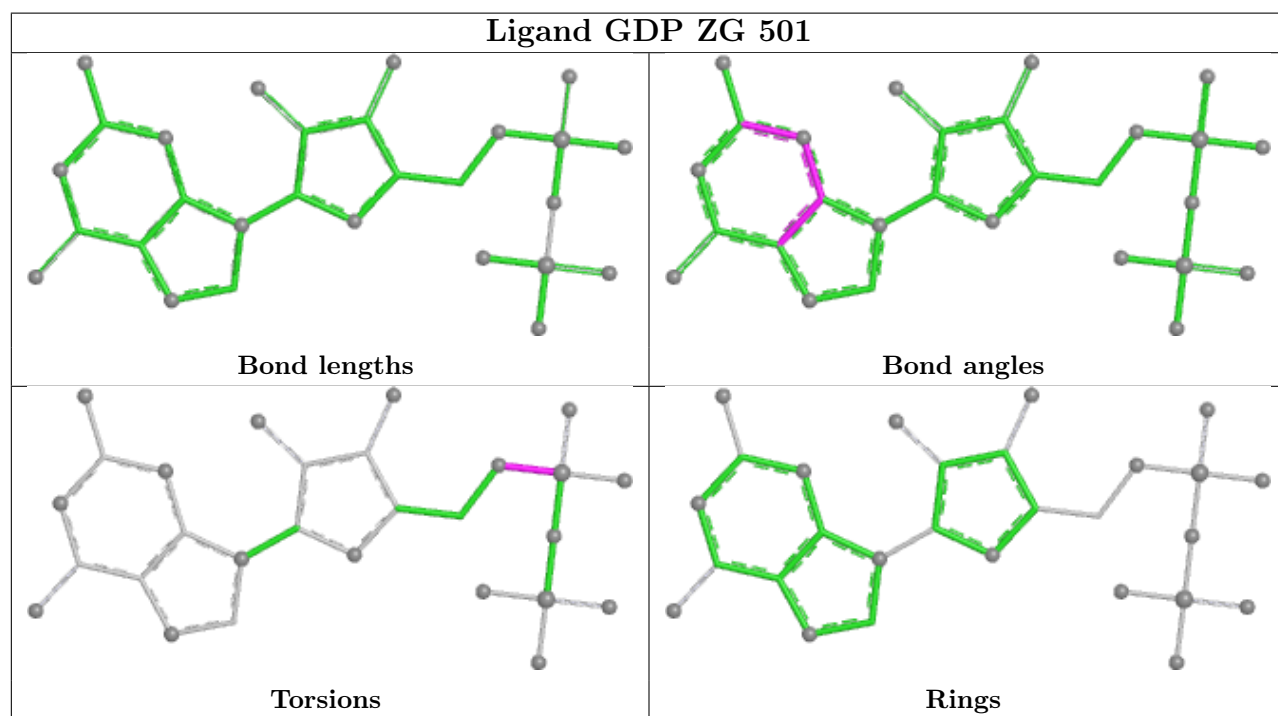
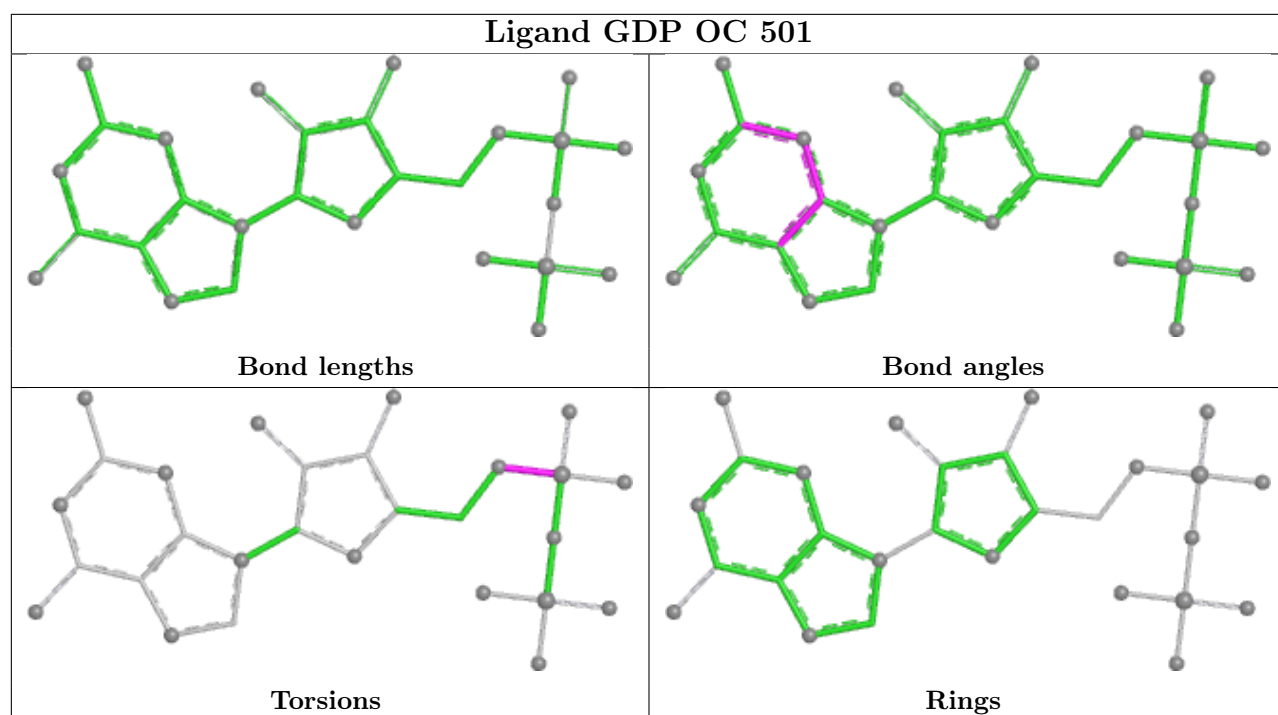
## Ligand GTP GA 602

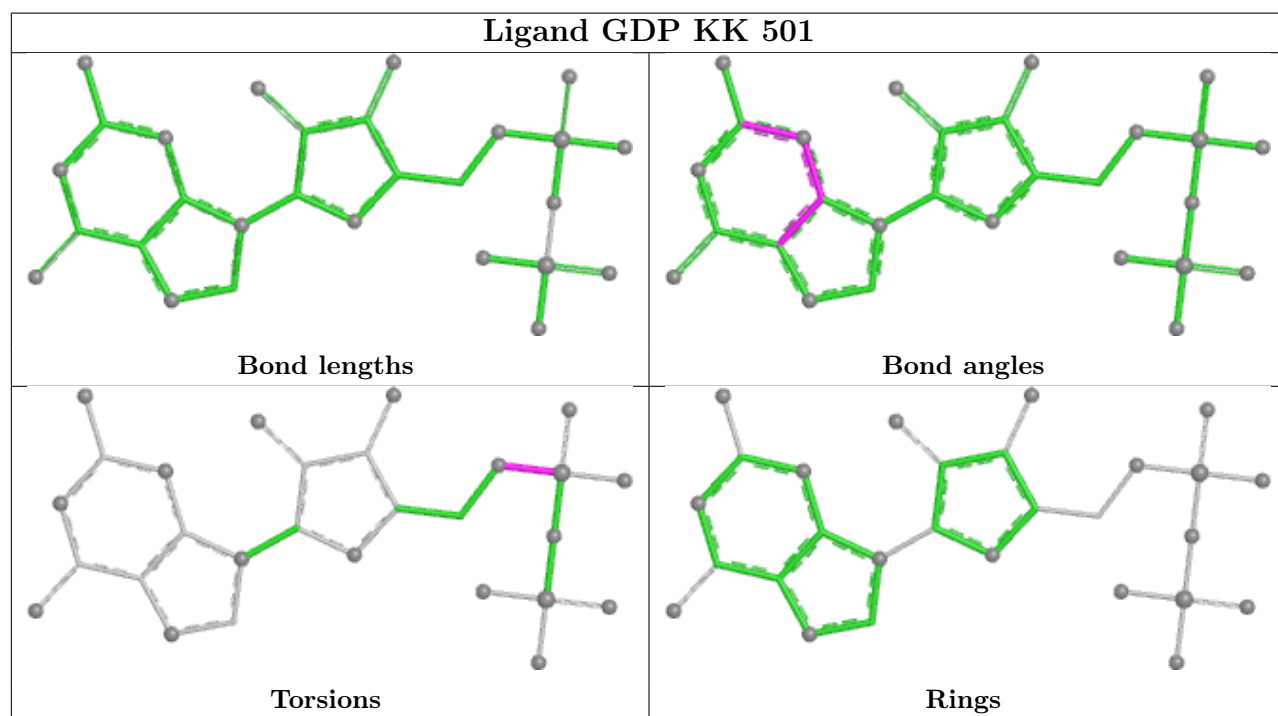
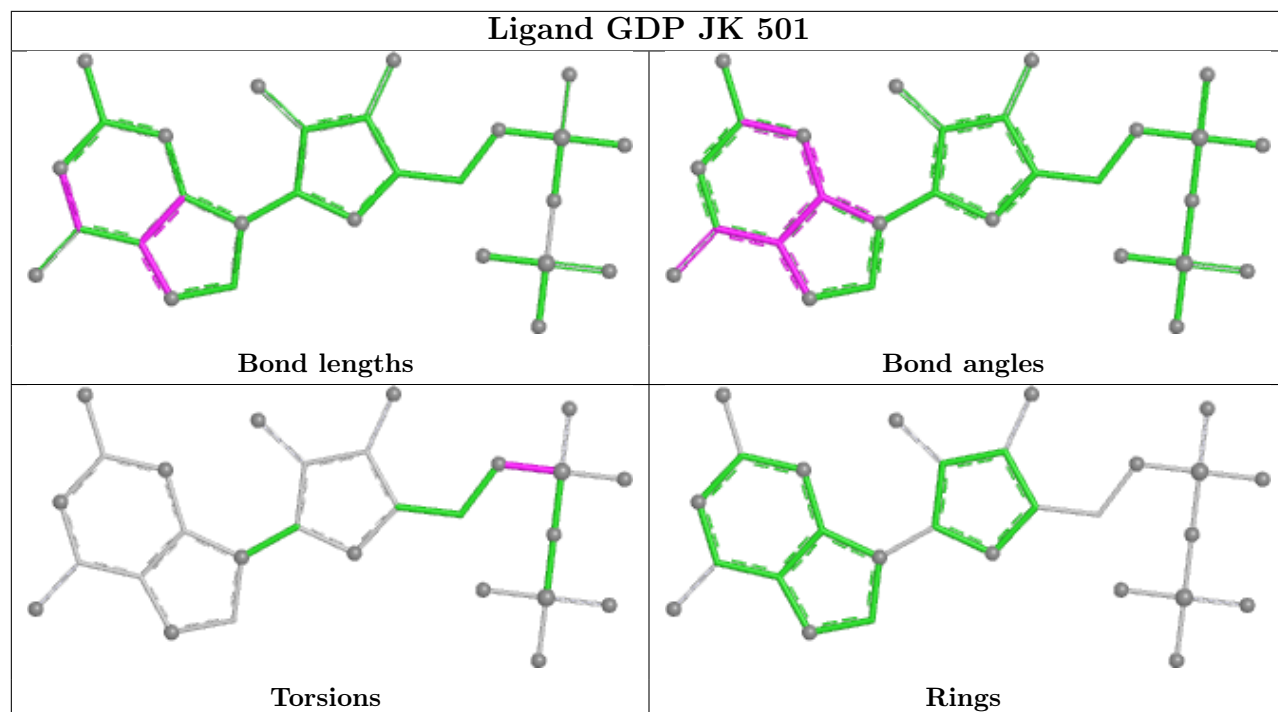


## Ligand GTP YC 501

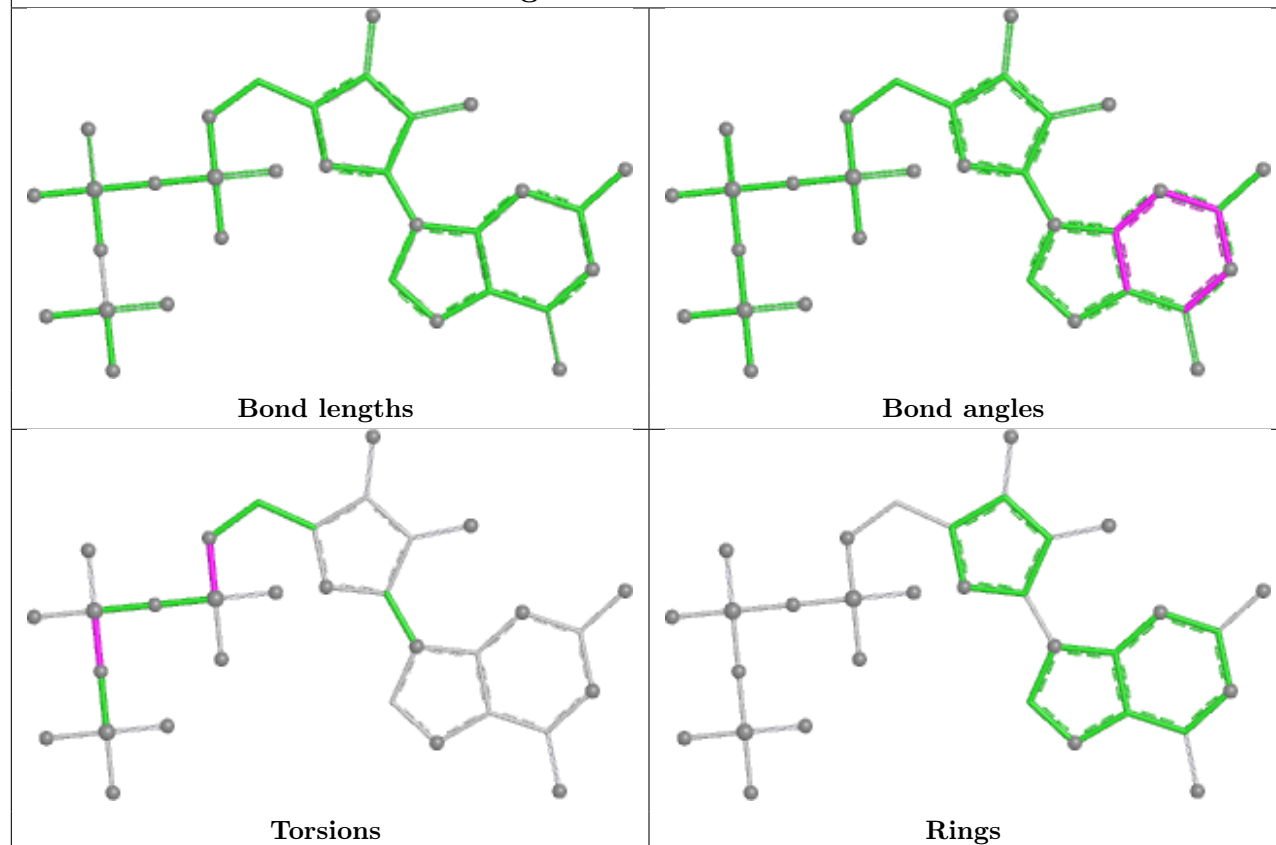




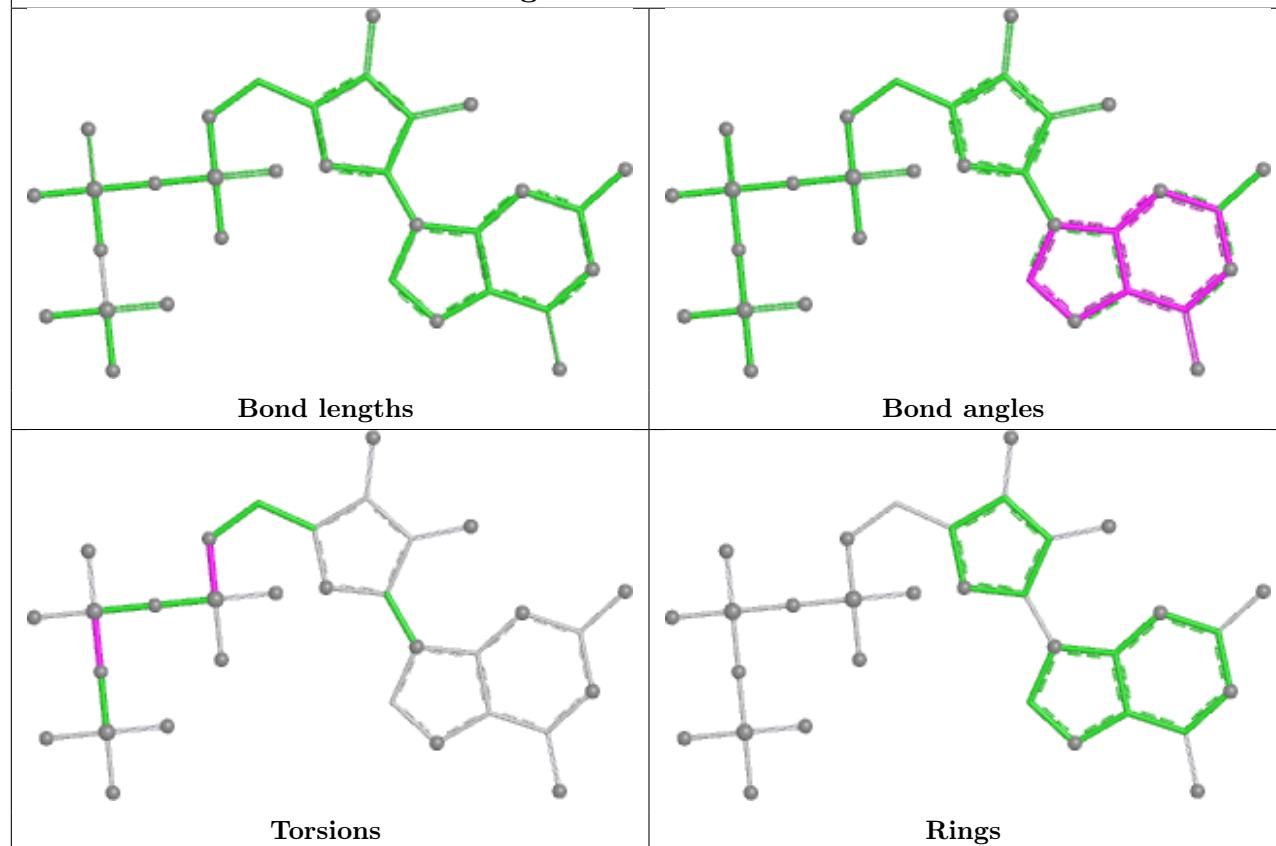




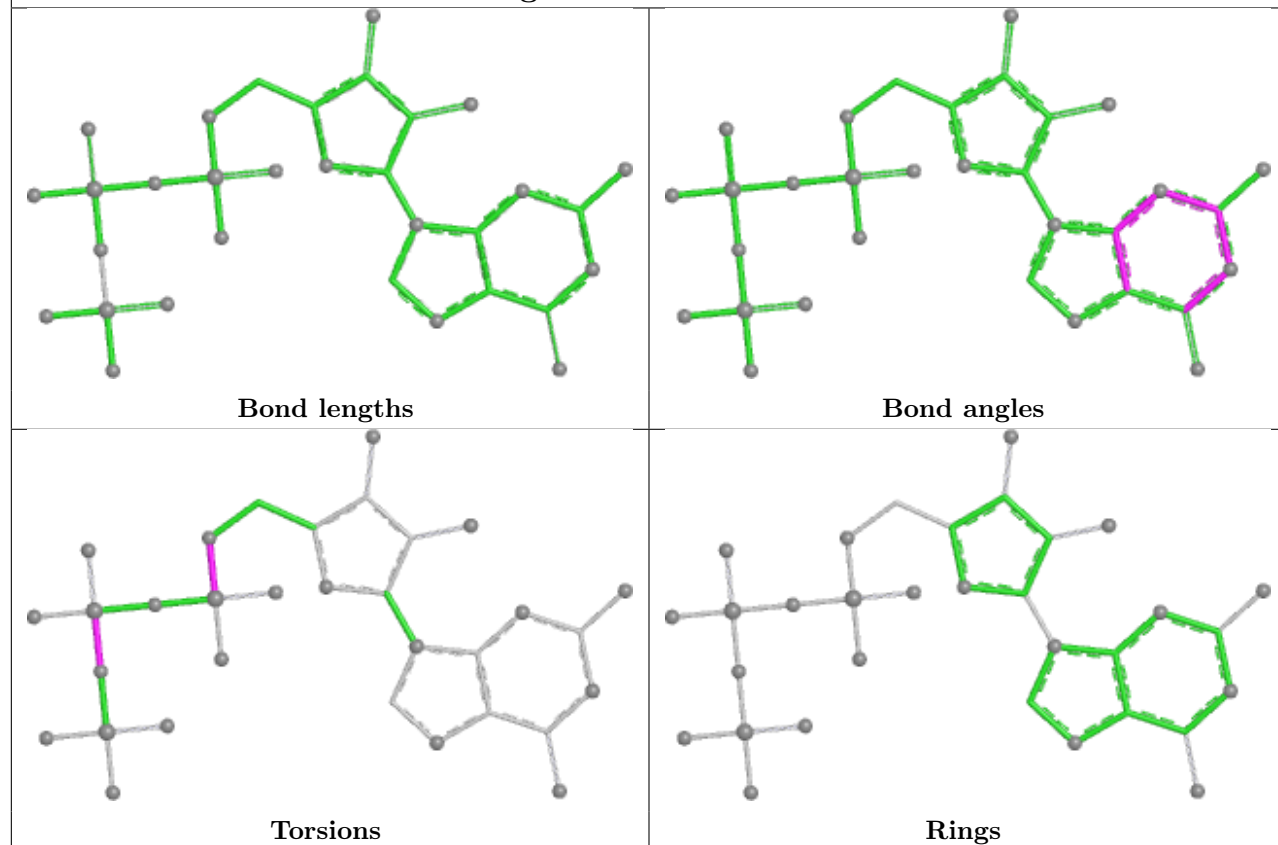
## Ligand GTP DJ 501



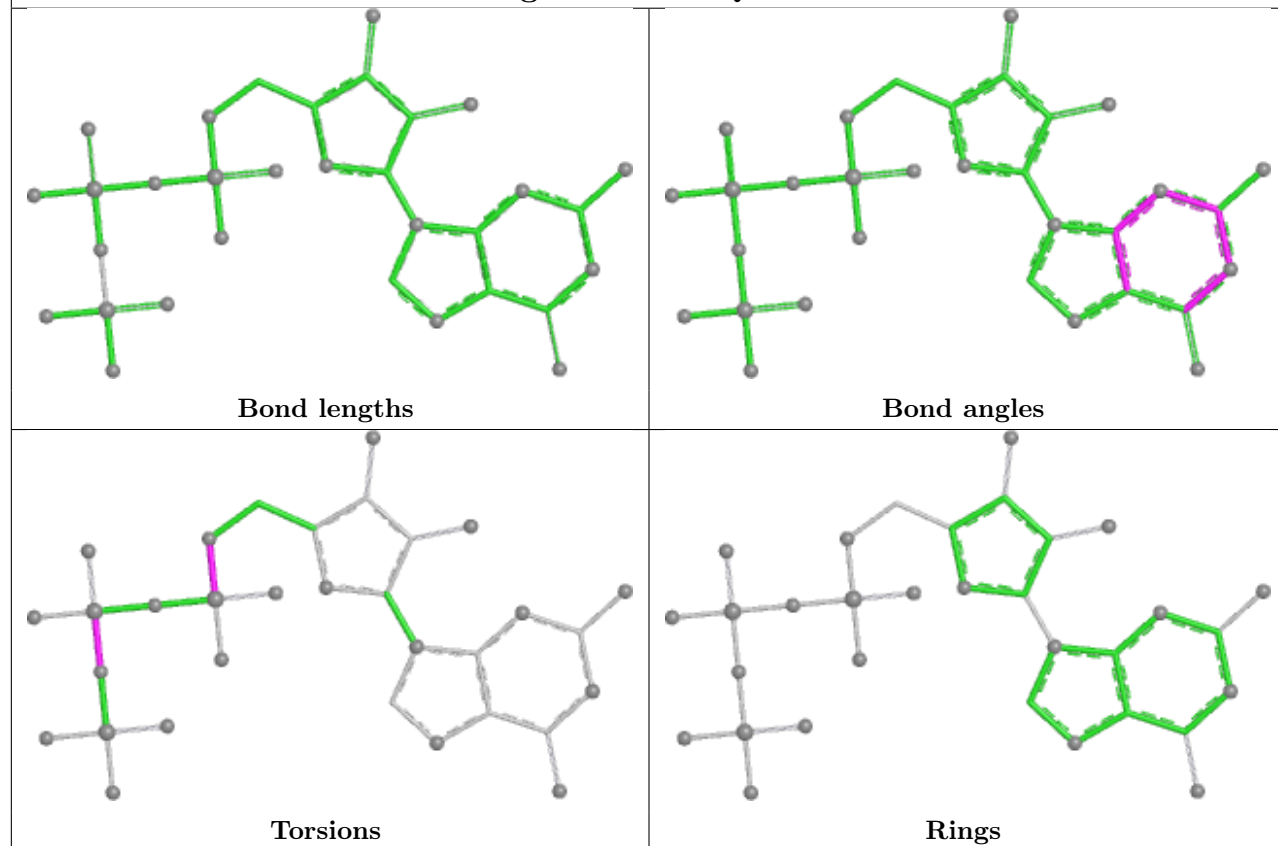
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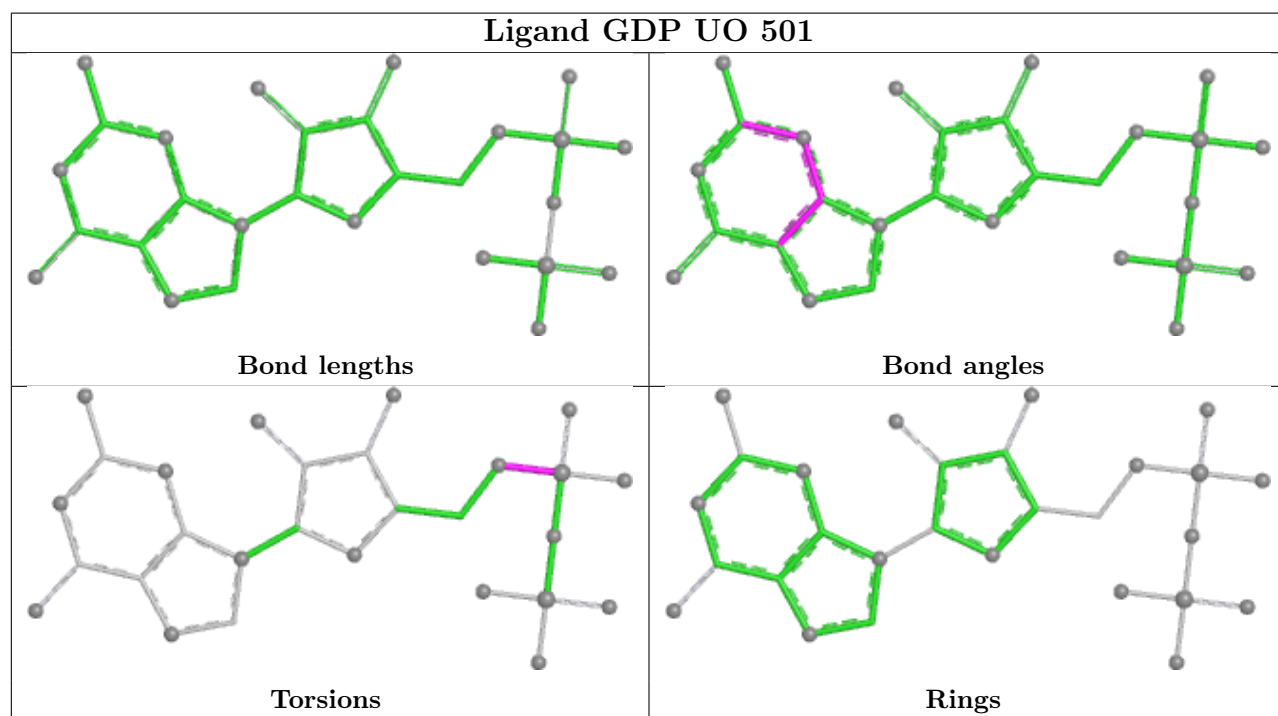
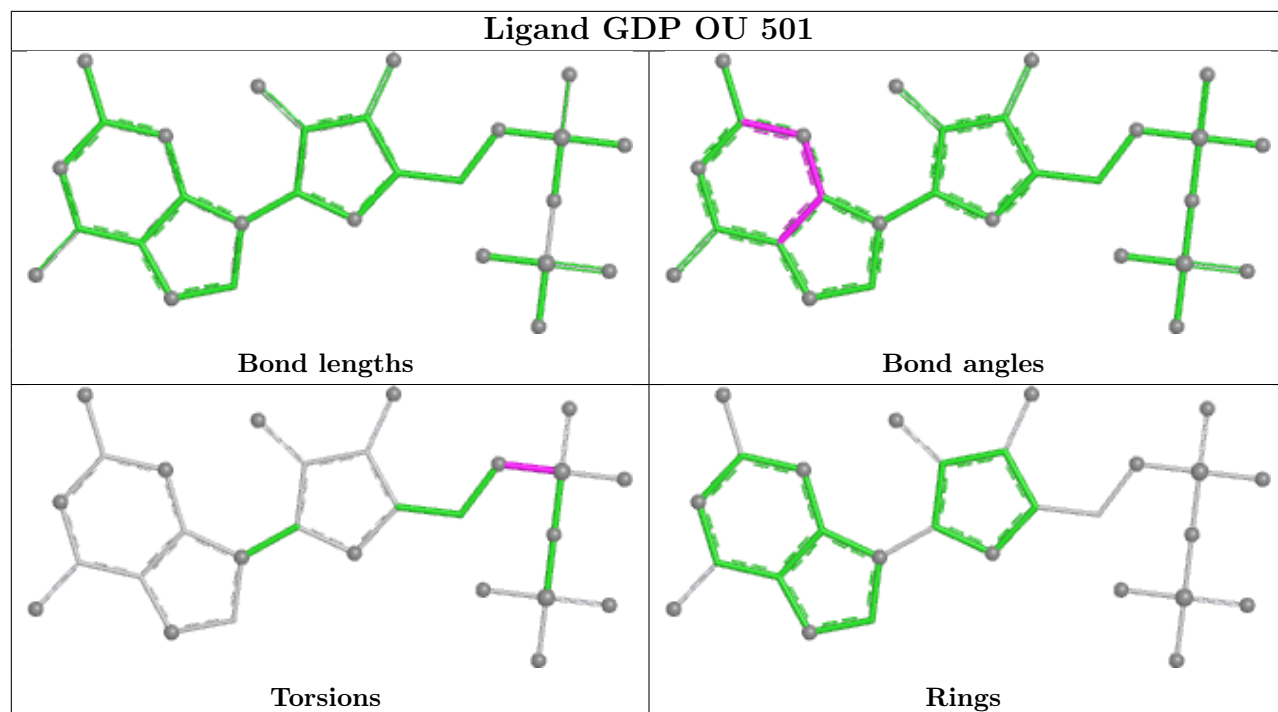


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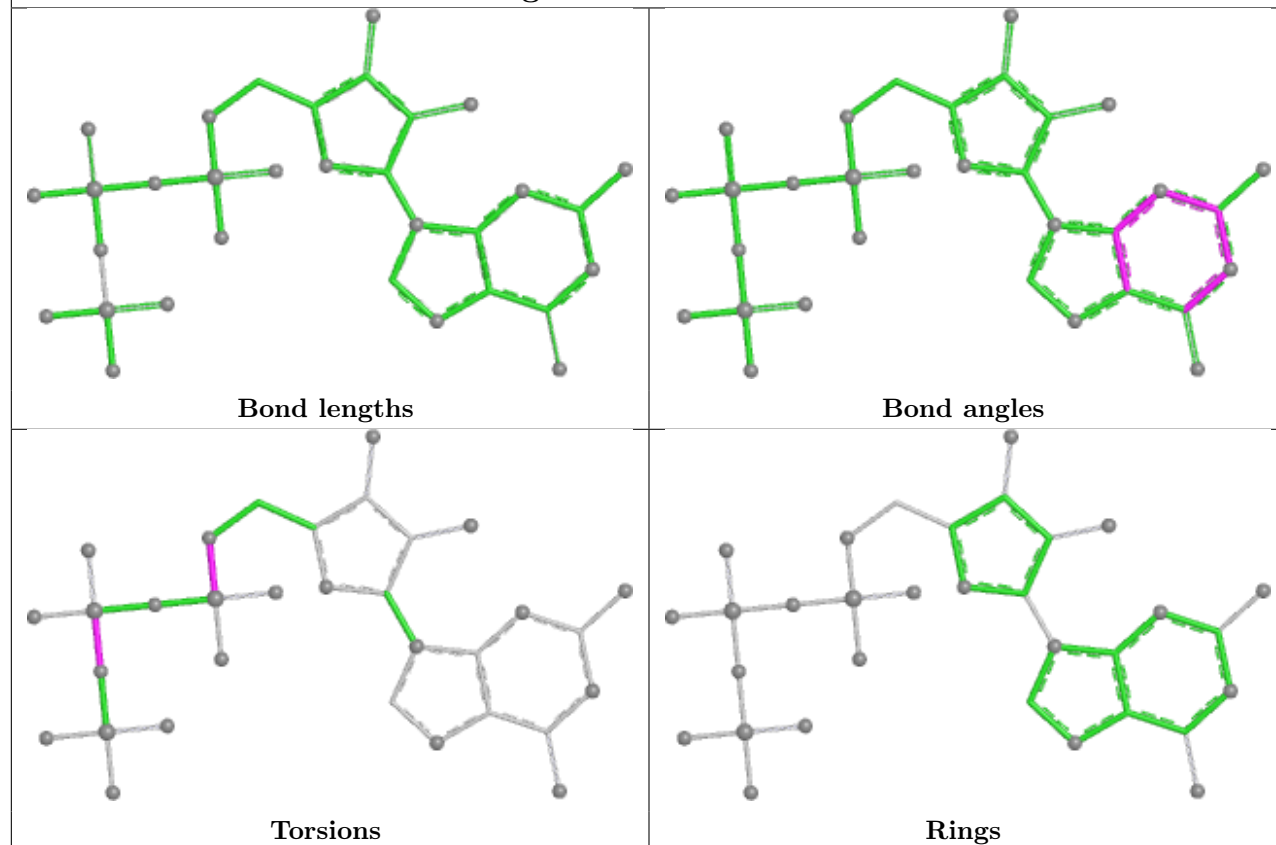


## Ligand GTP SQ 602

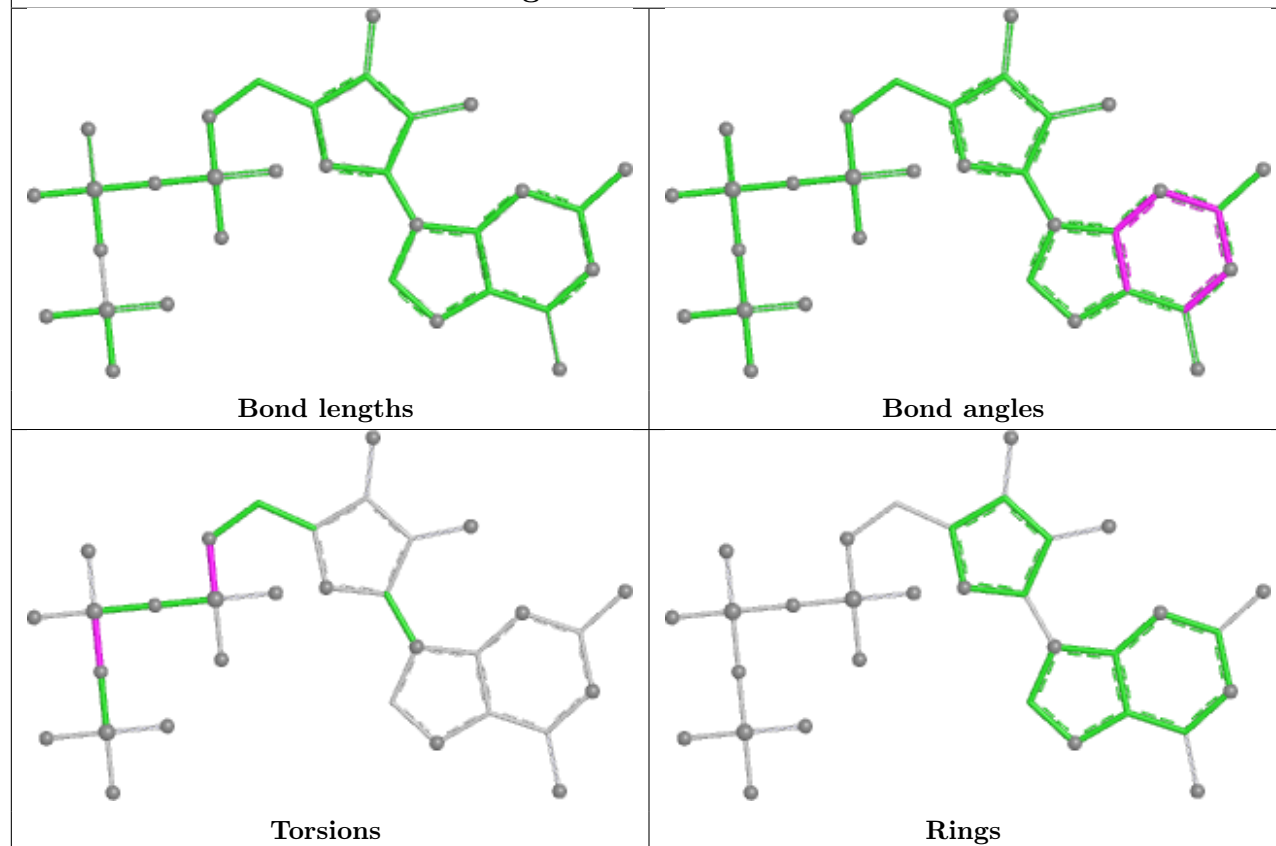


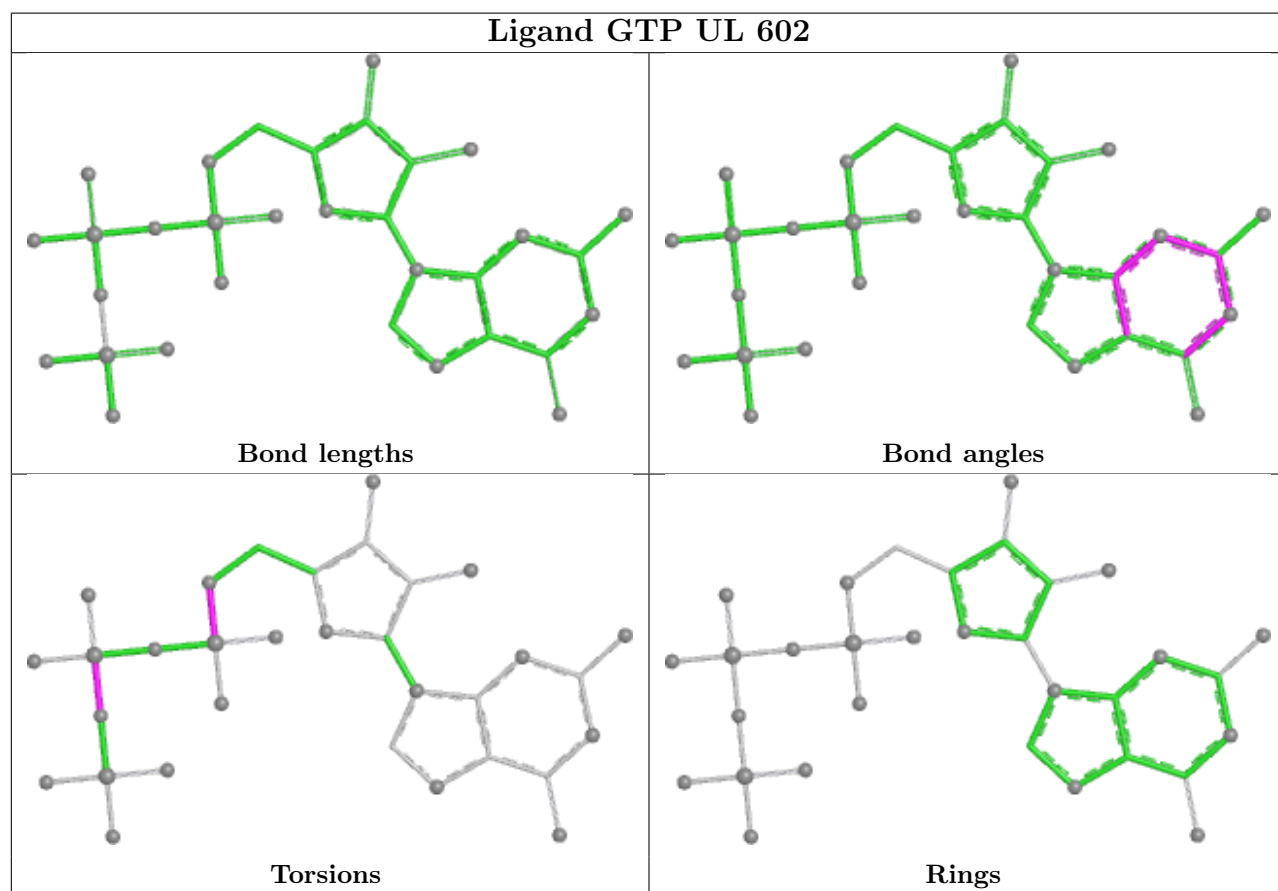
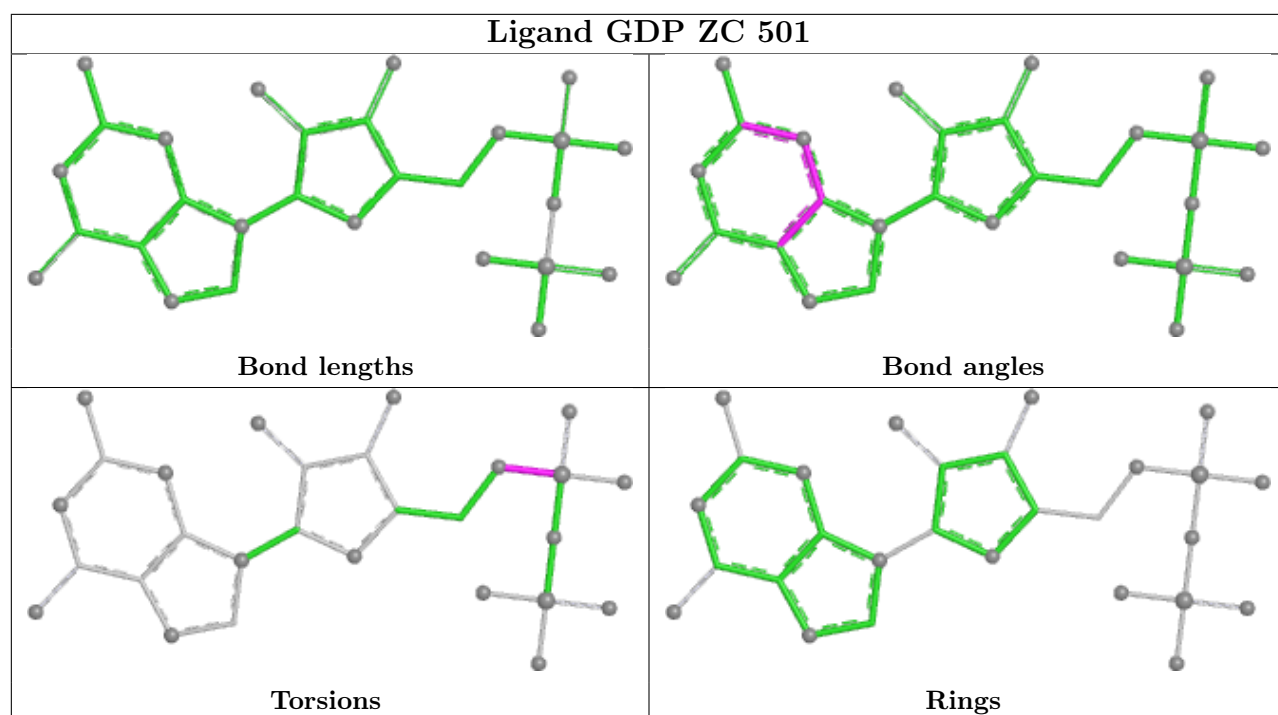


## Ligand GTP LZ 501

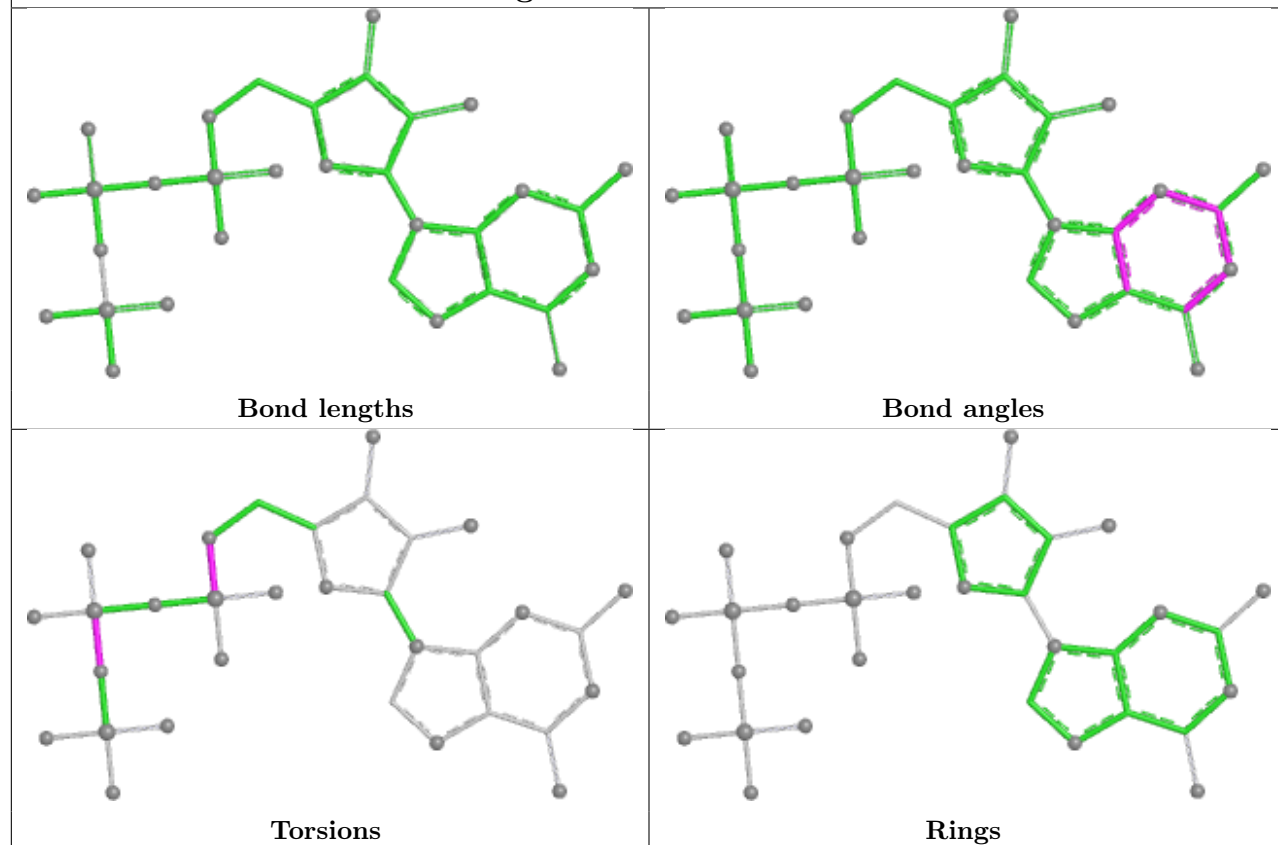


## Ligand GTP FS 602

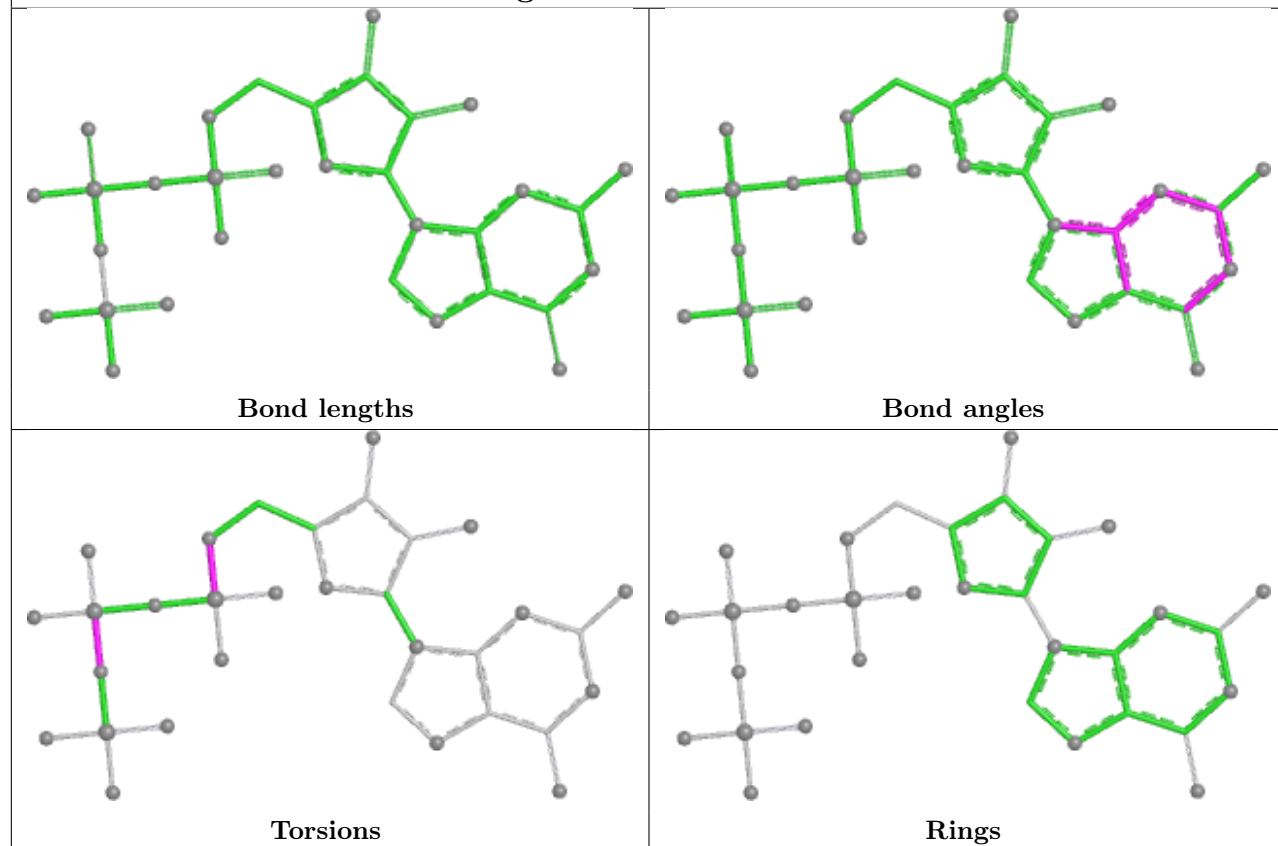




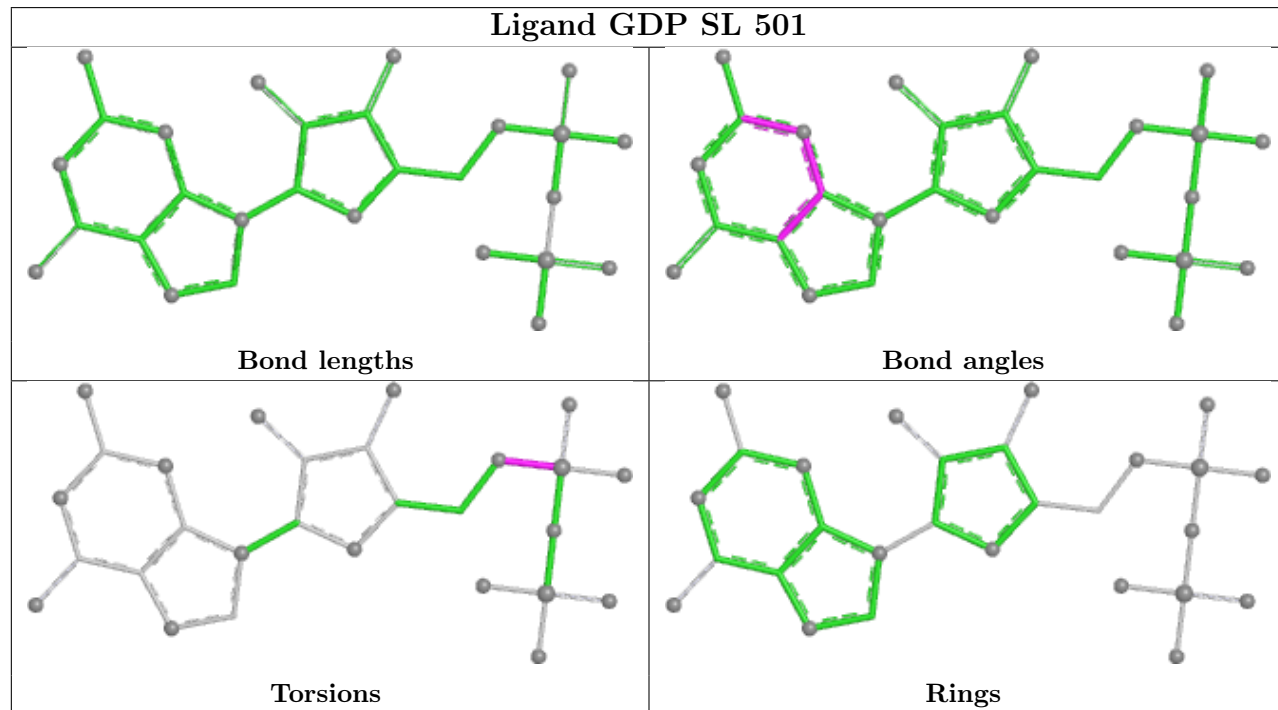
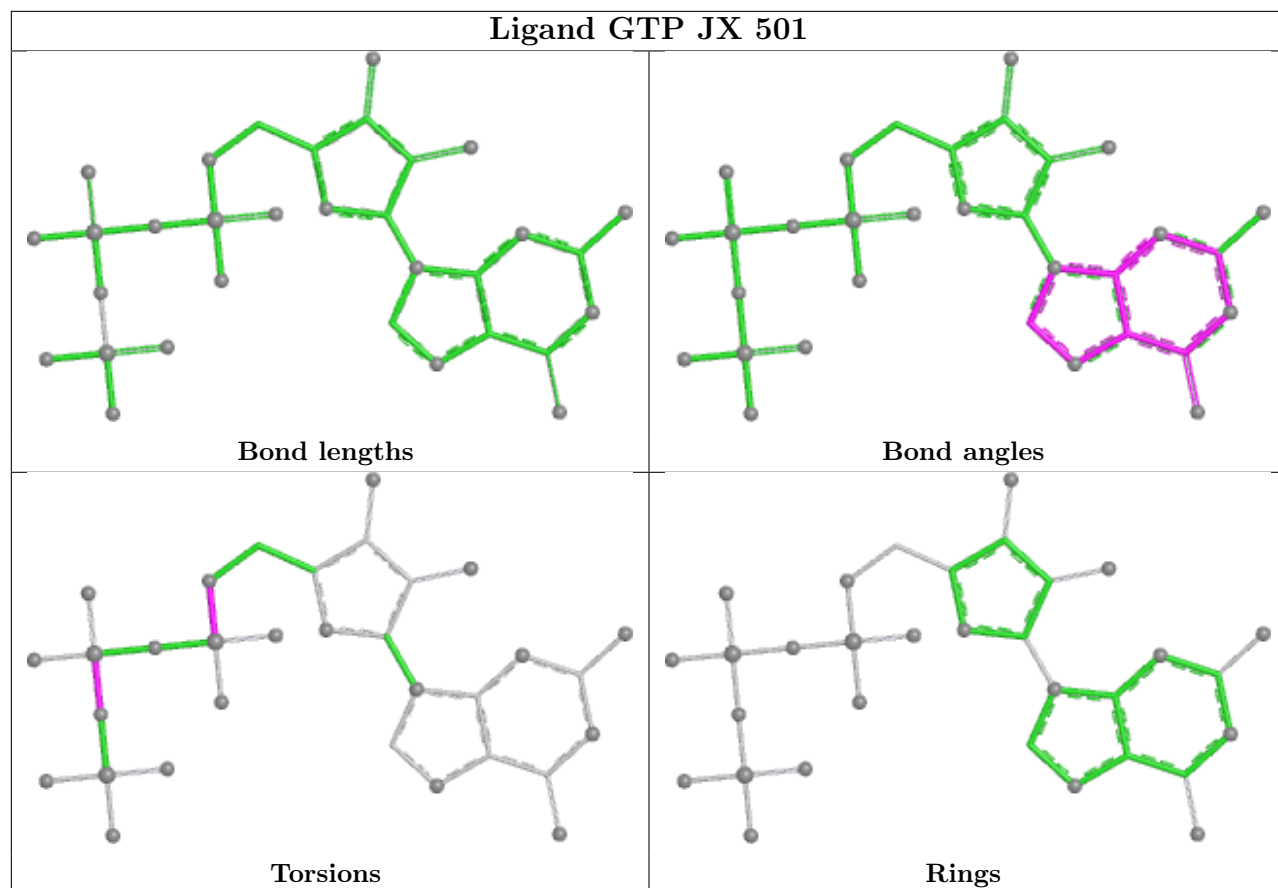
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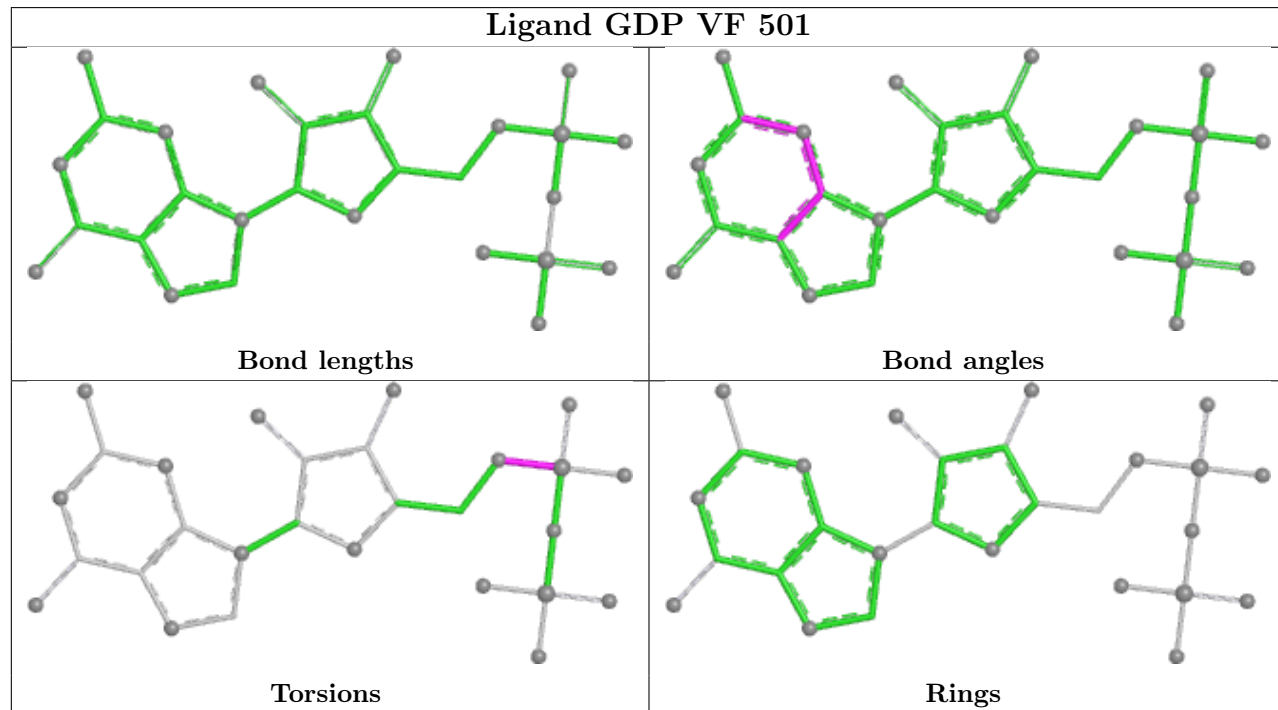
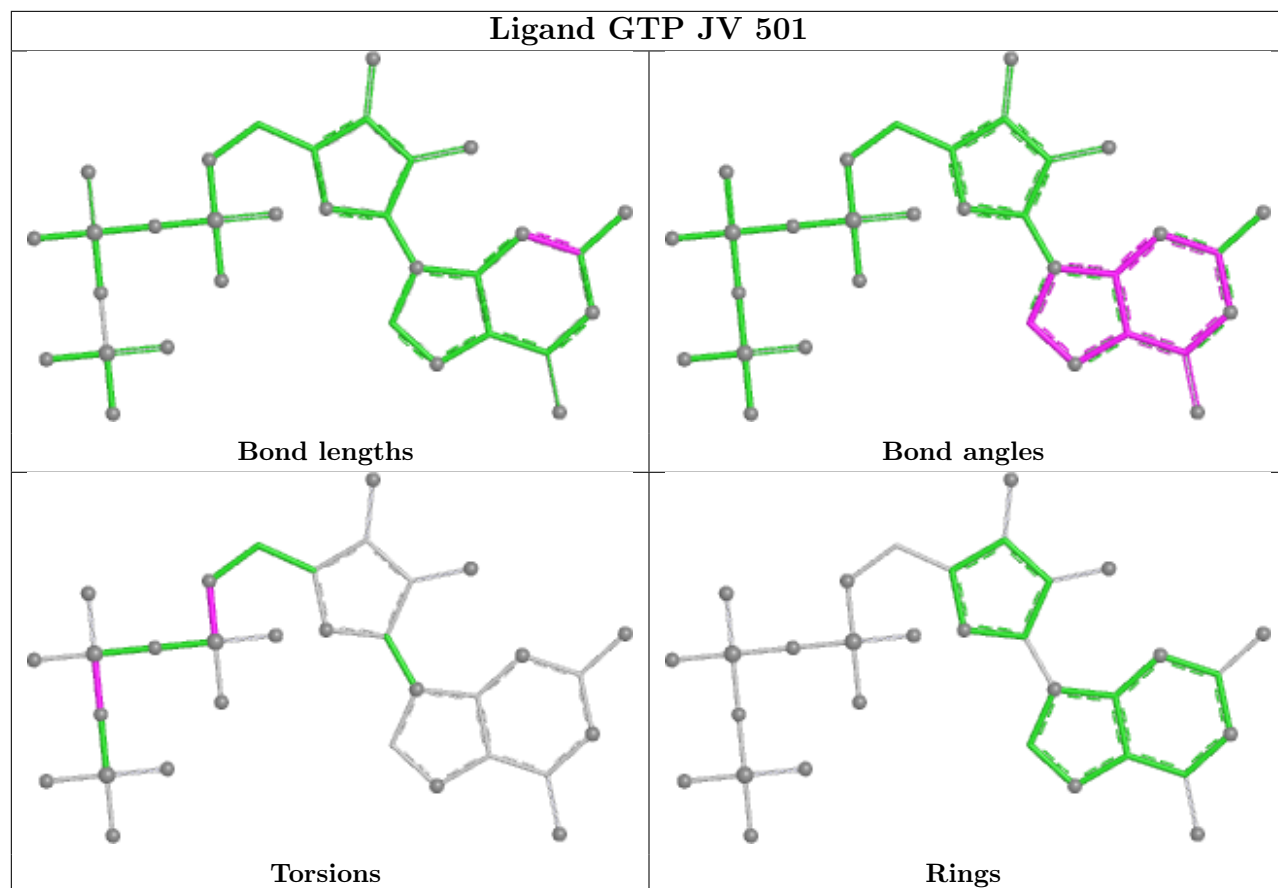


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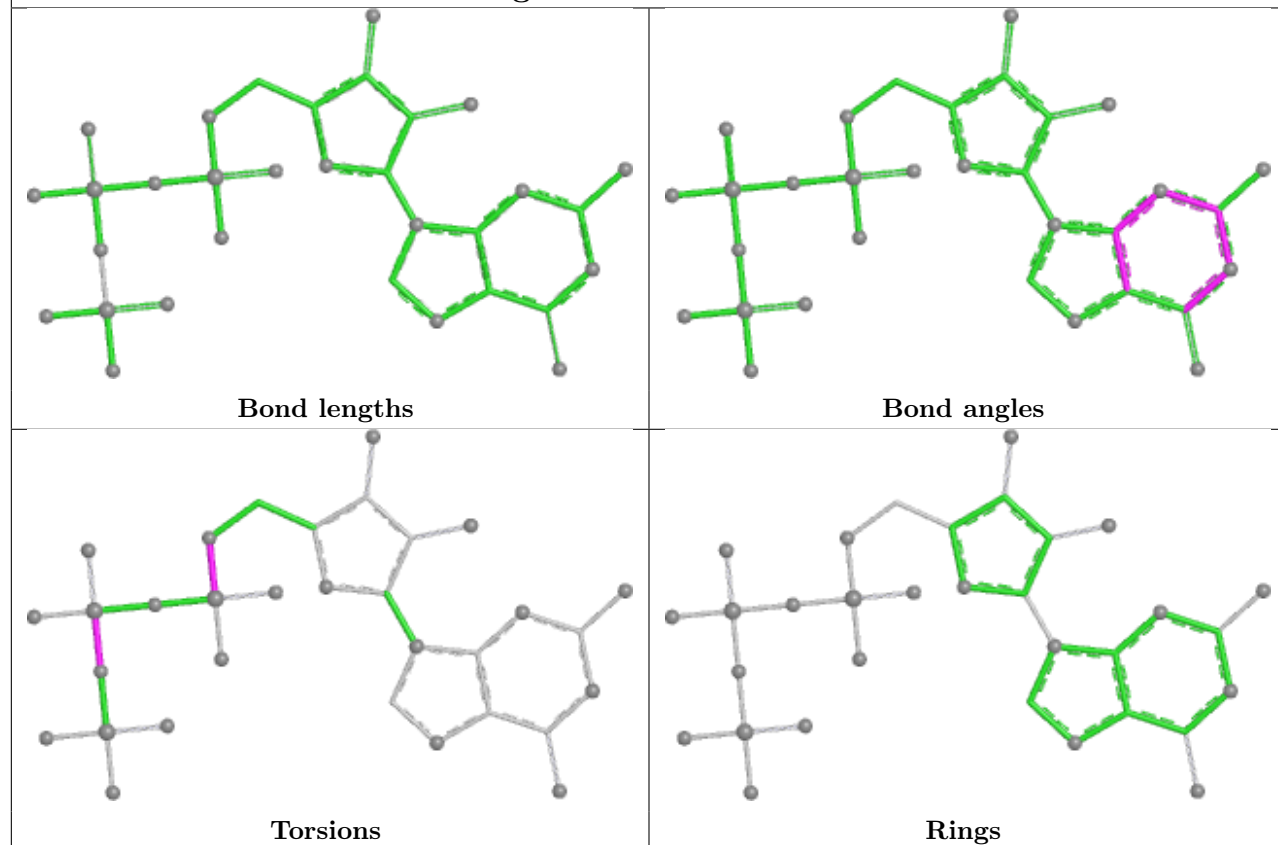




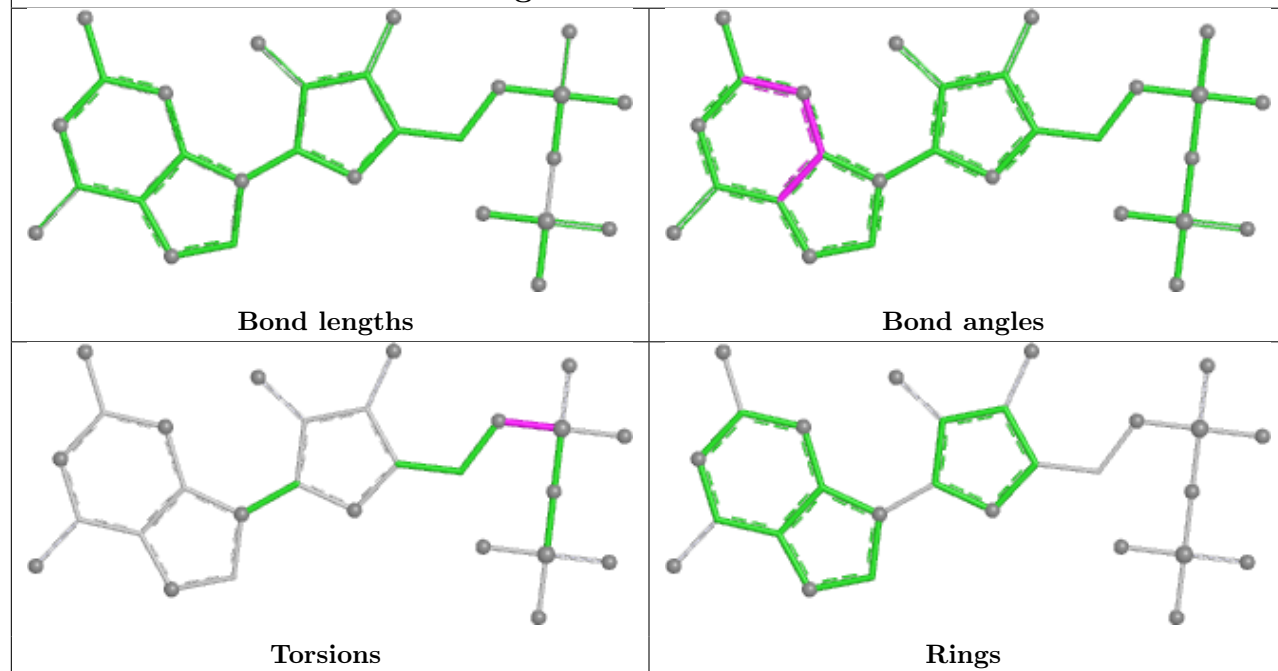




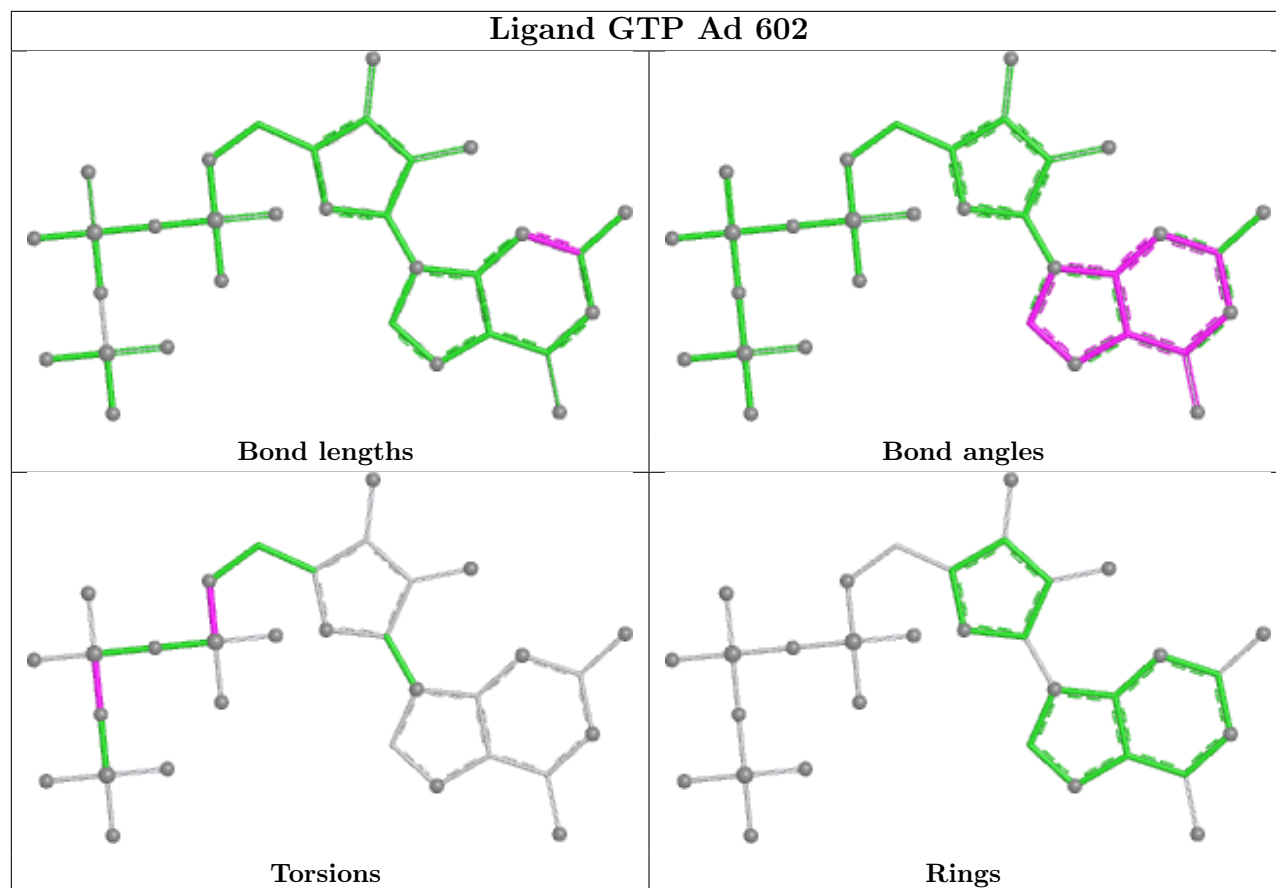
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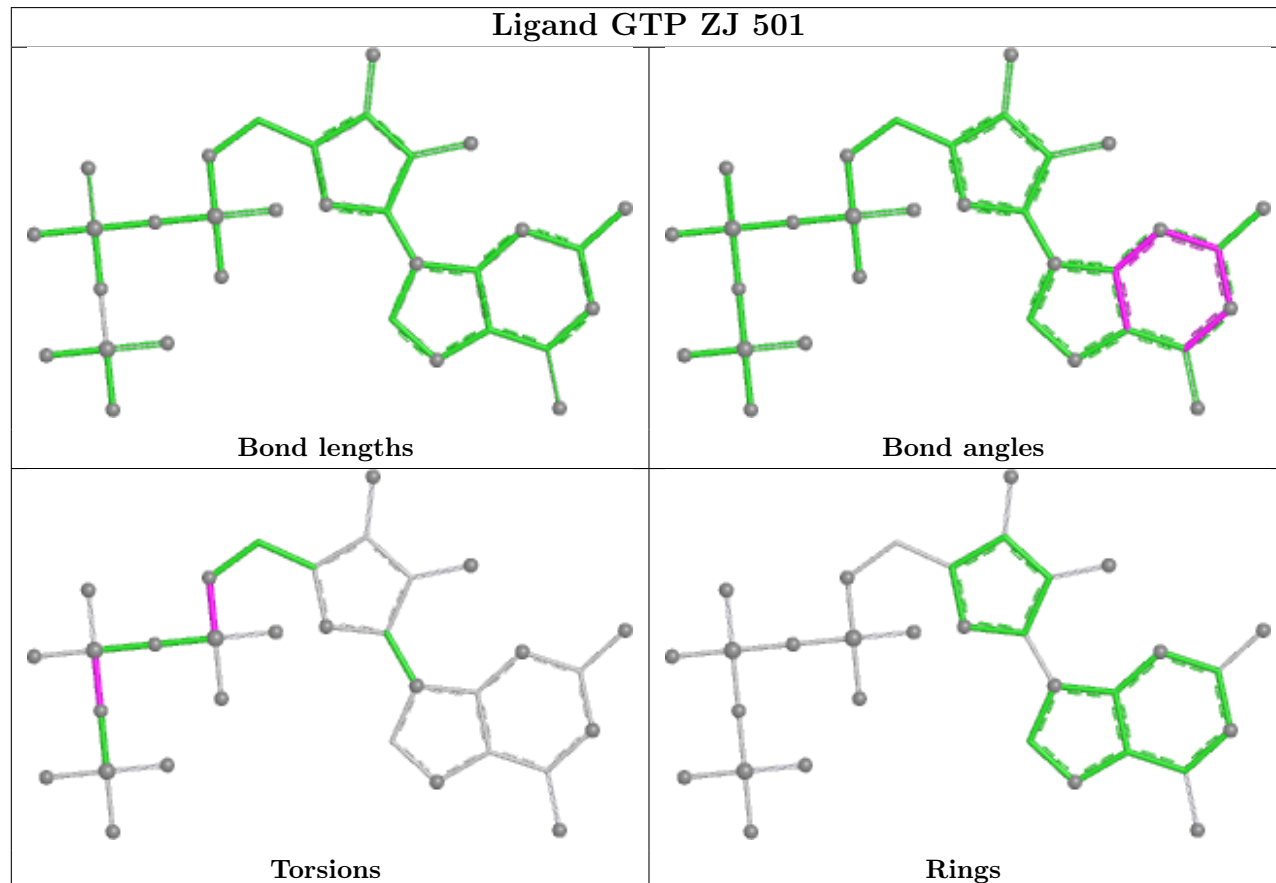
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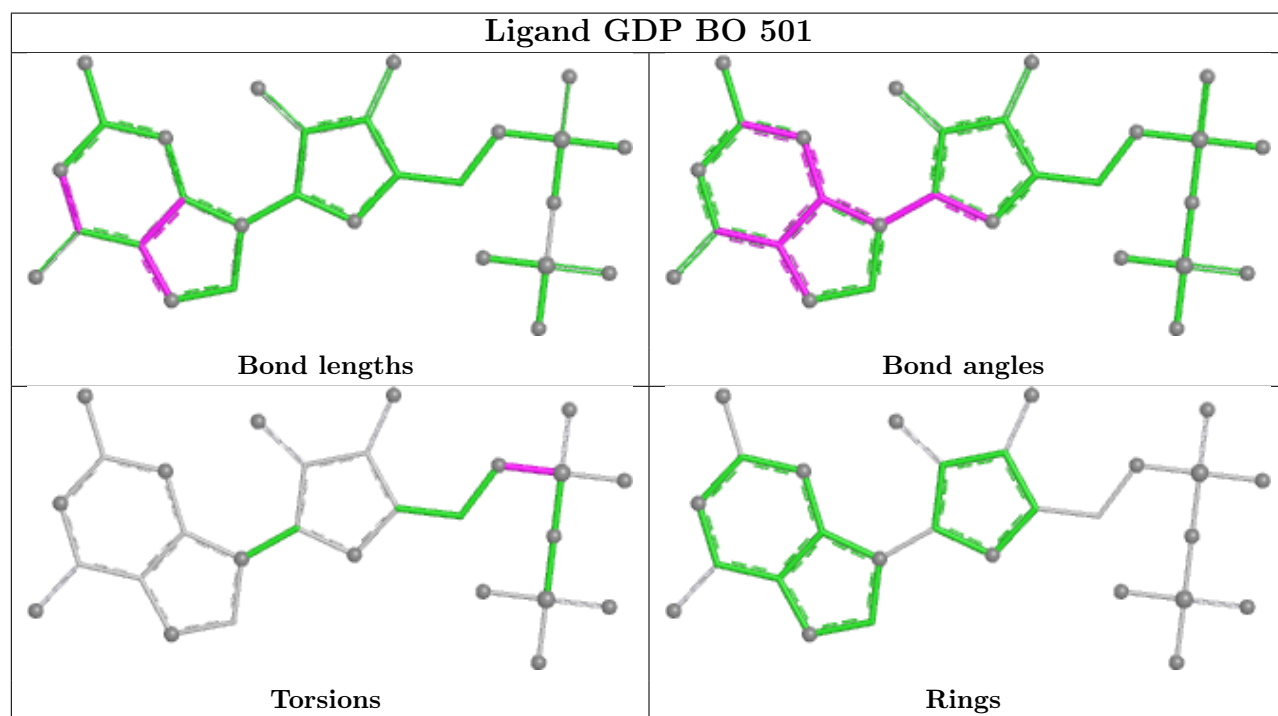
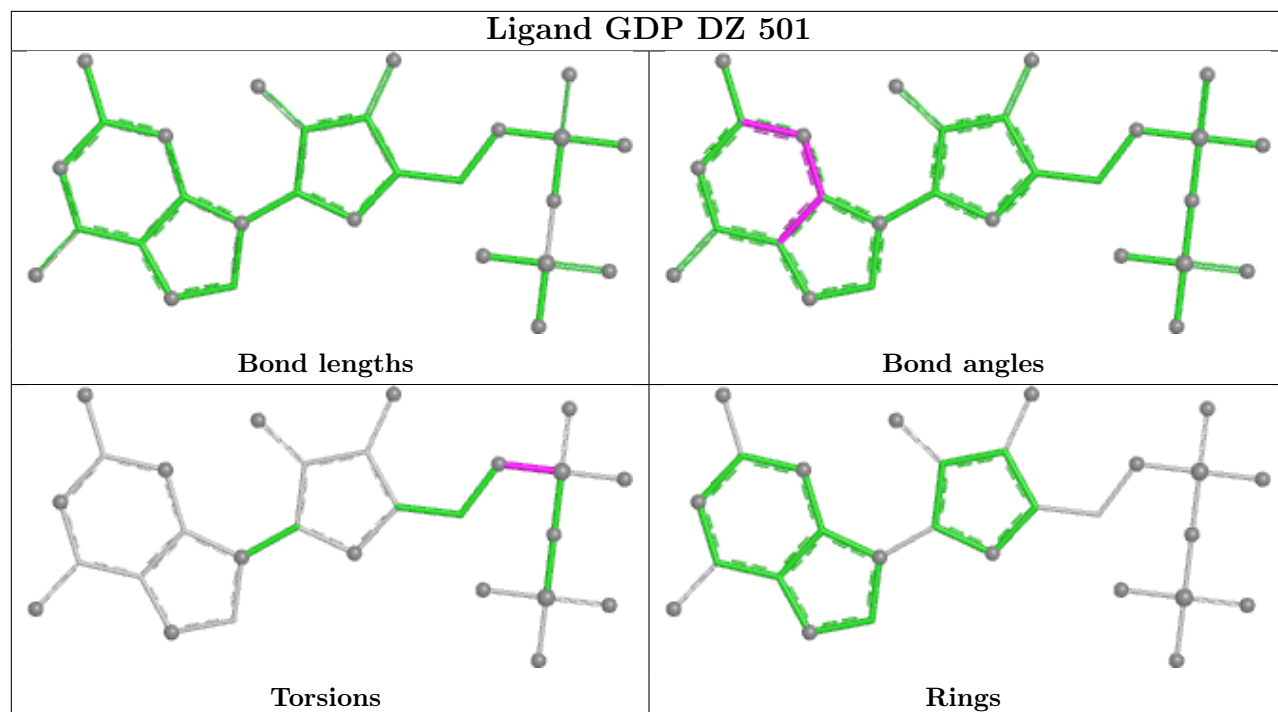


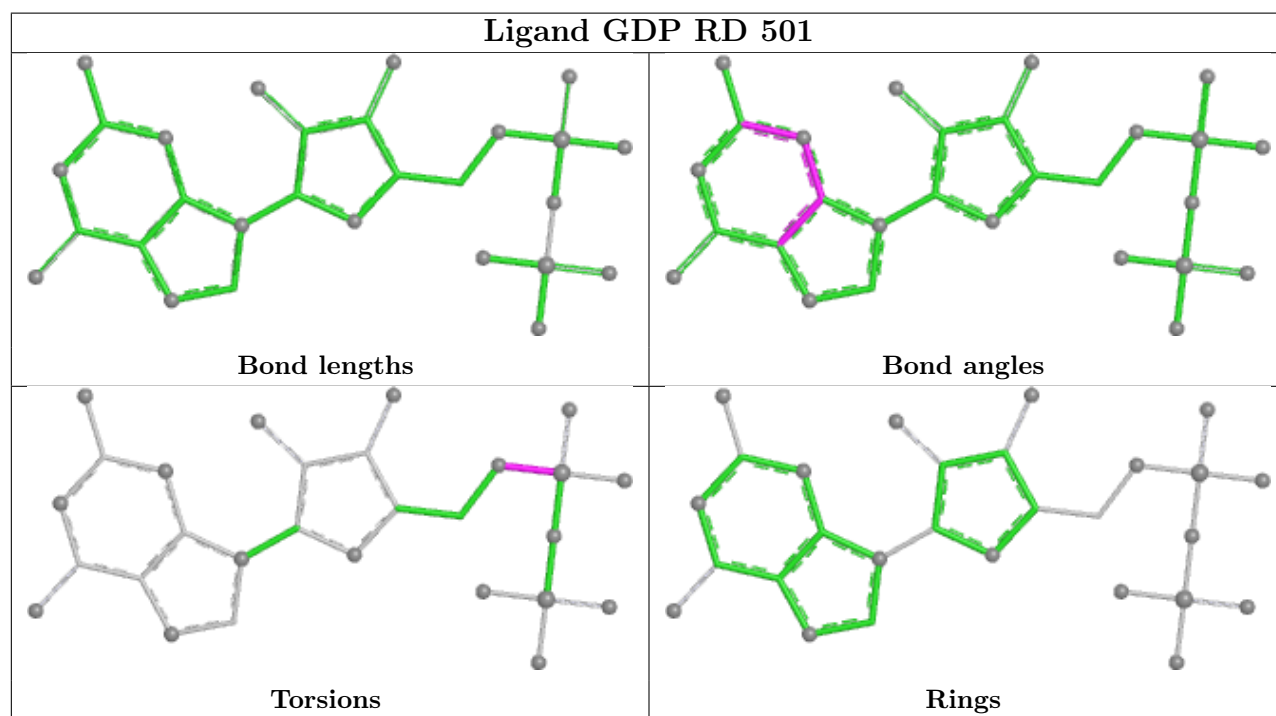
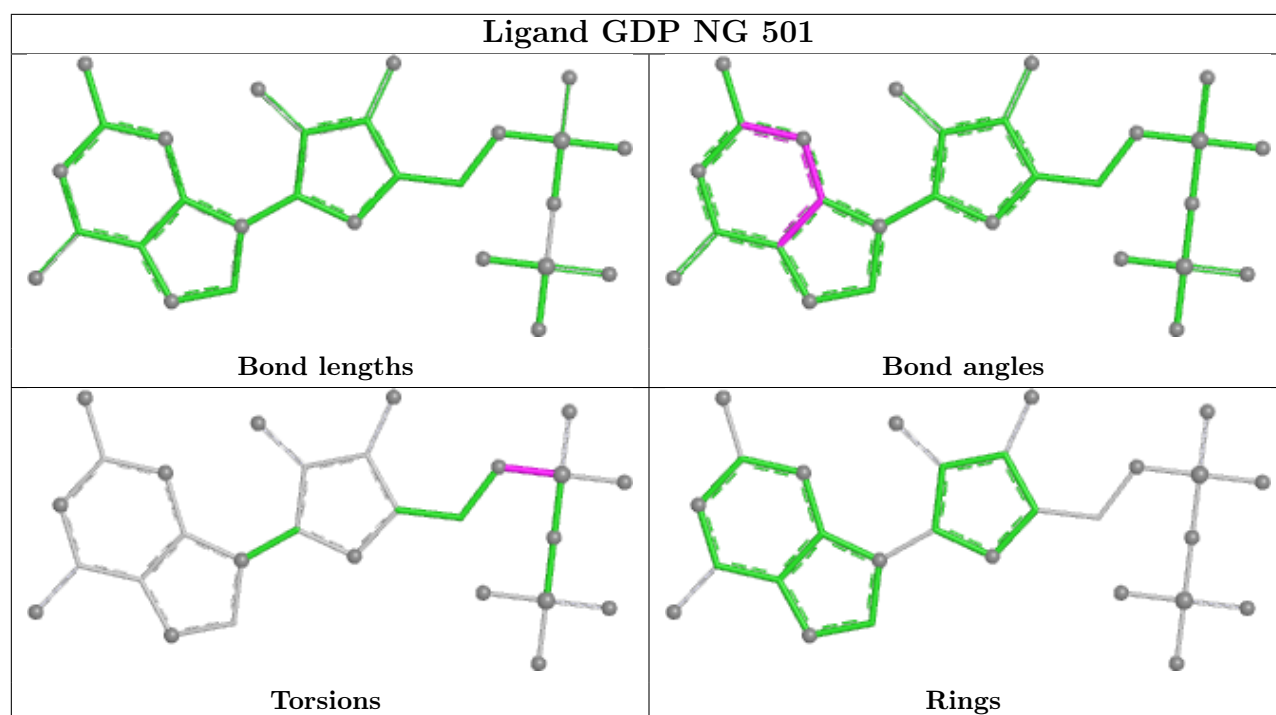
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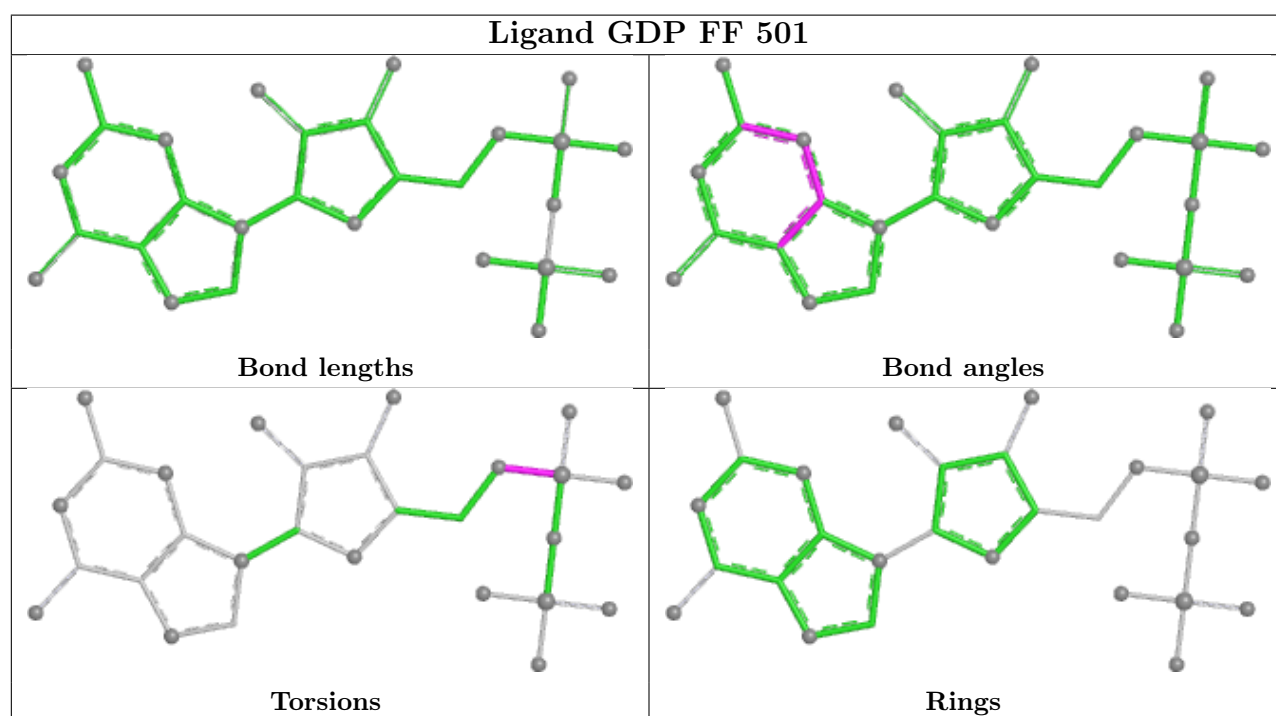
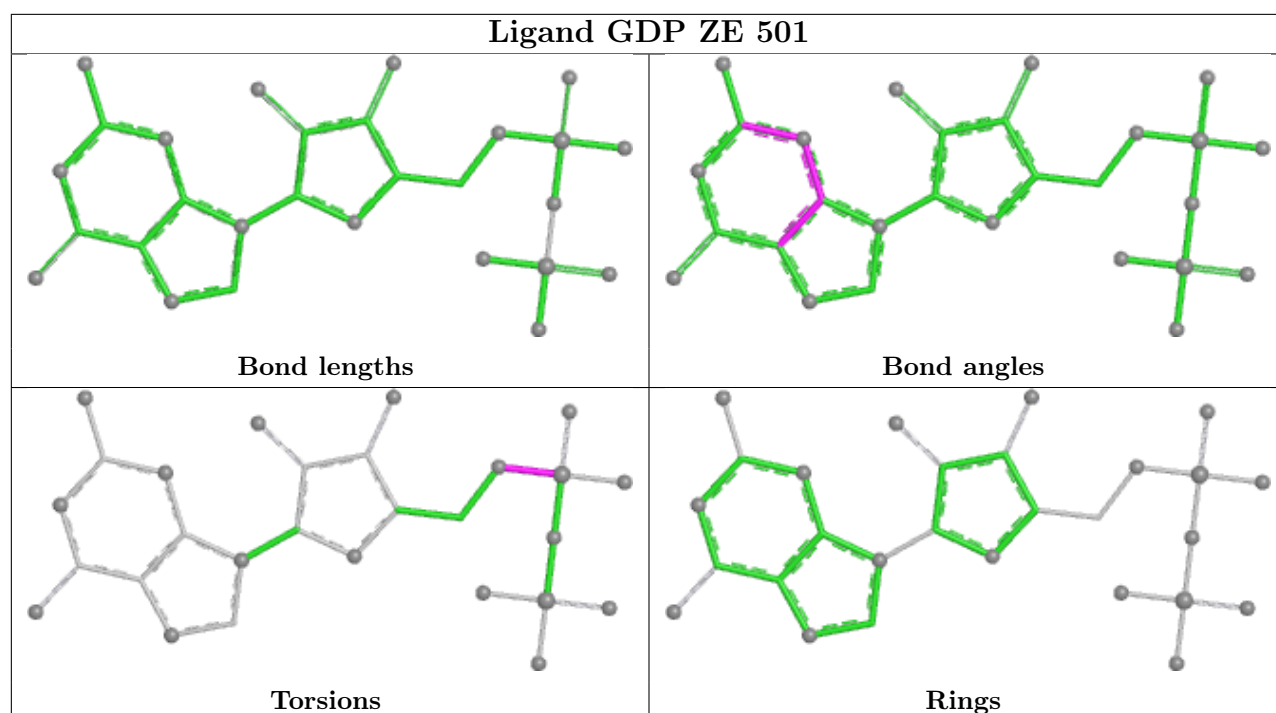


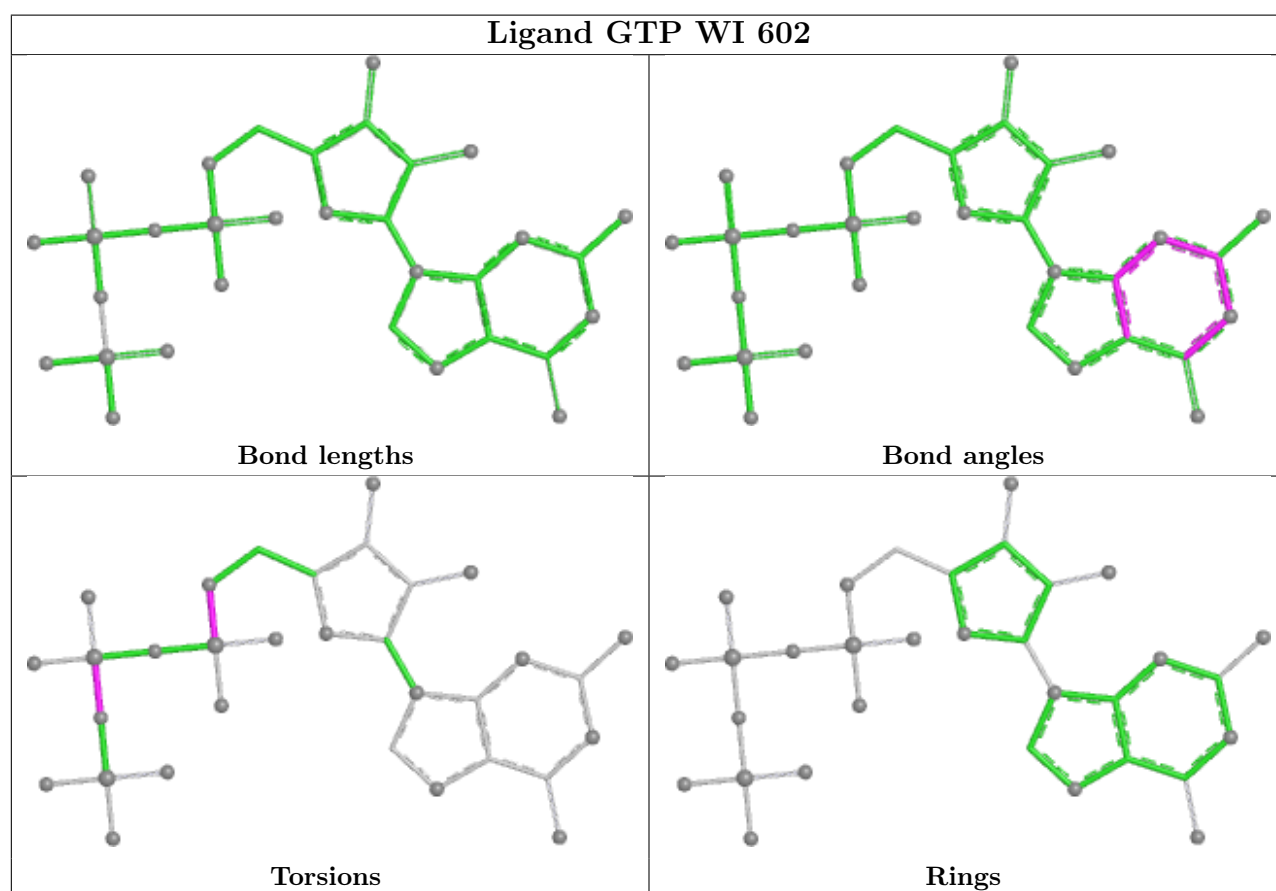
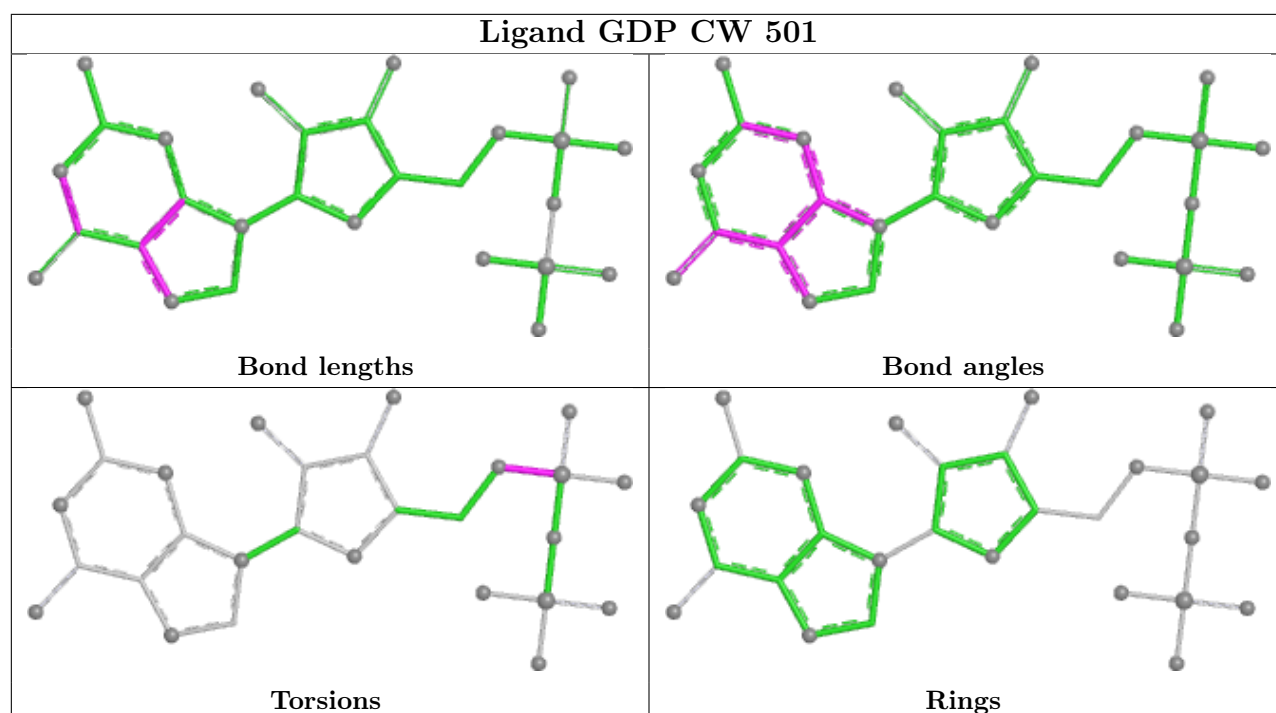
## Ligand GTP ZJ 501



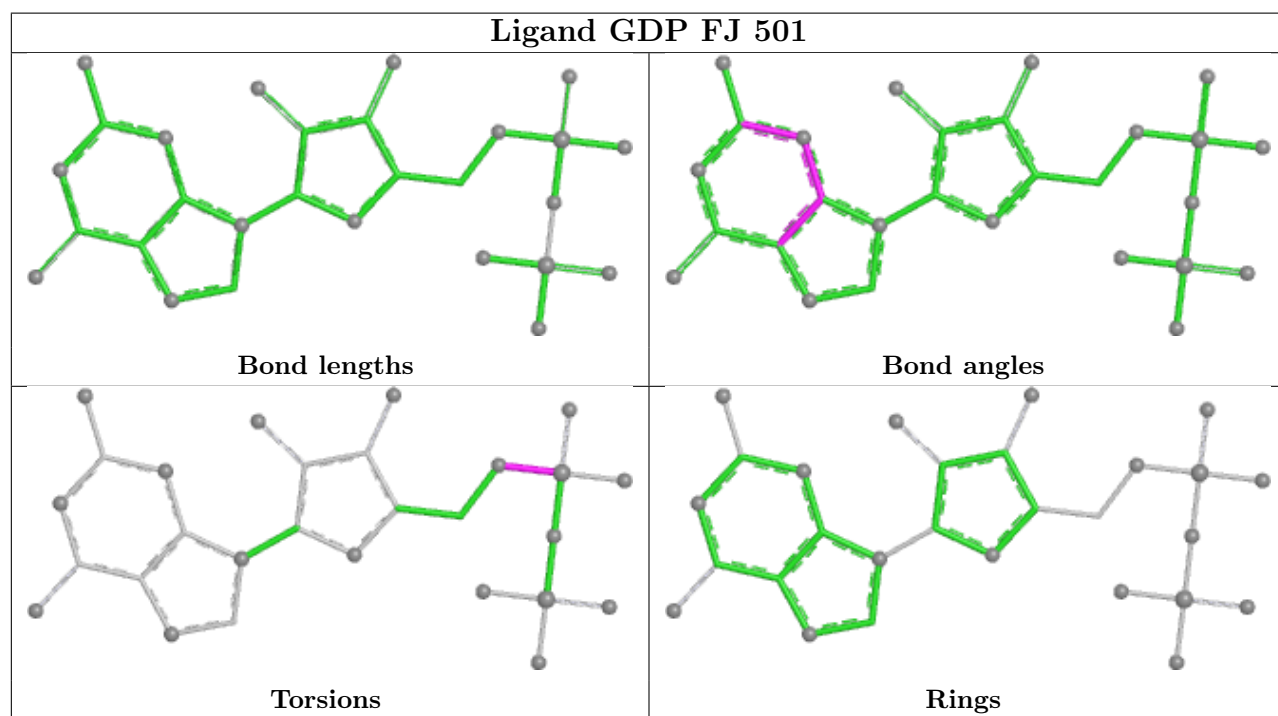
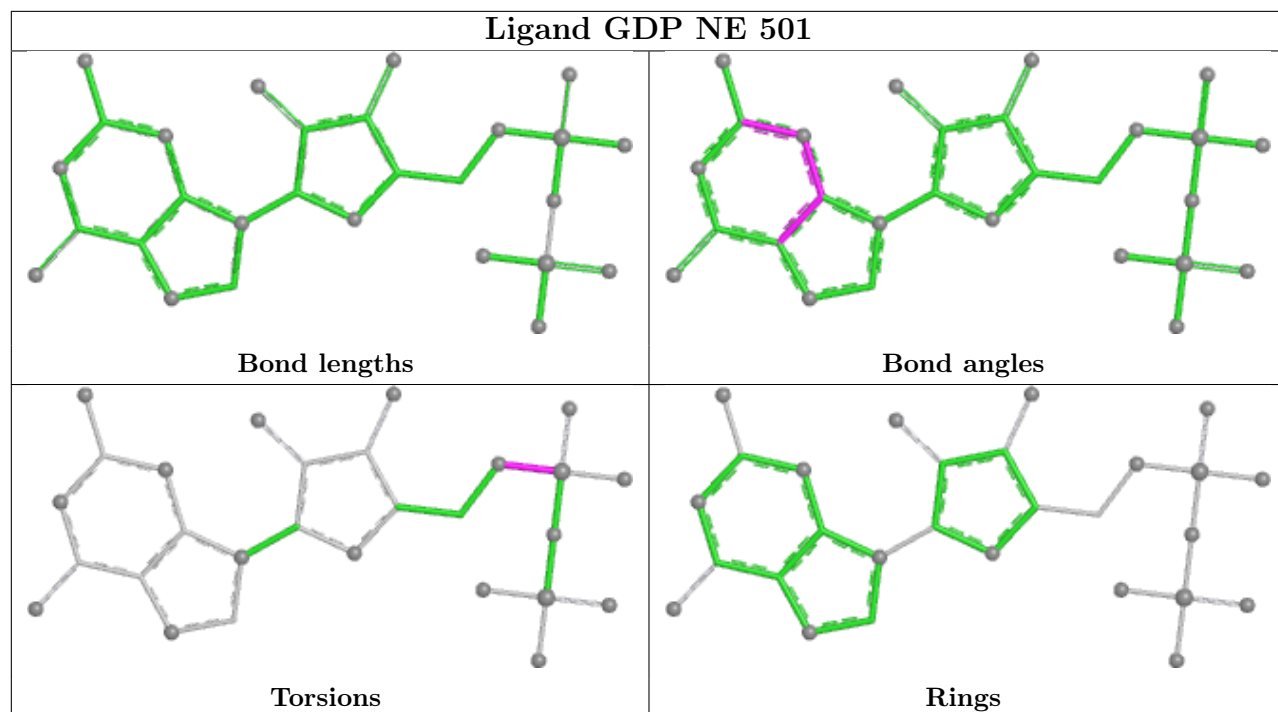


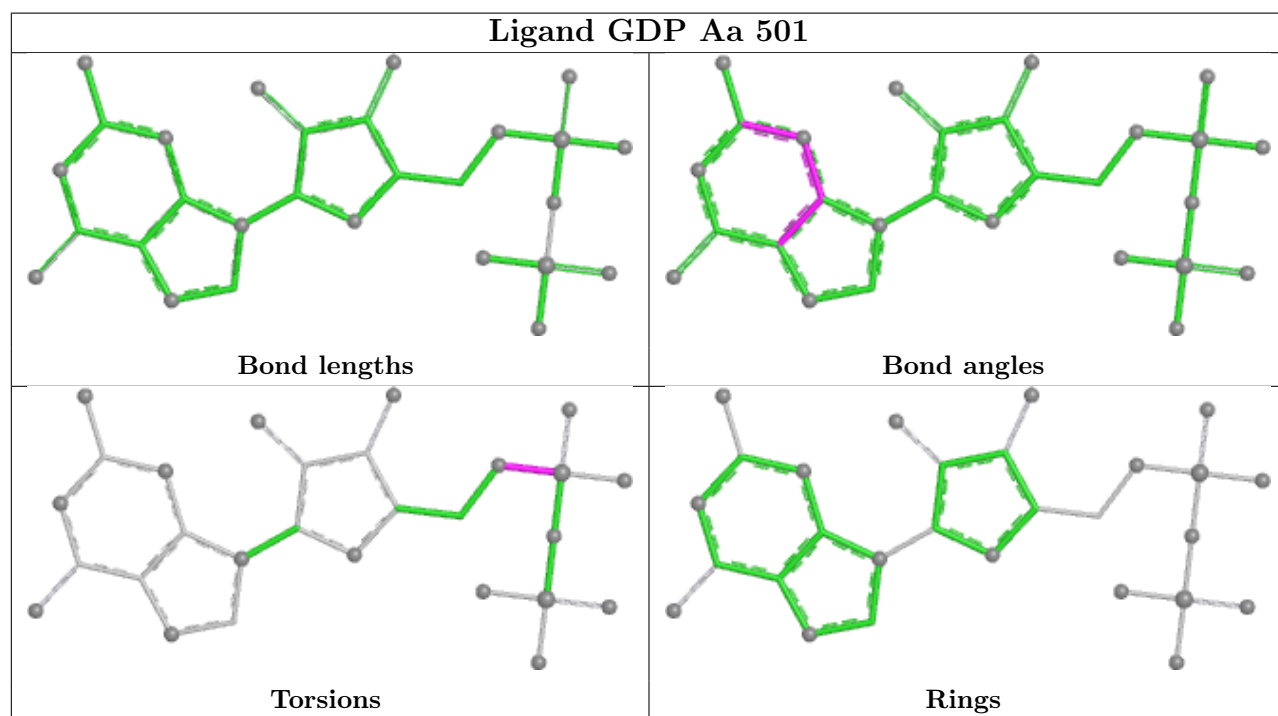
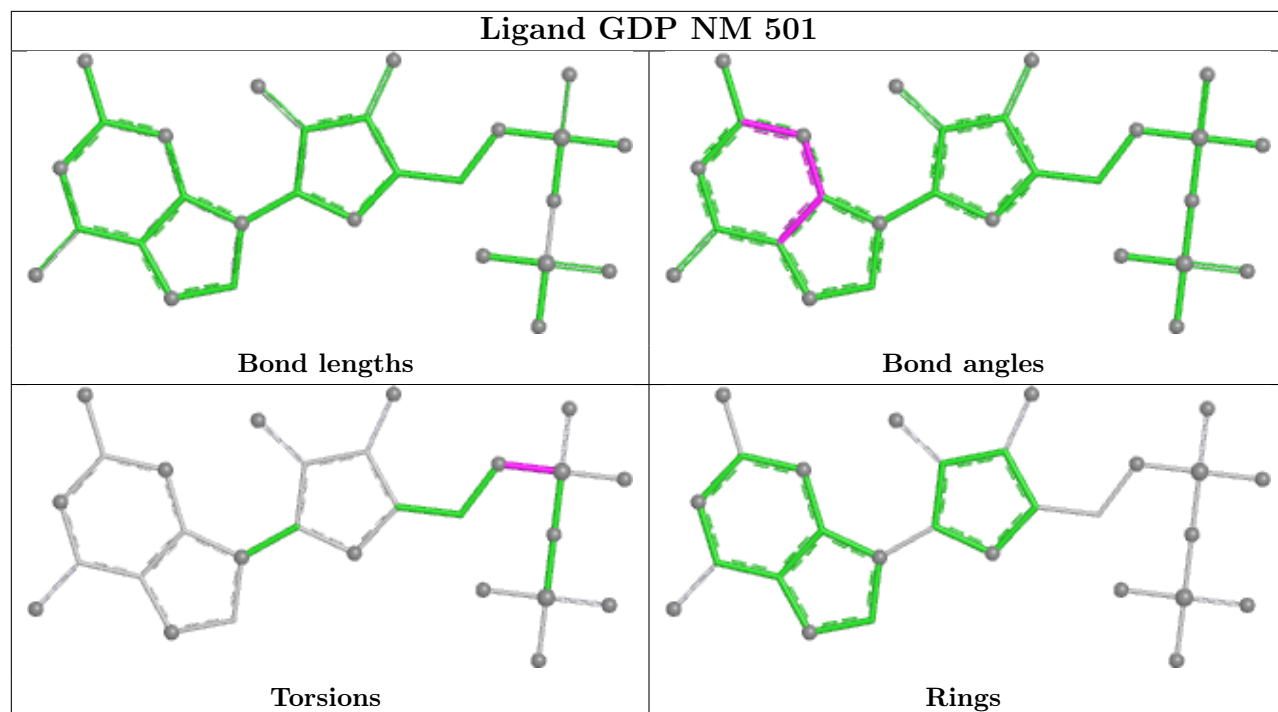




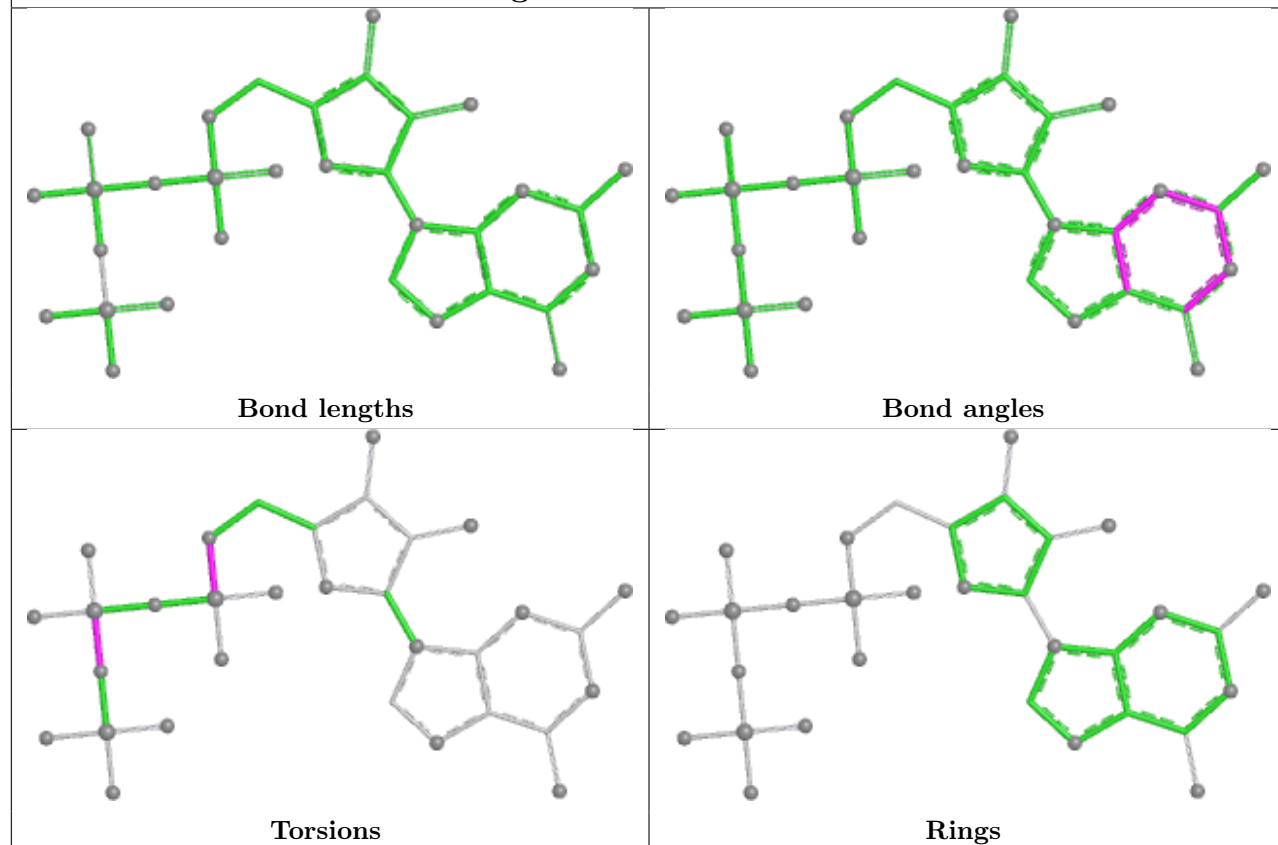




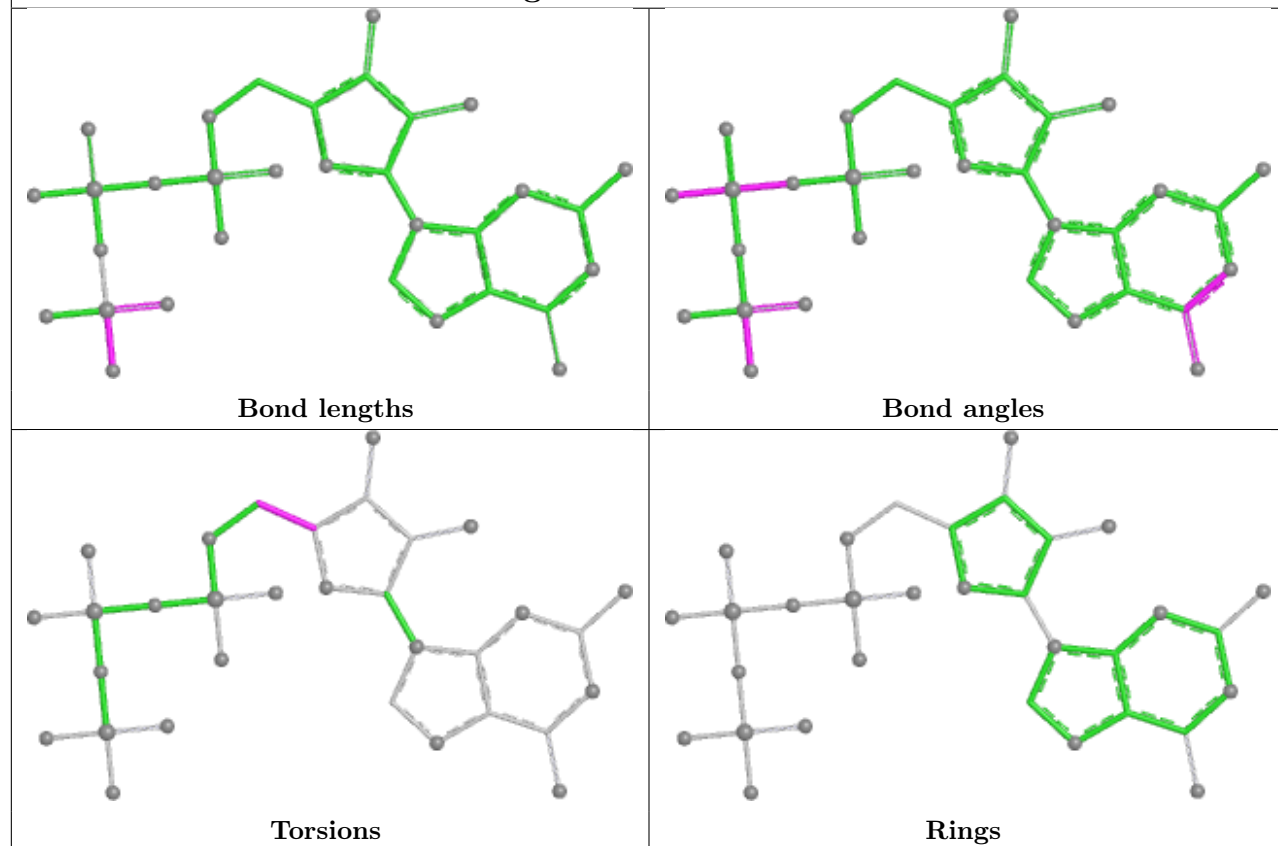


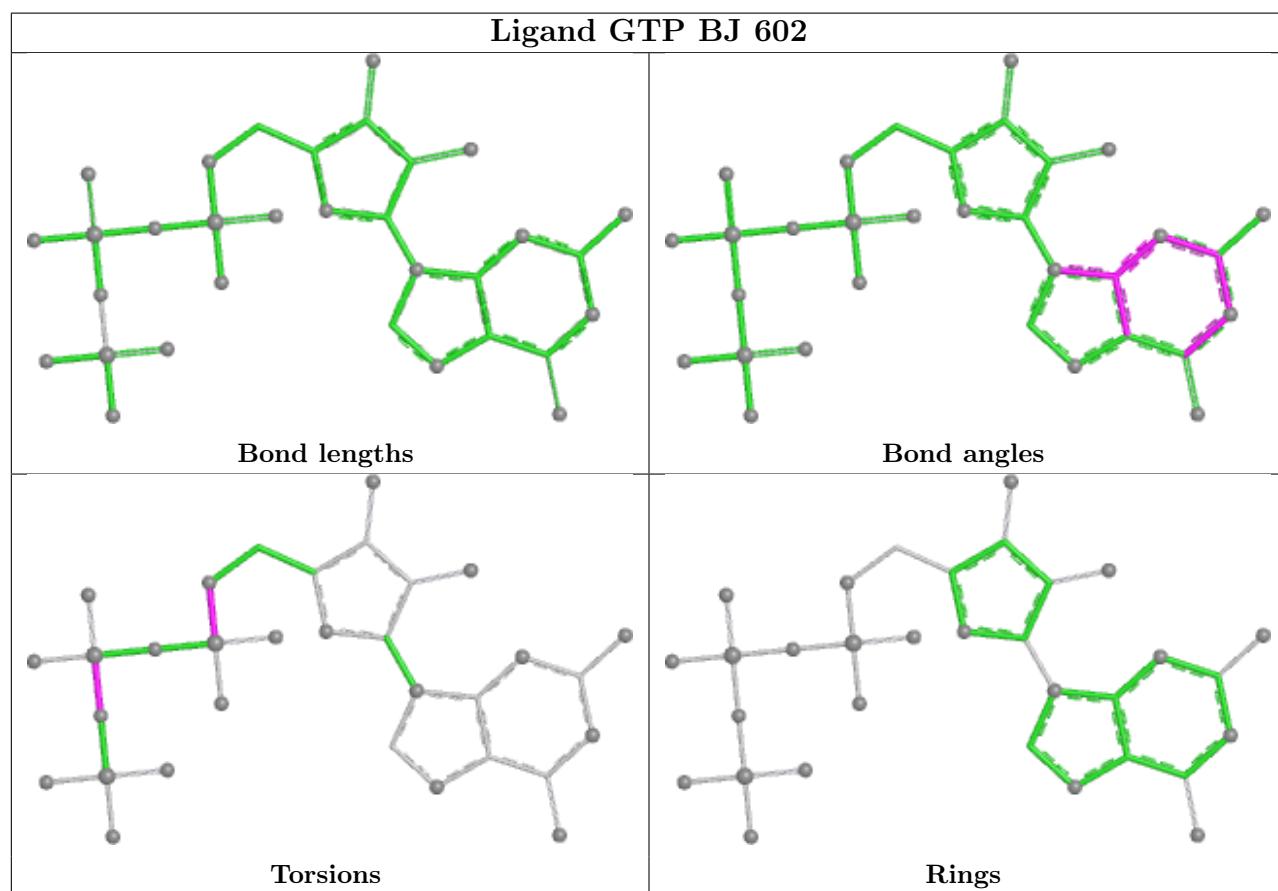
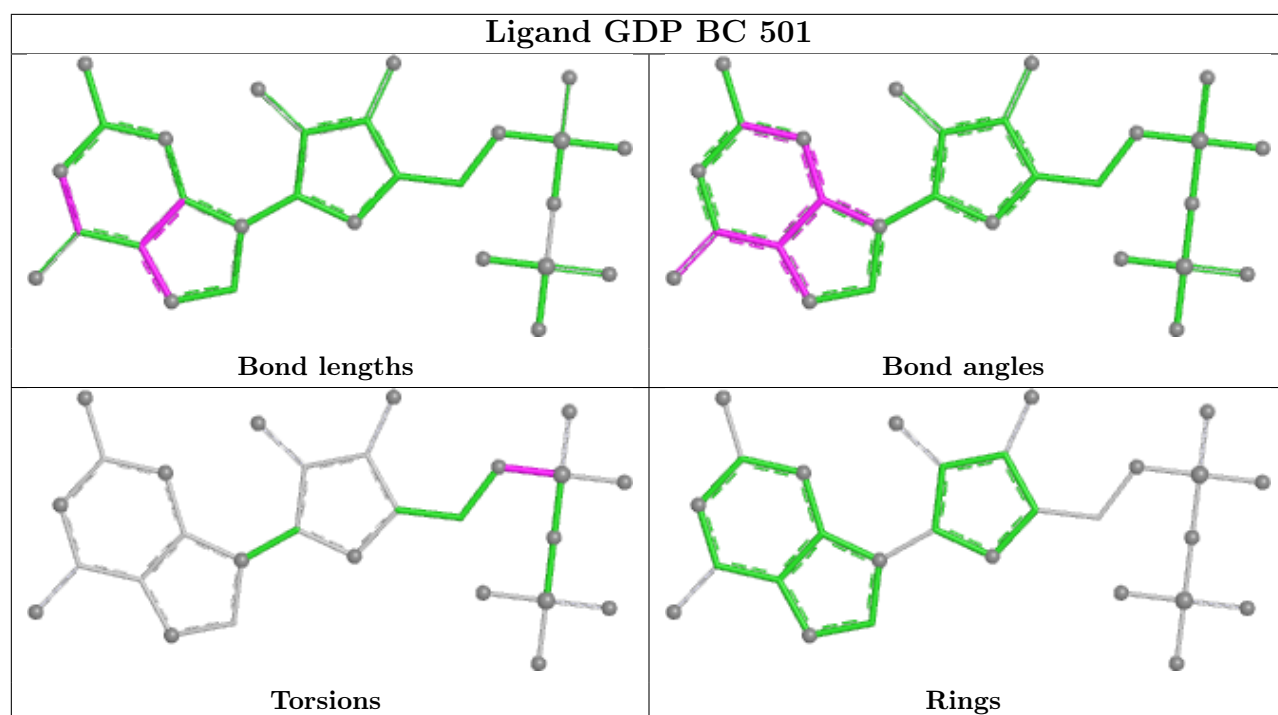


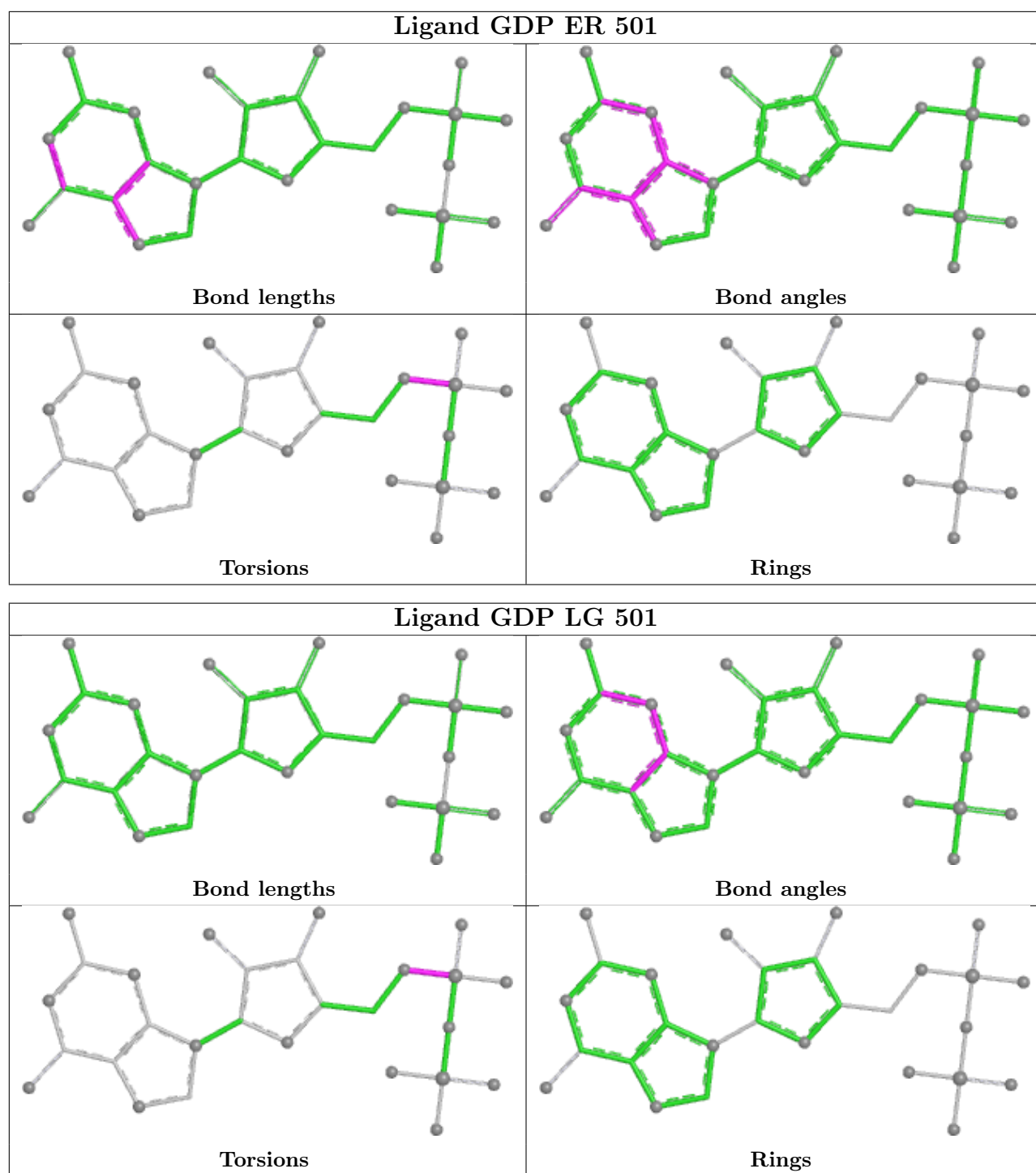
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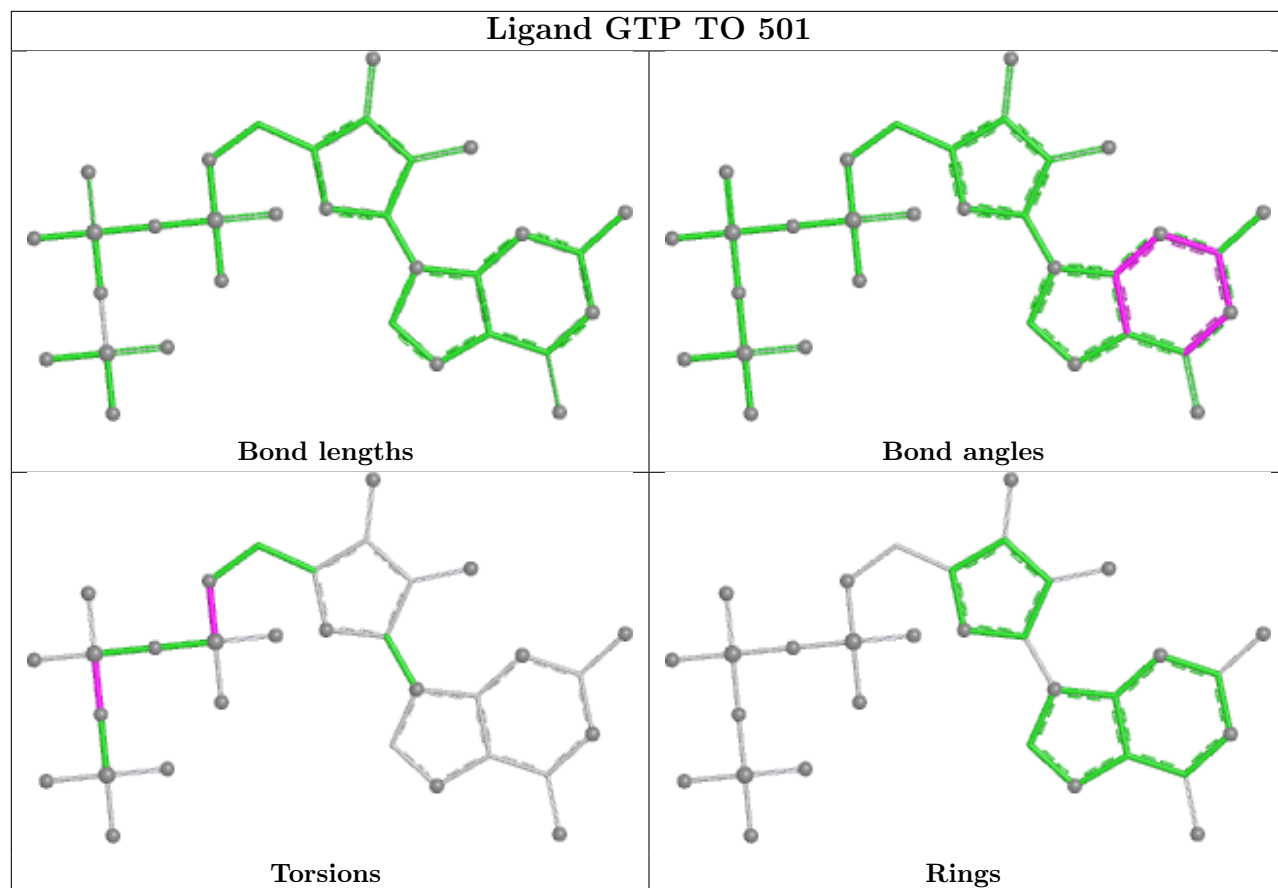
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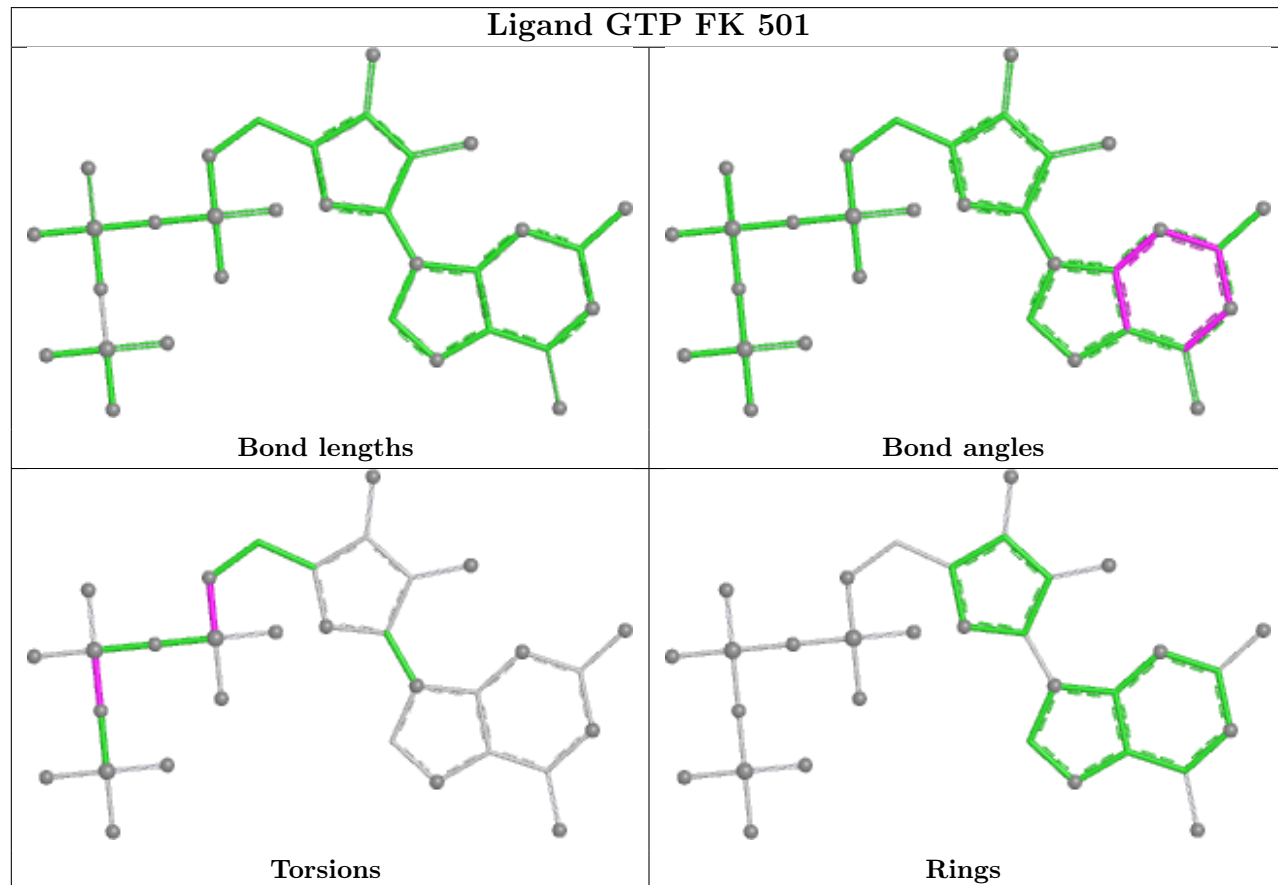


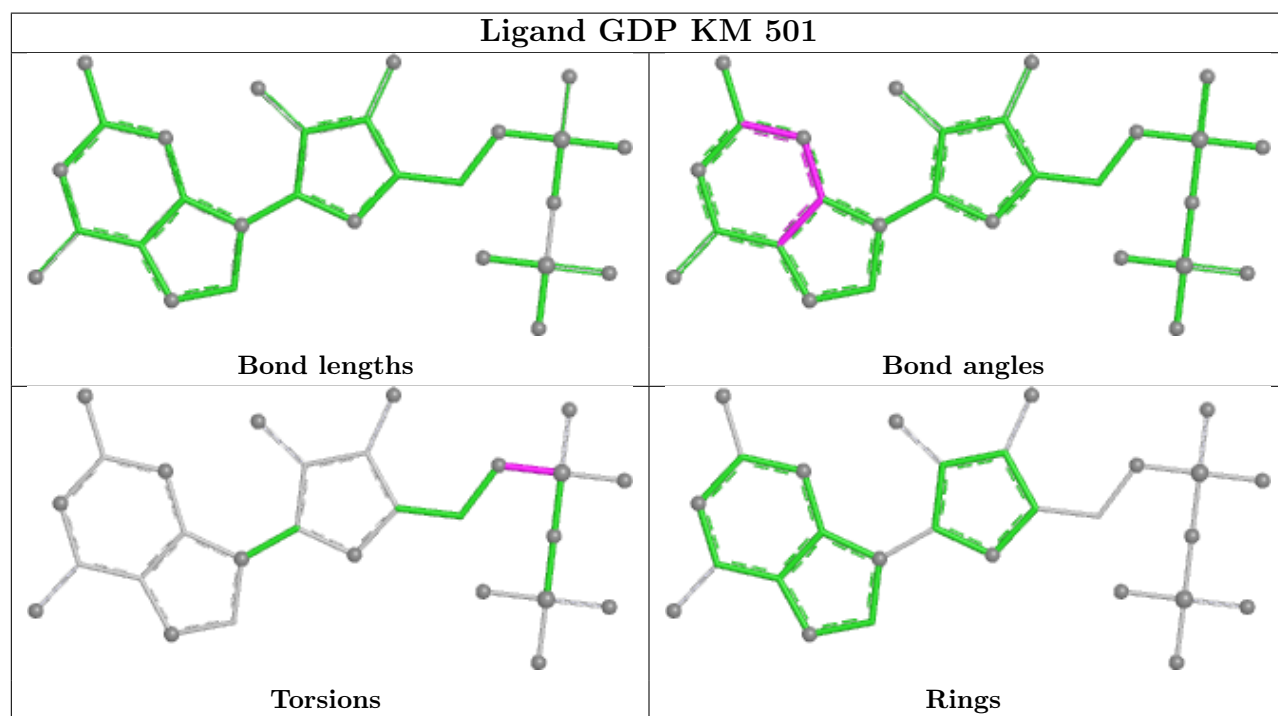
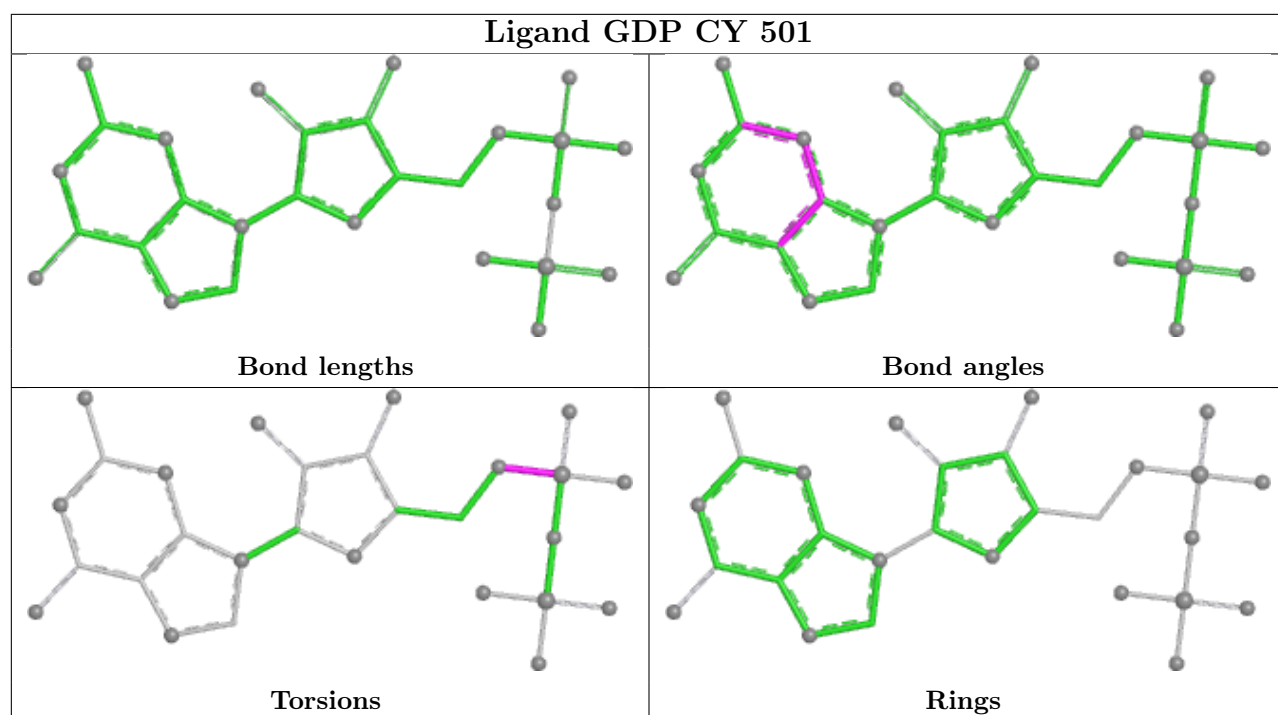


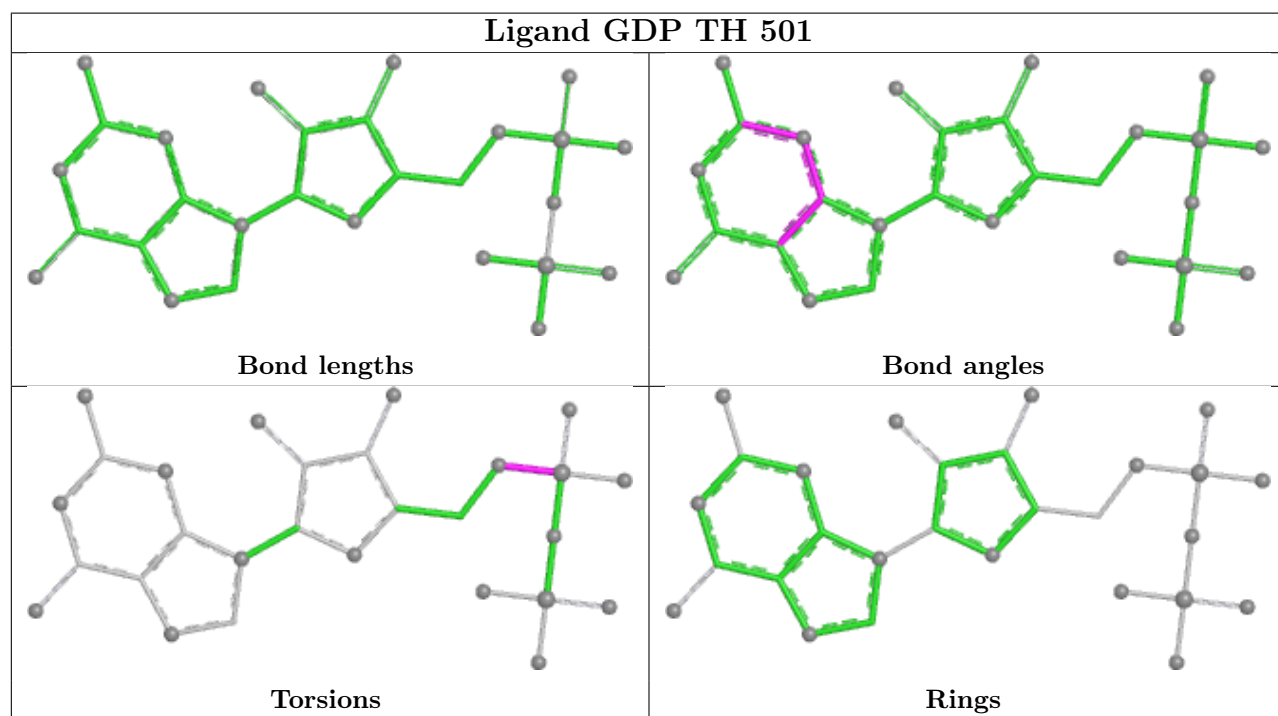
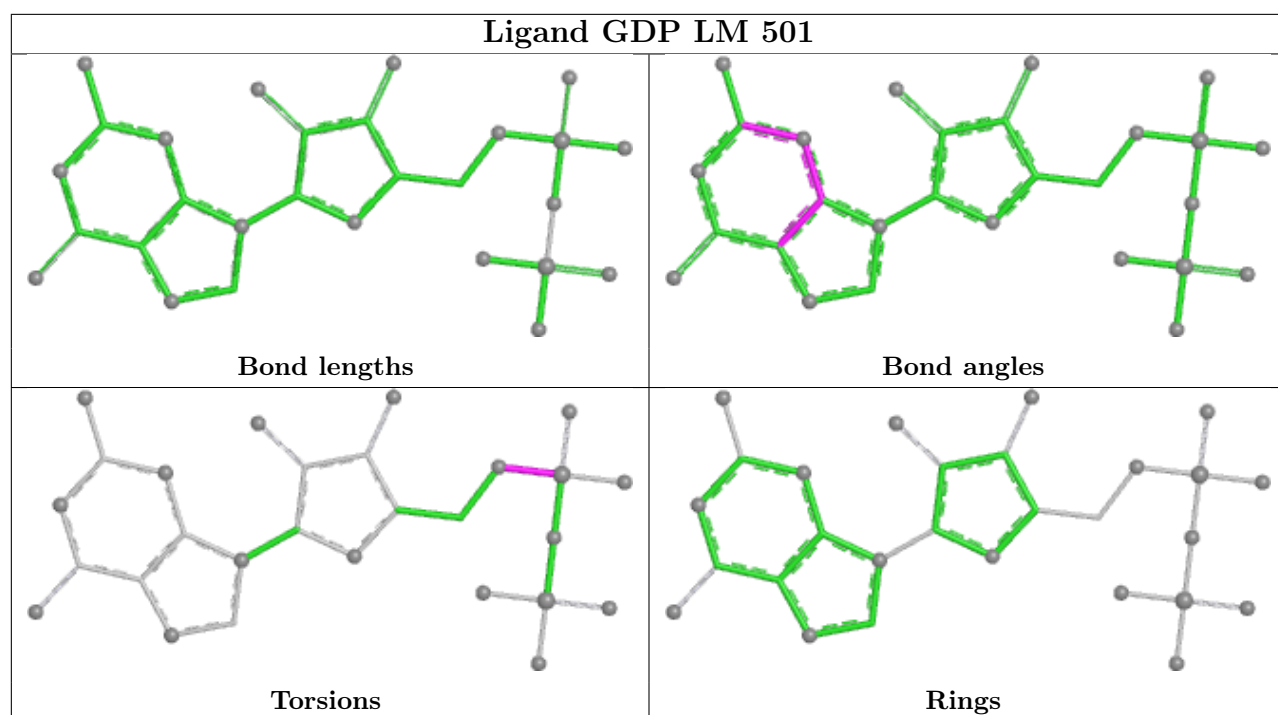
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## Ligand GTP FK 501

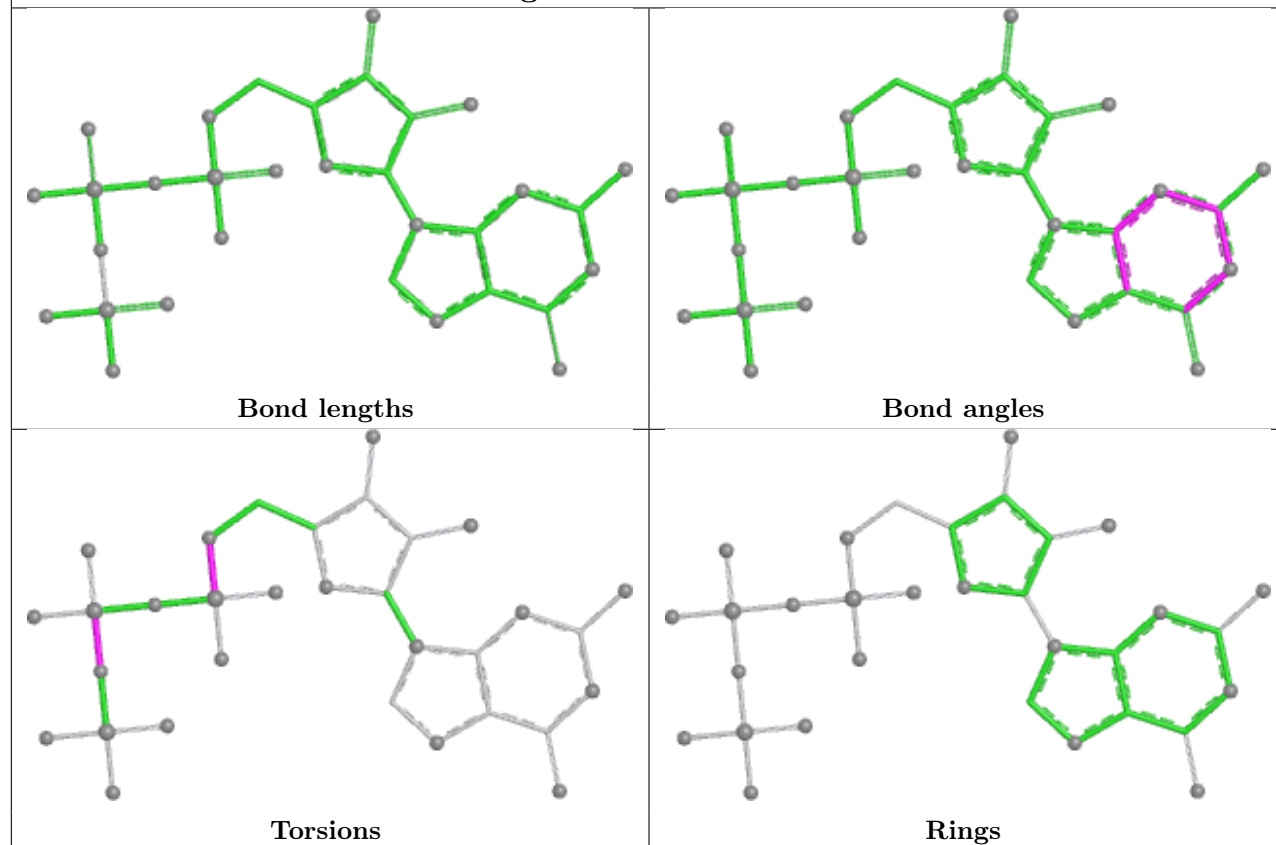




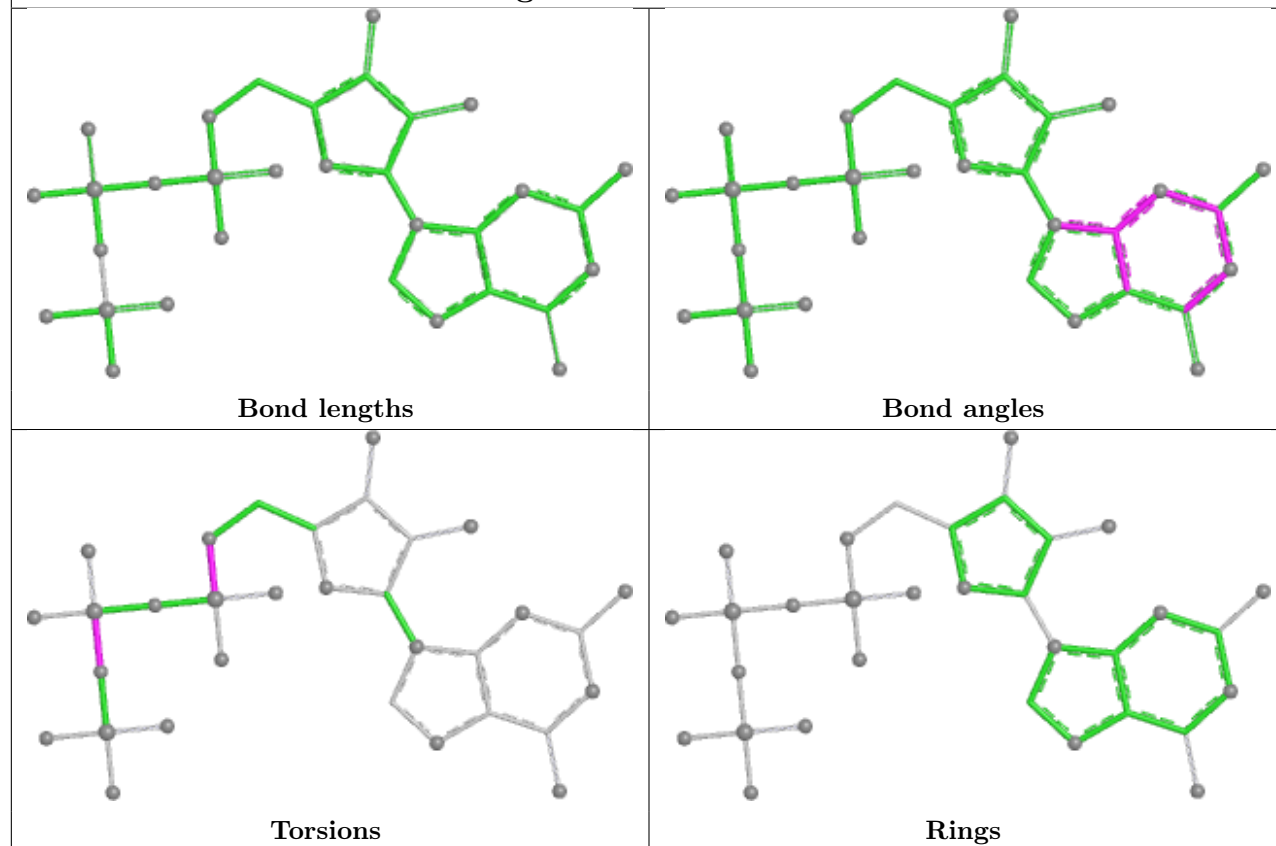




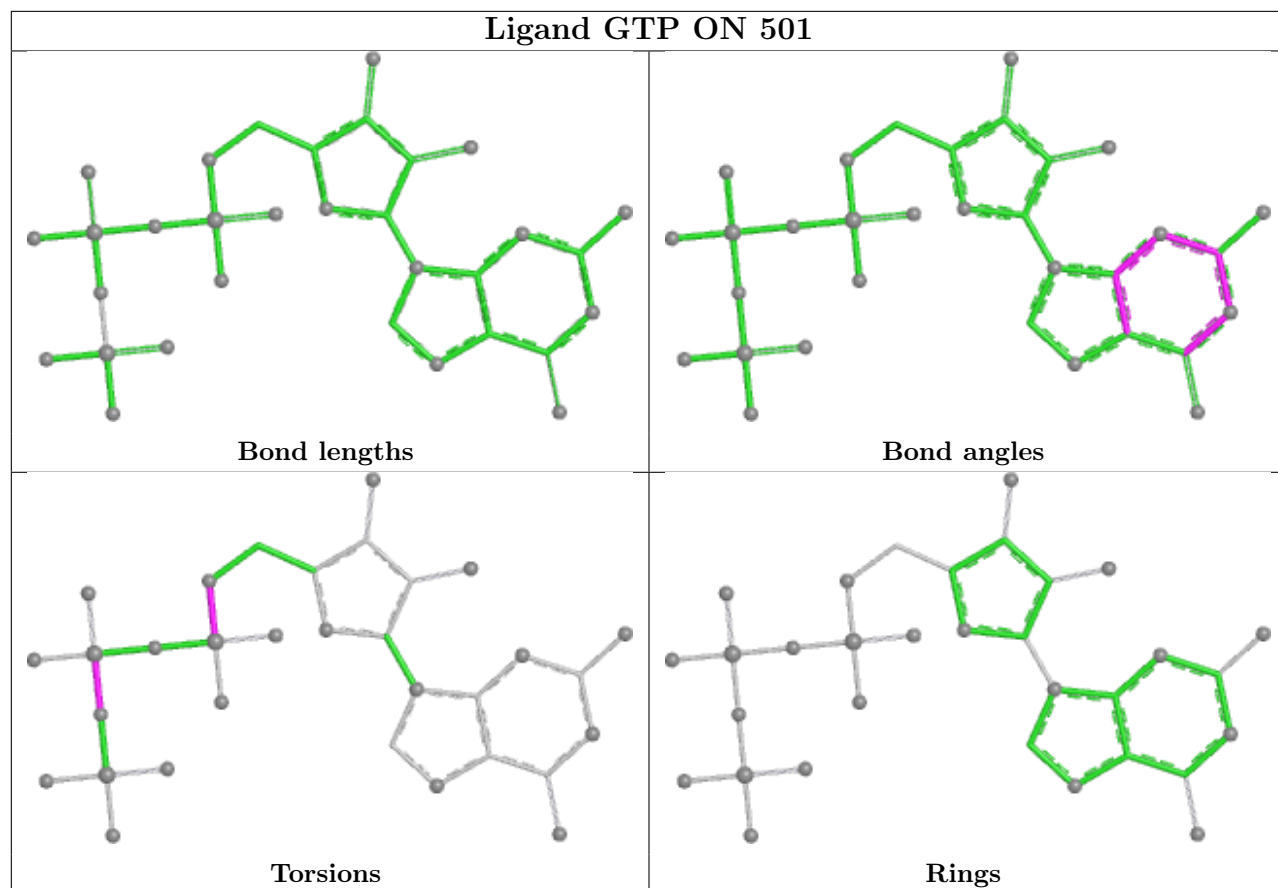
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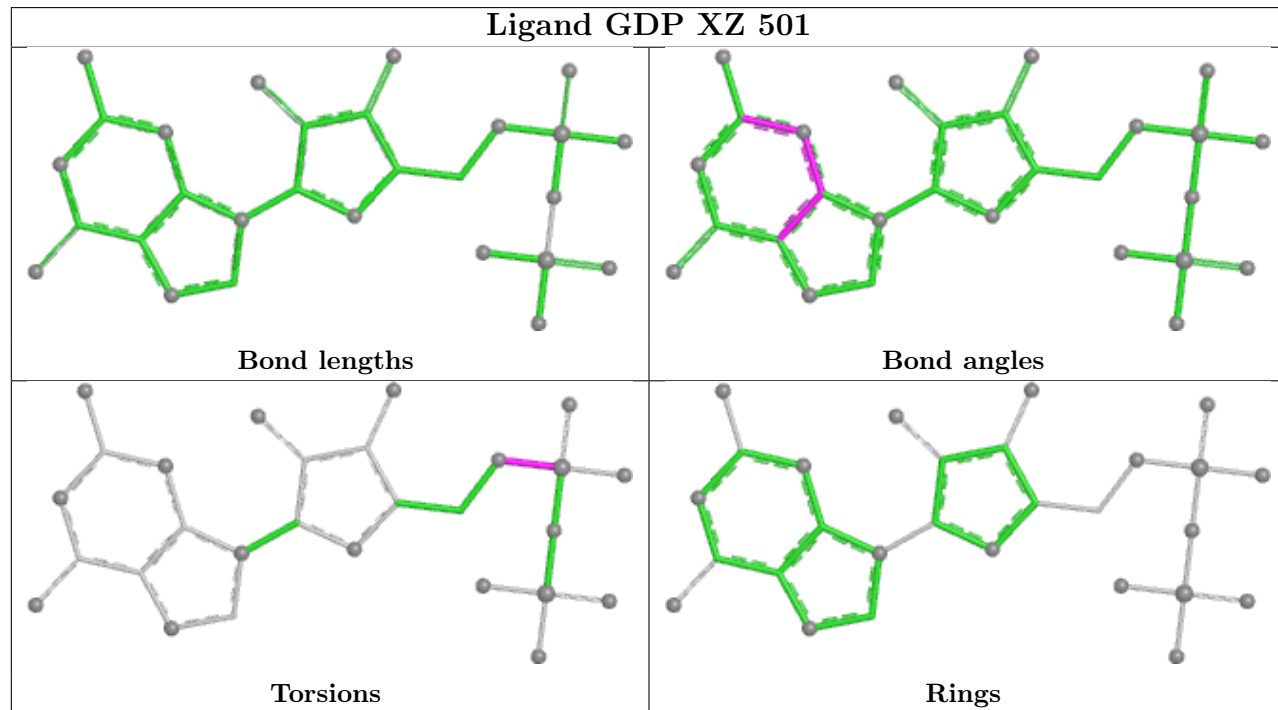
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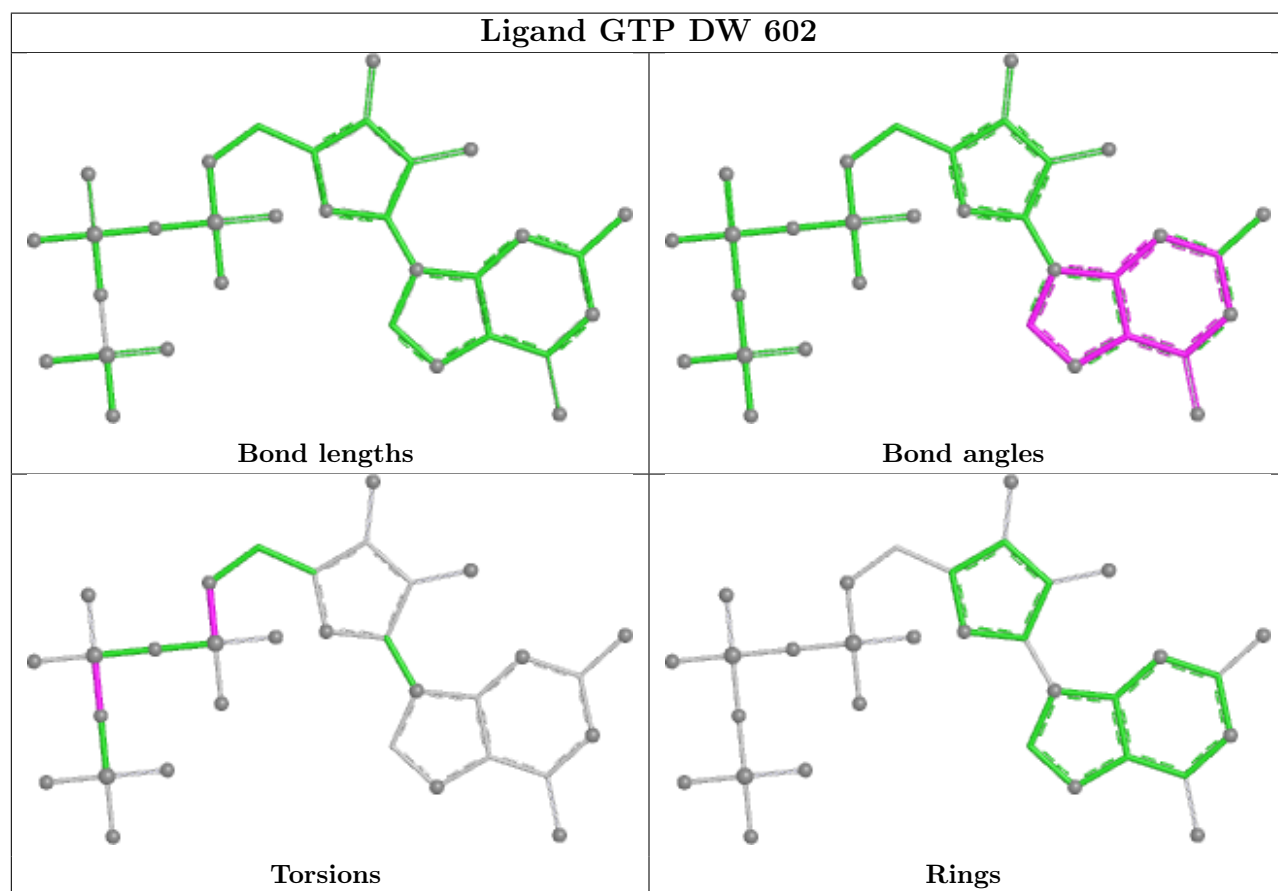
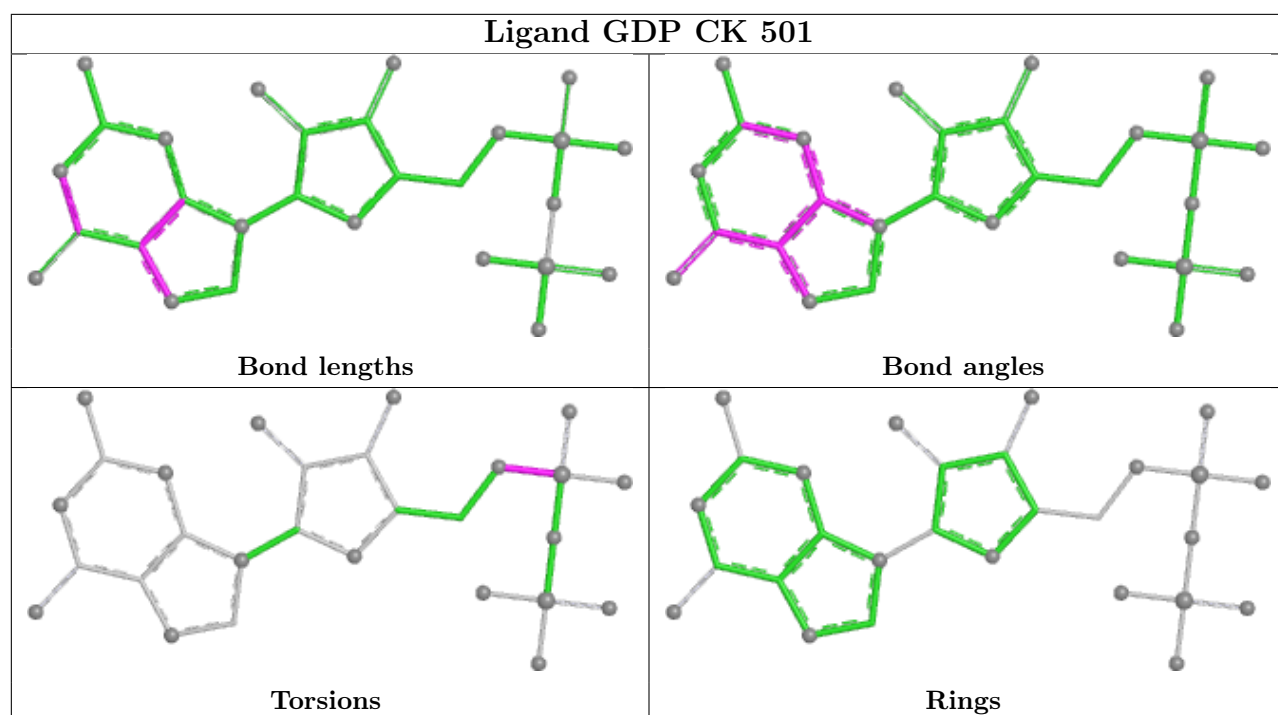


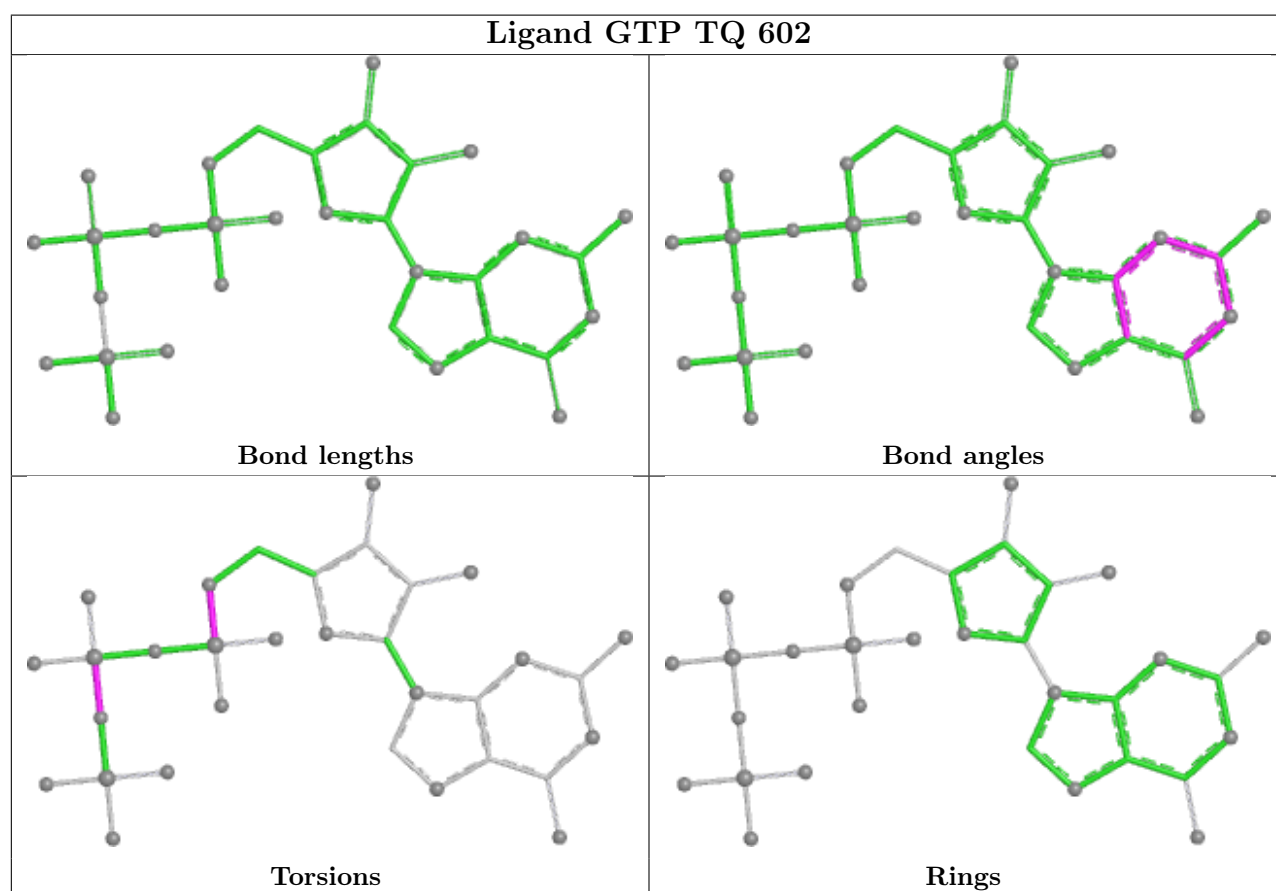
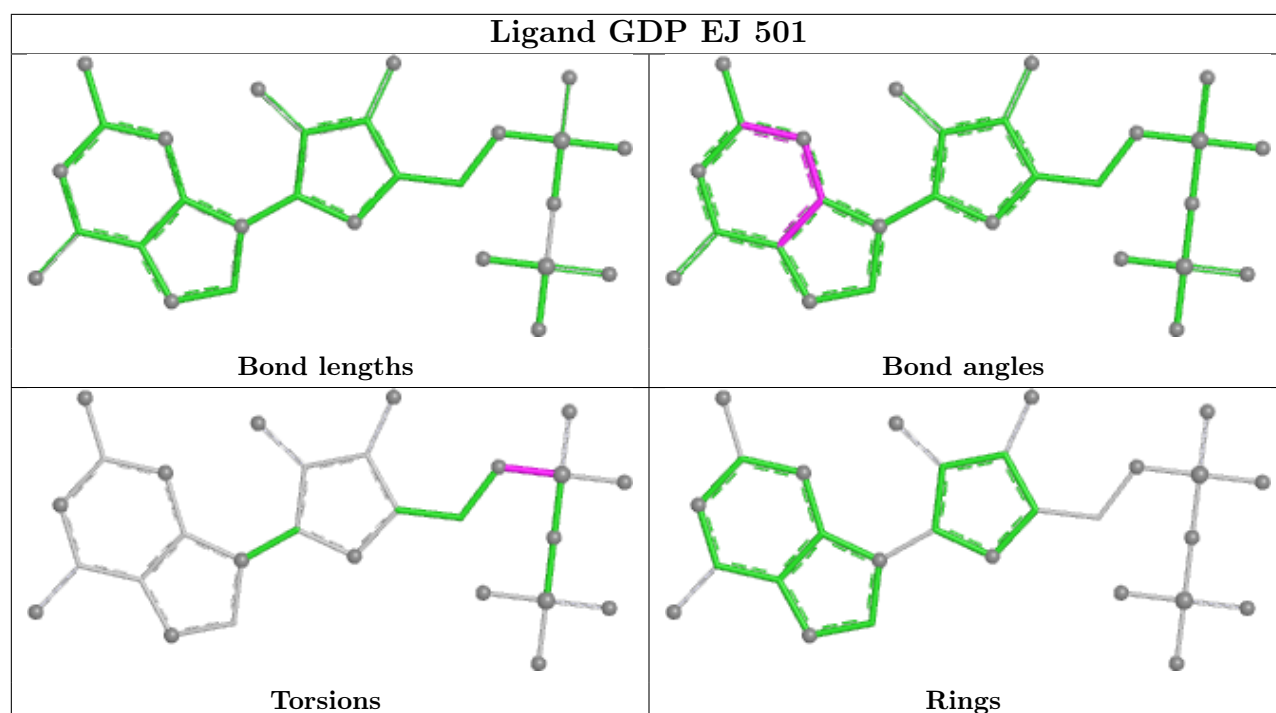
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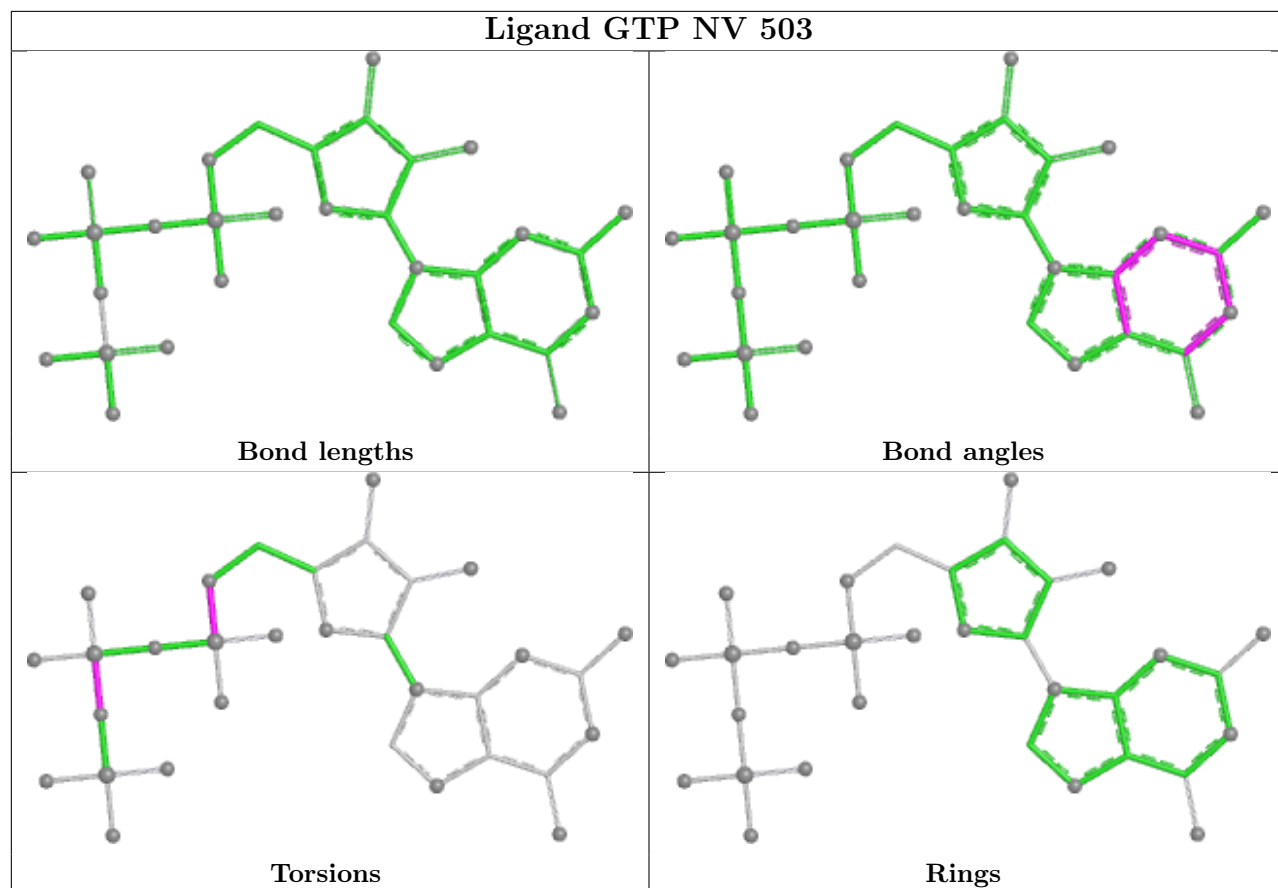
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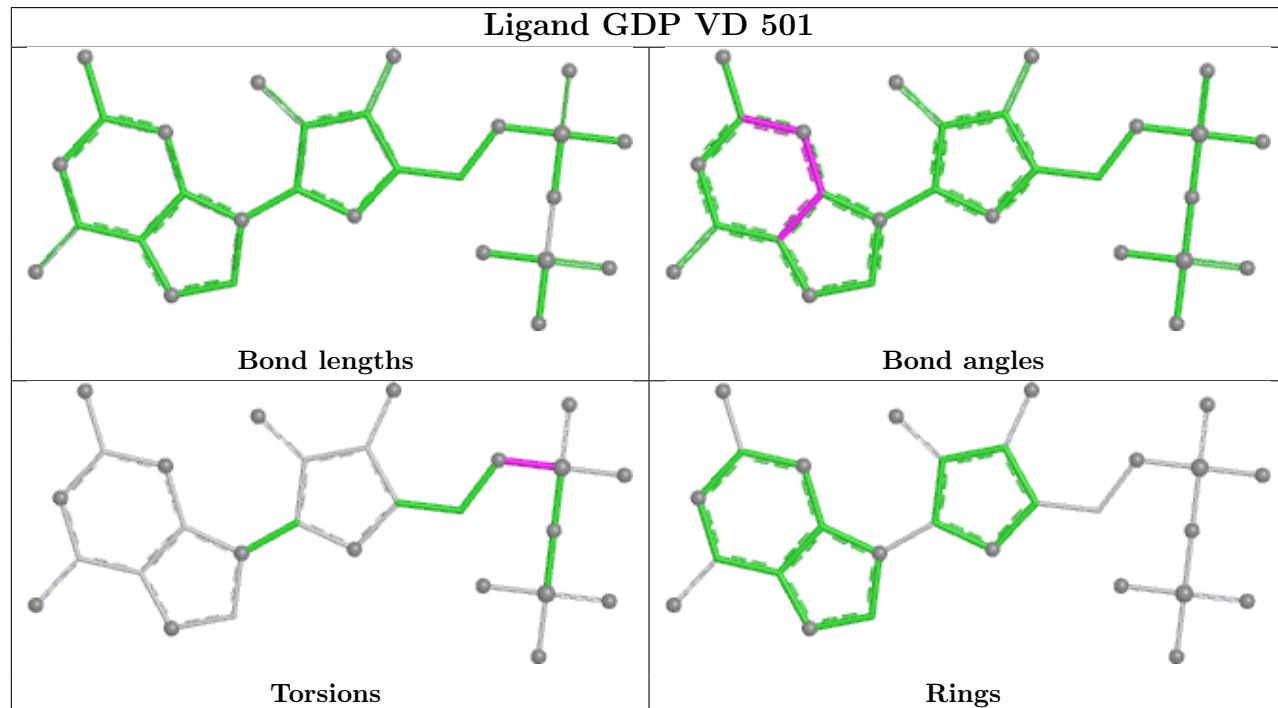


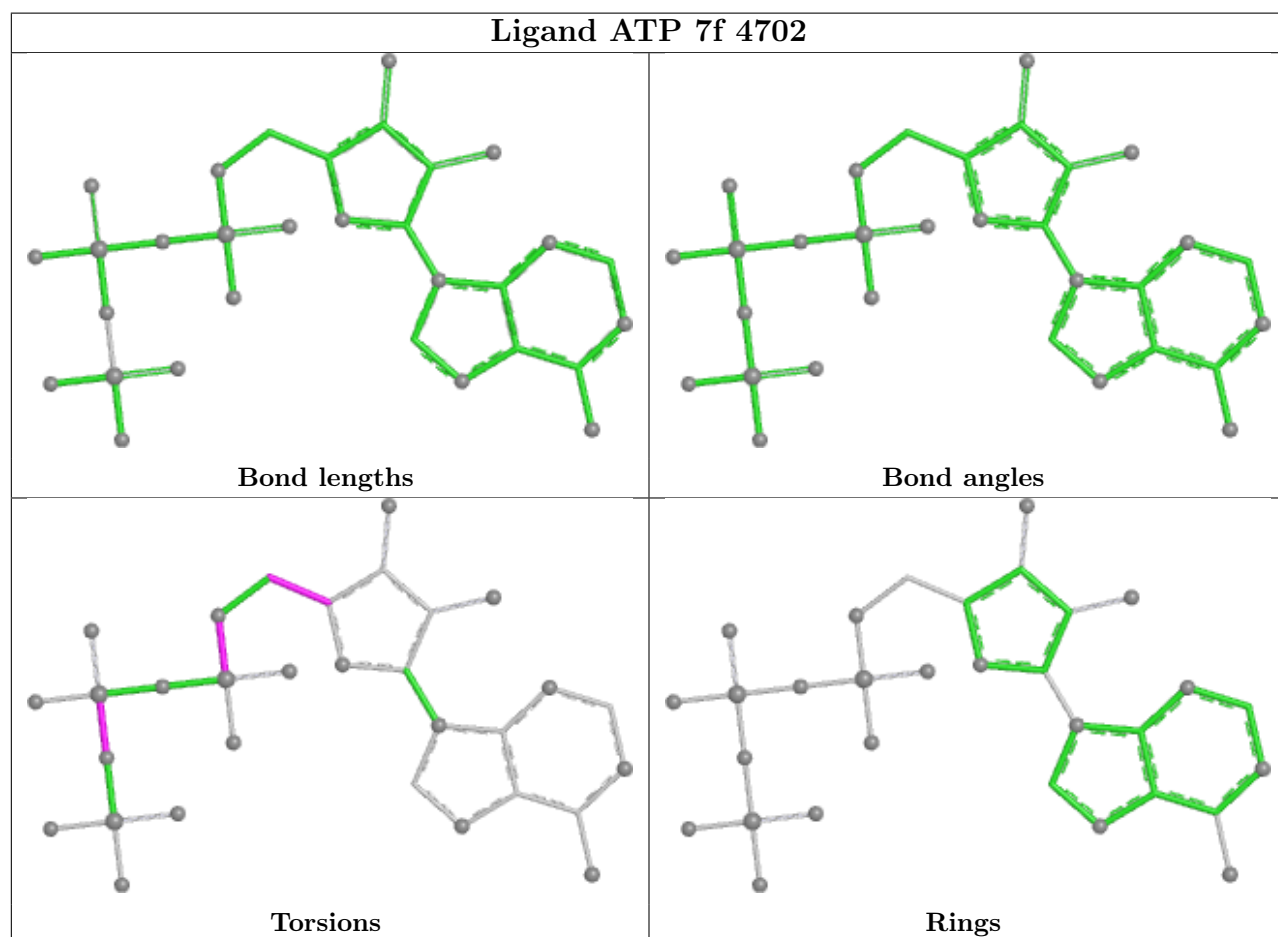
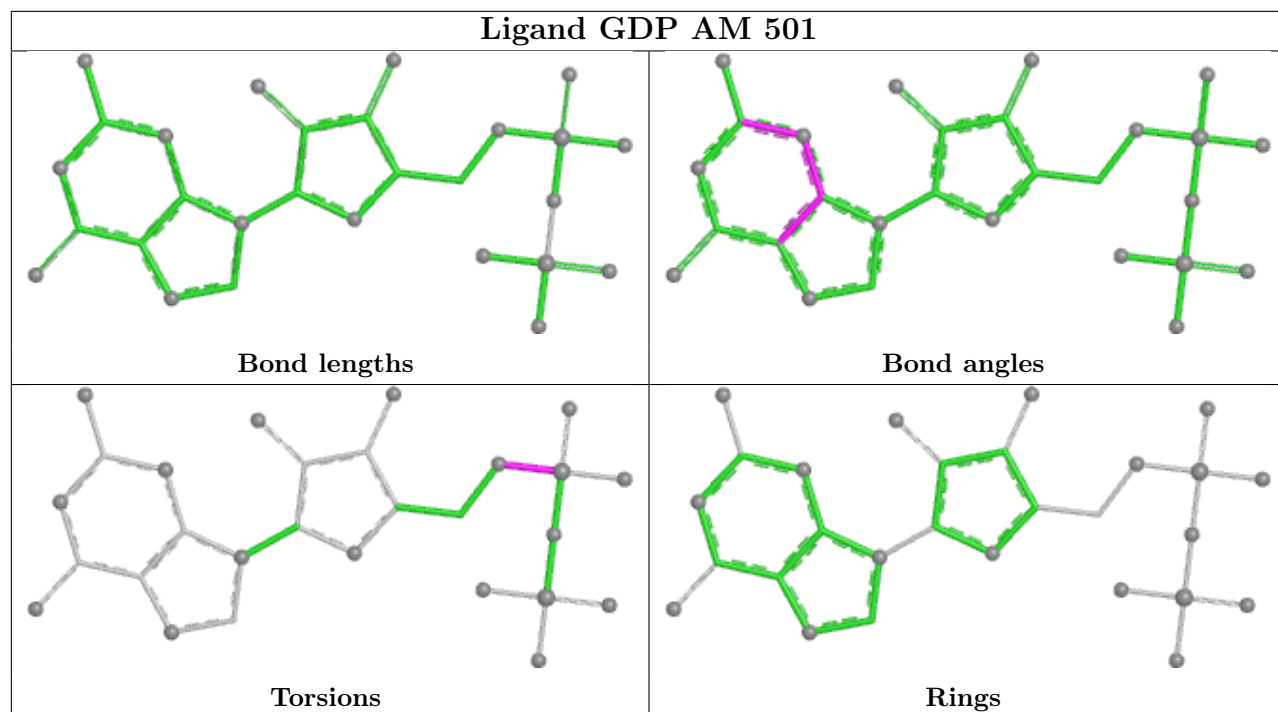


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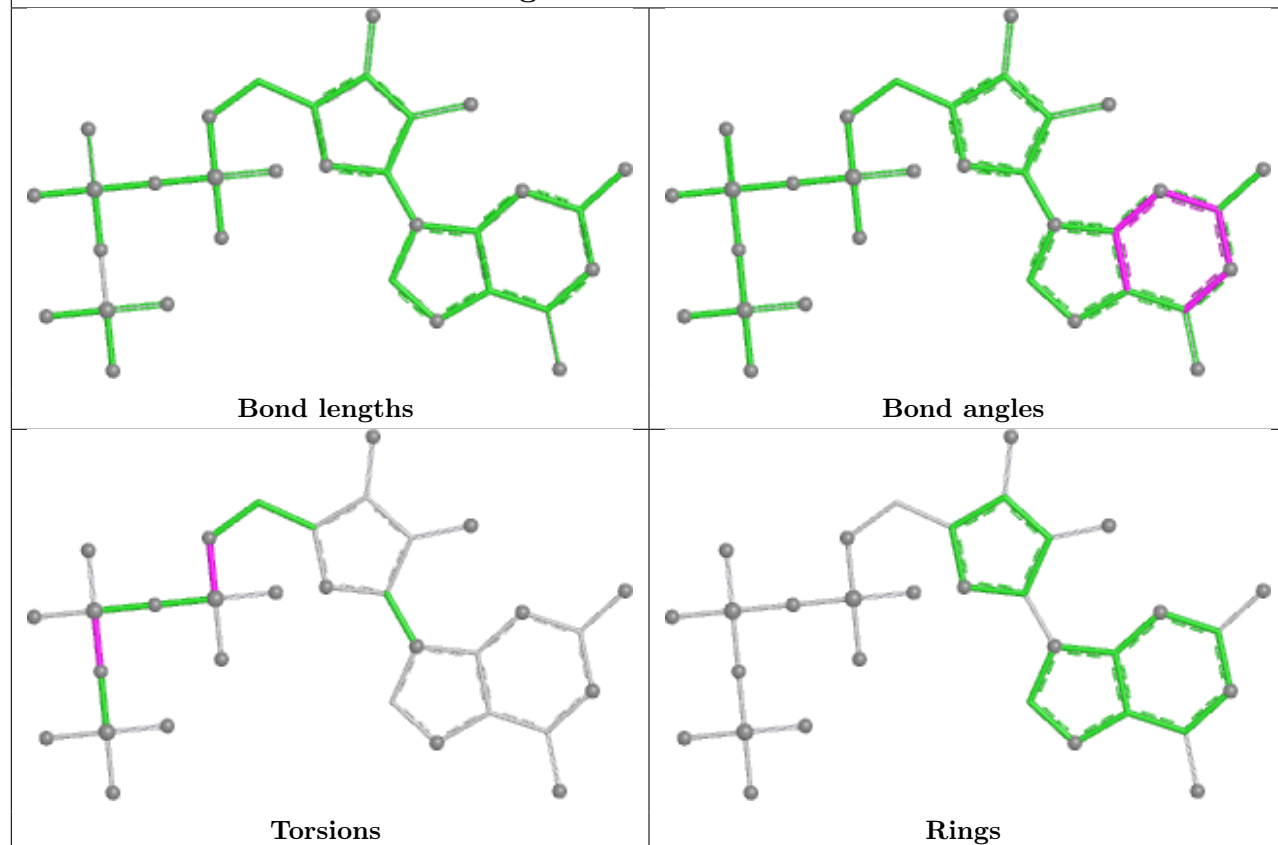


## Ligand GDP VD 501

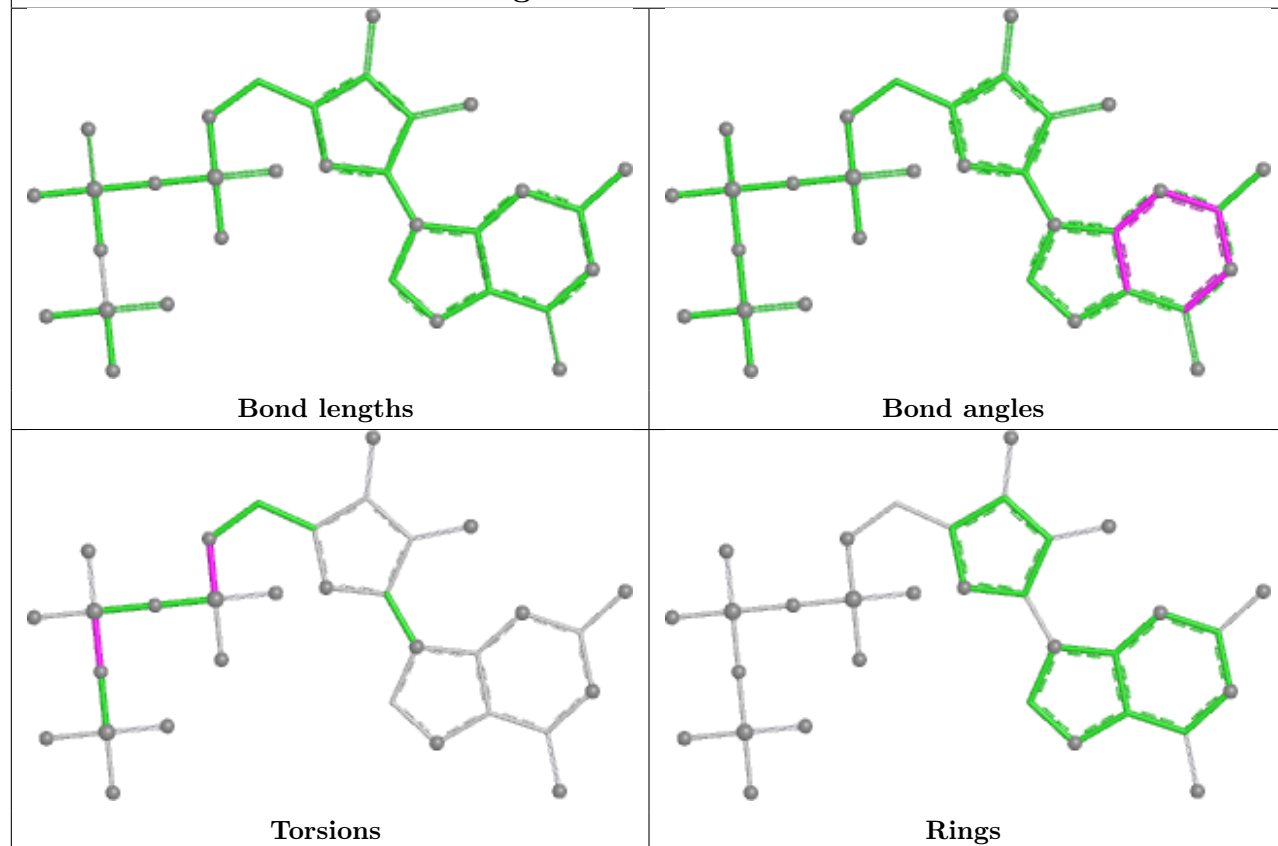




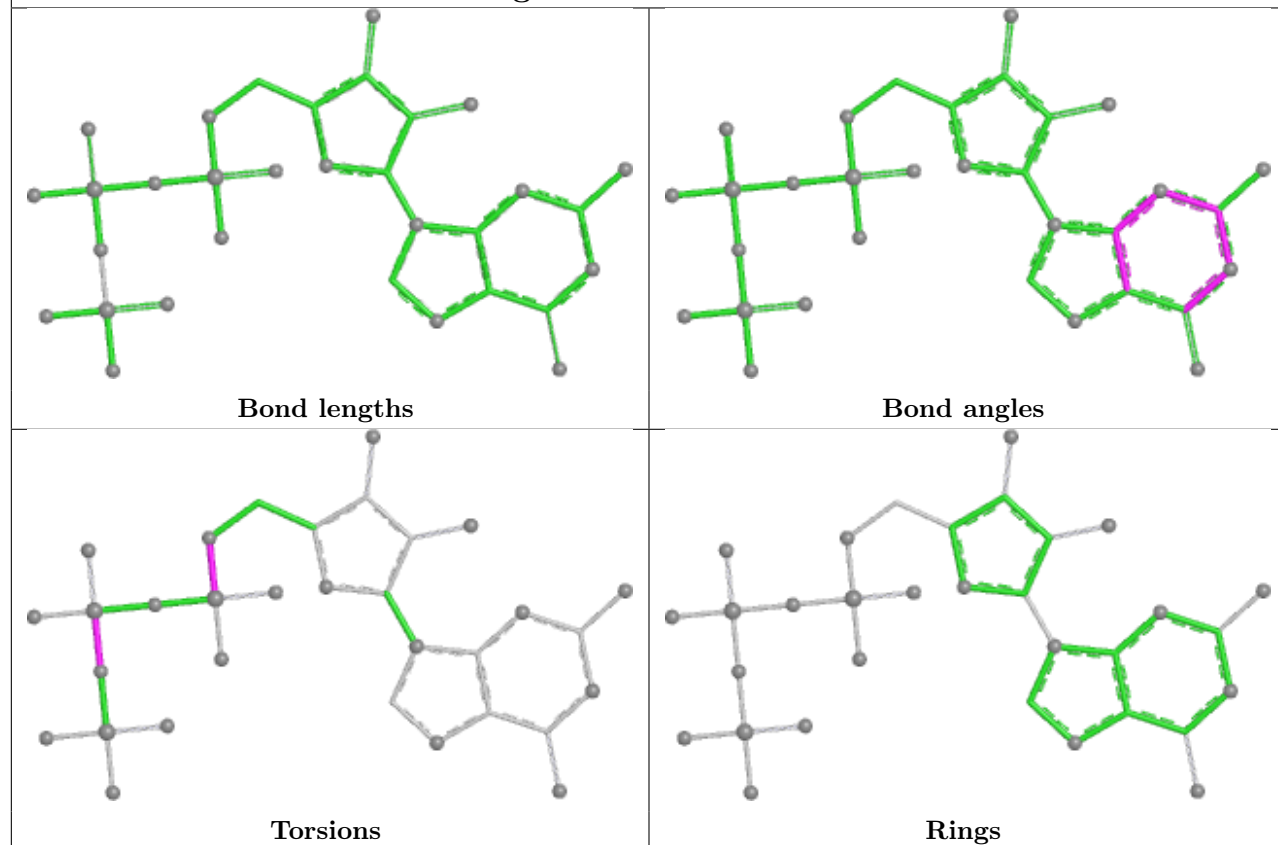
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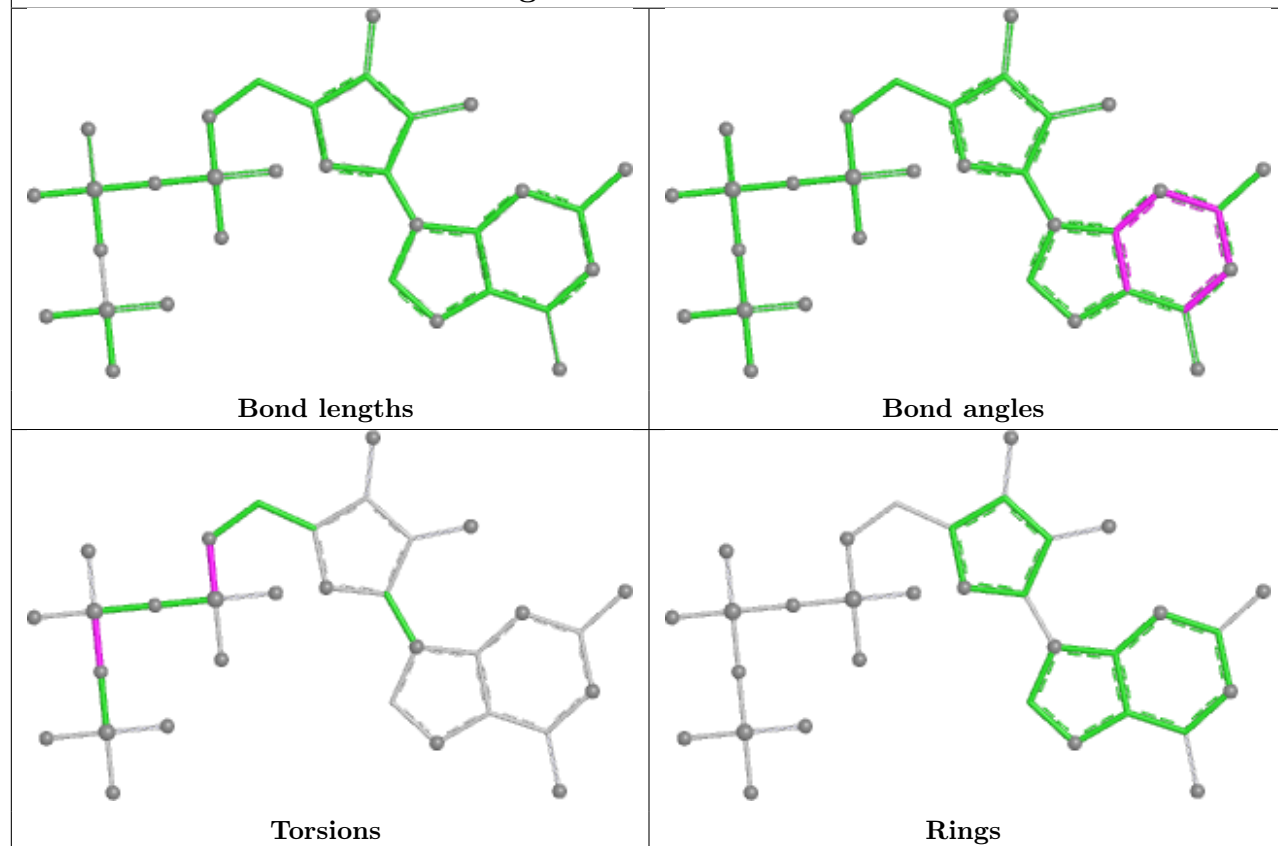
## Ligand GTP MD 502



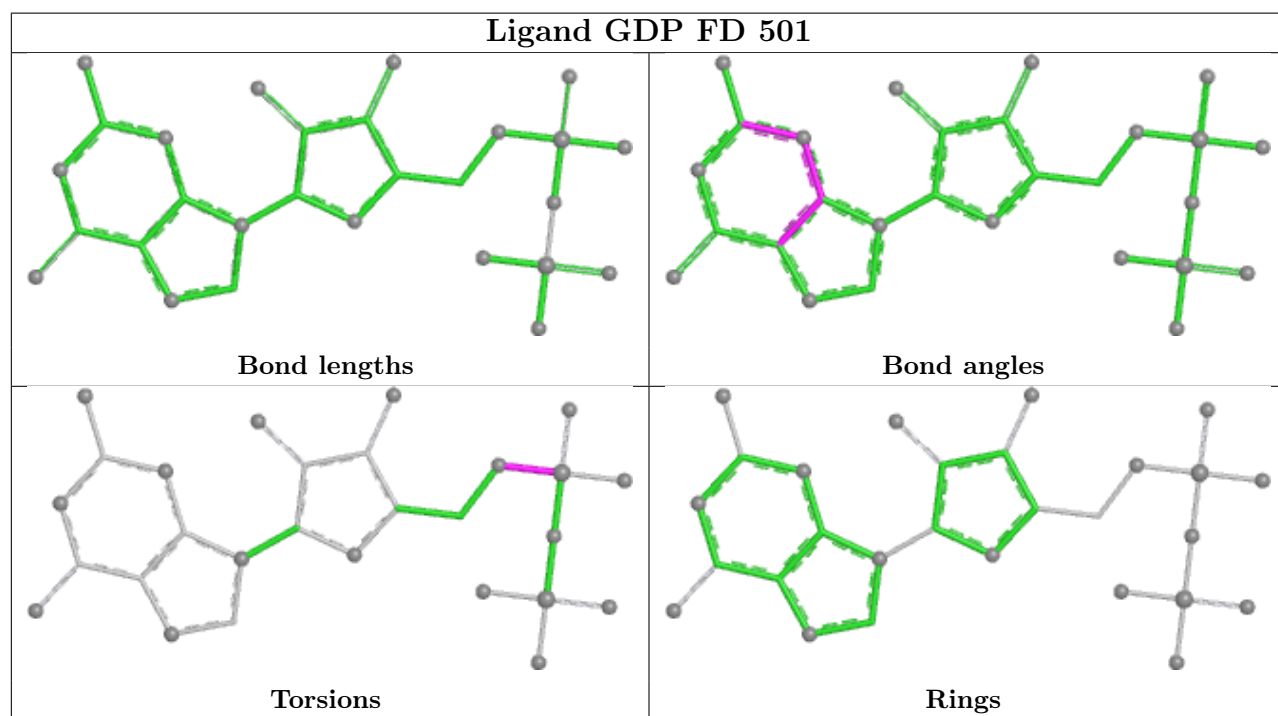
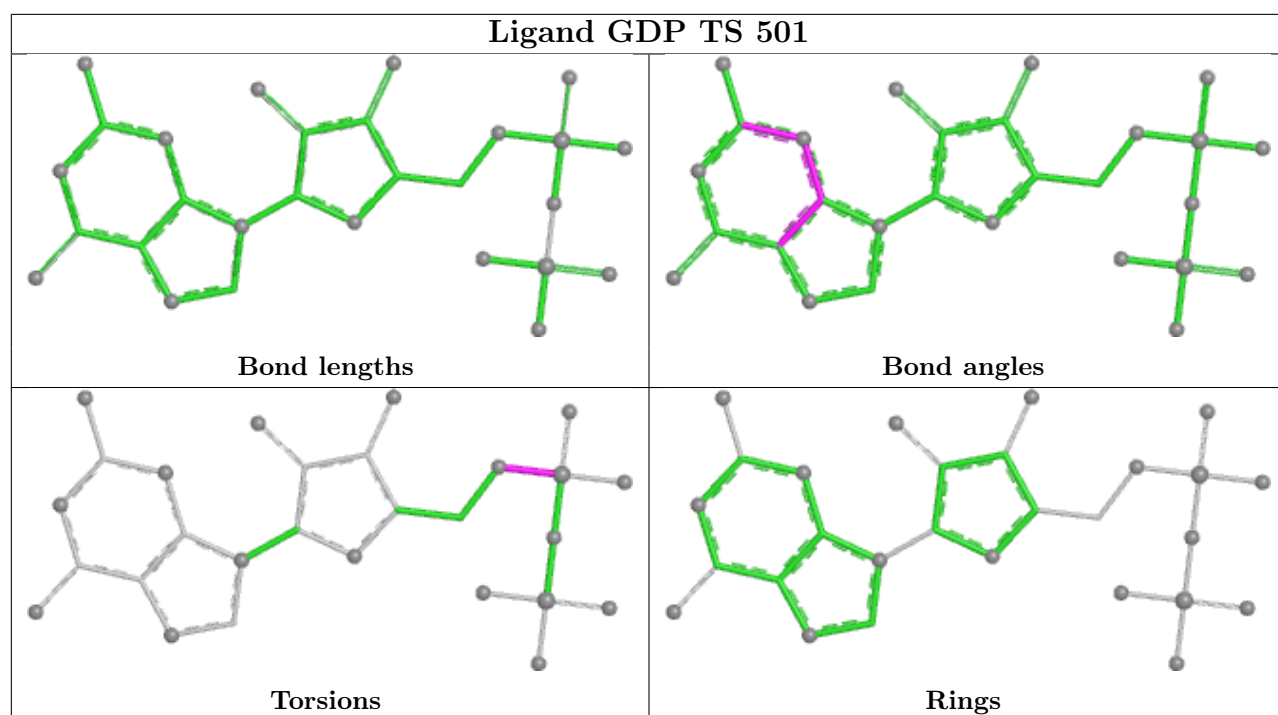
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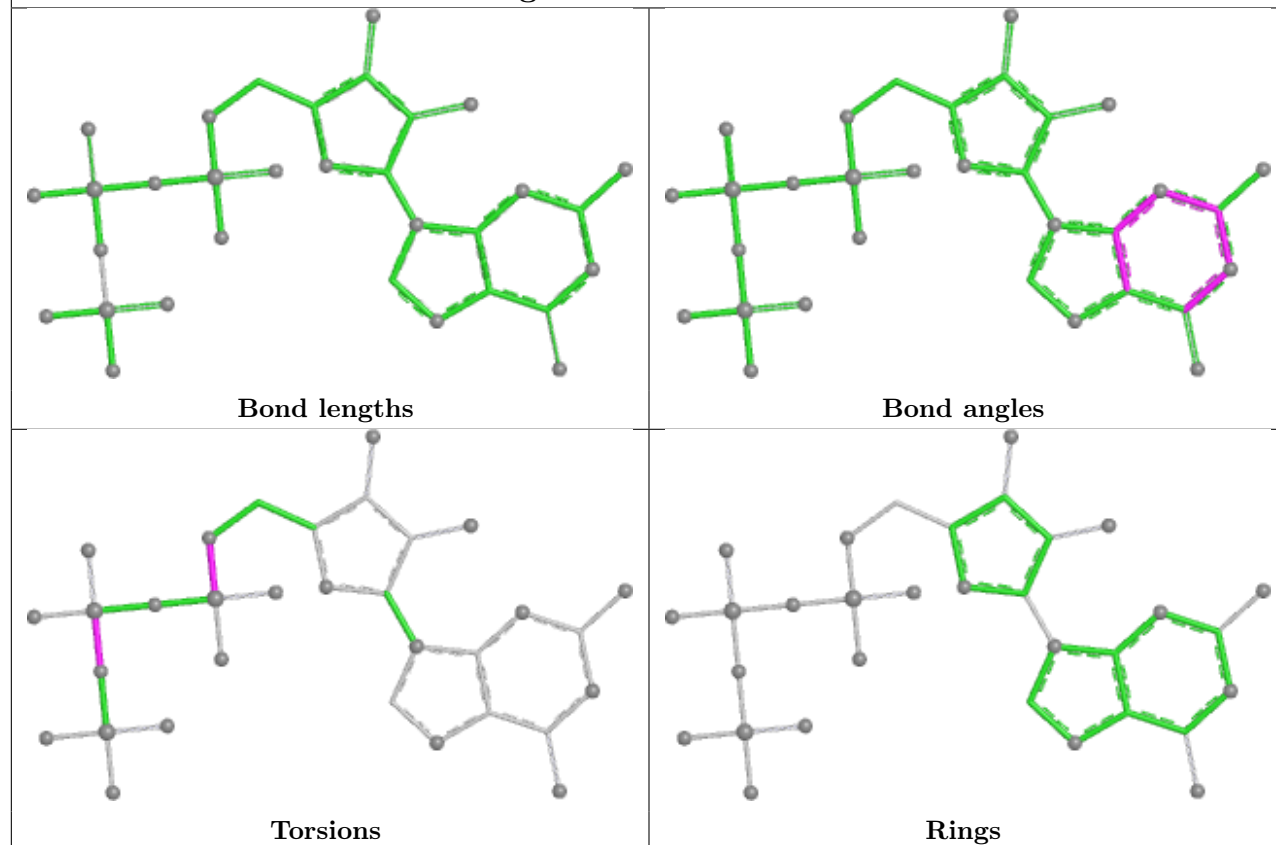
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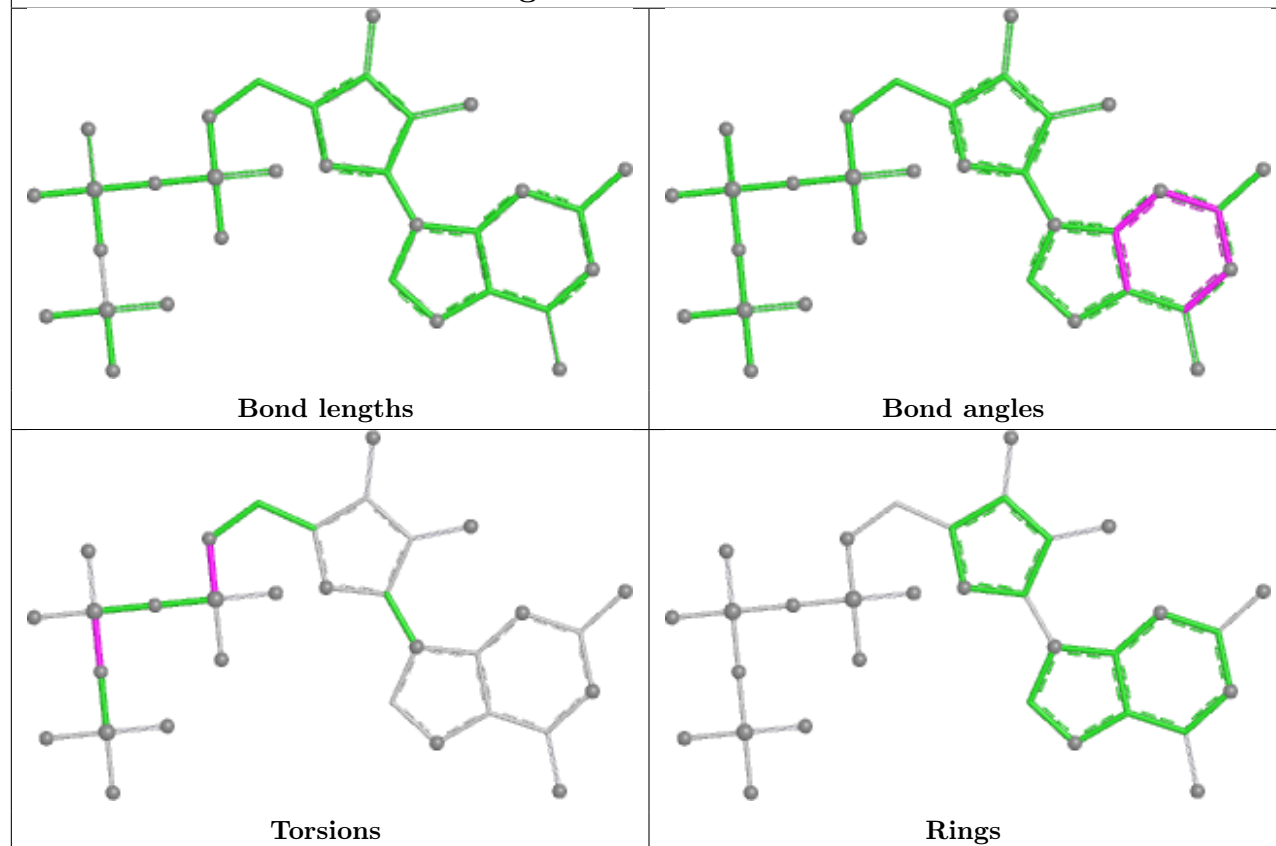




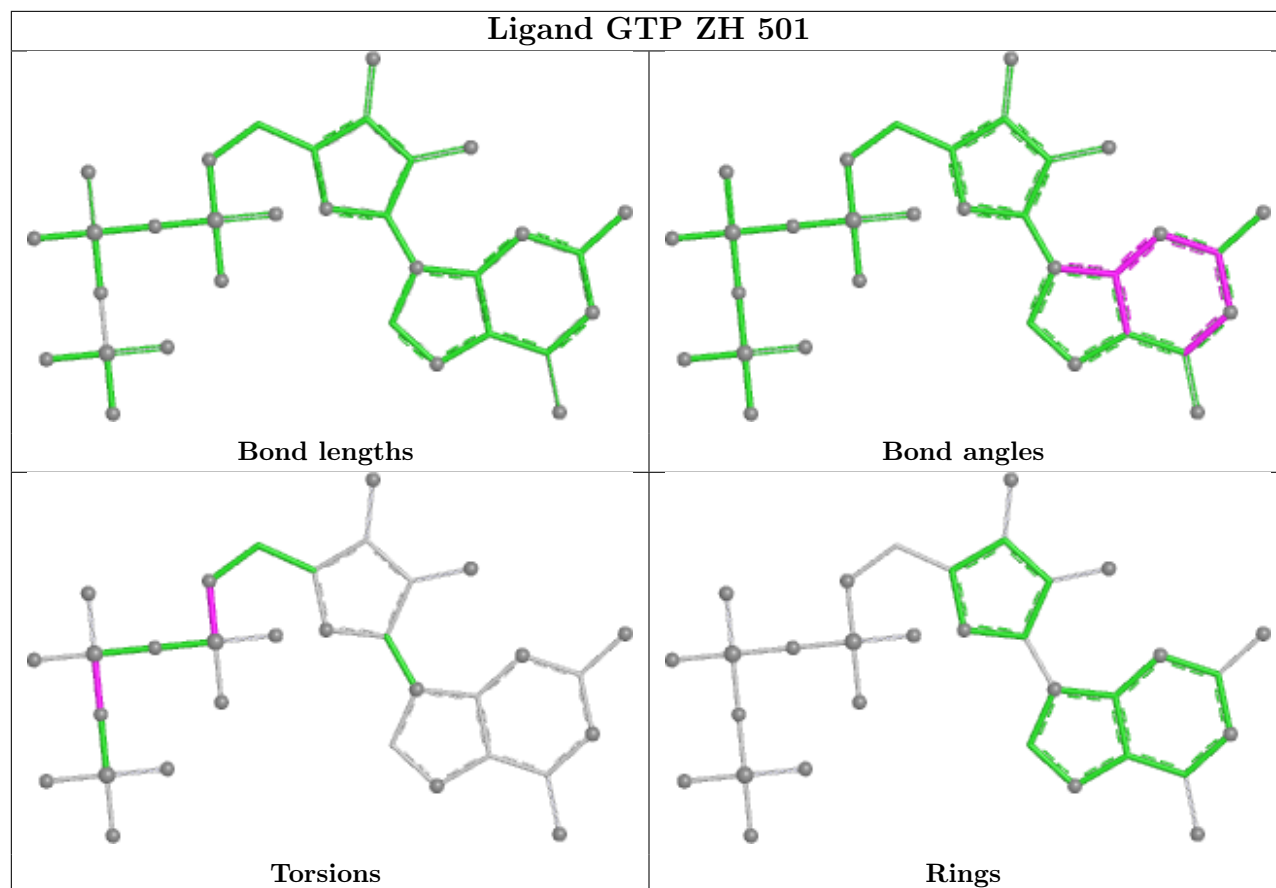
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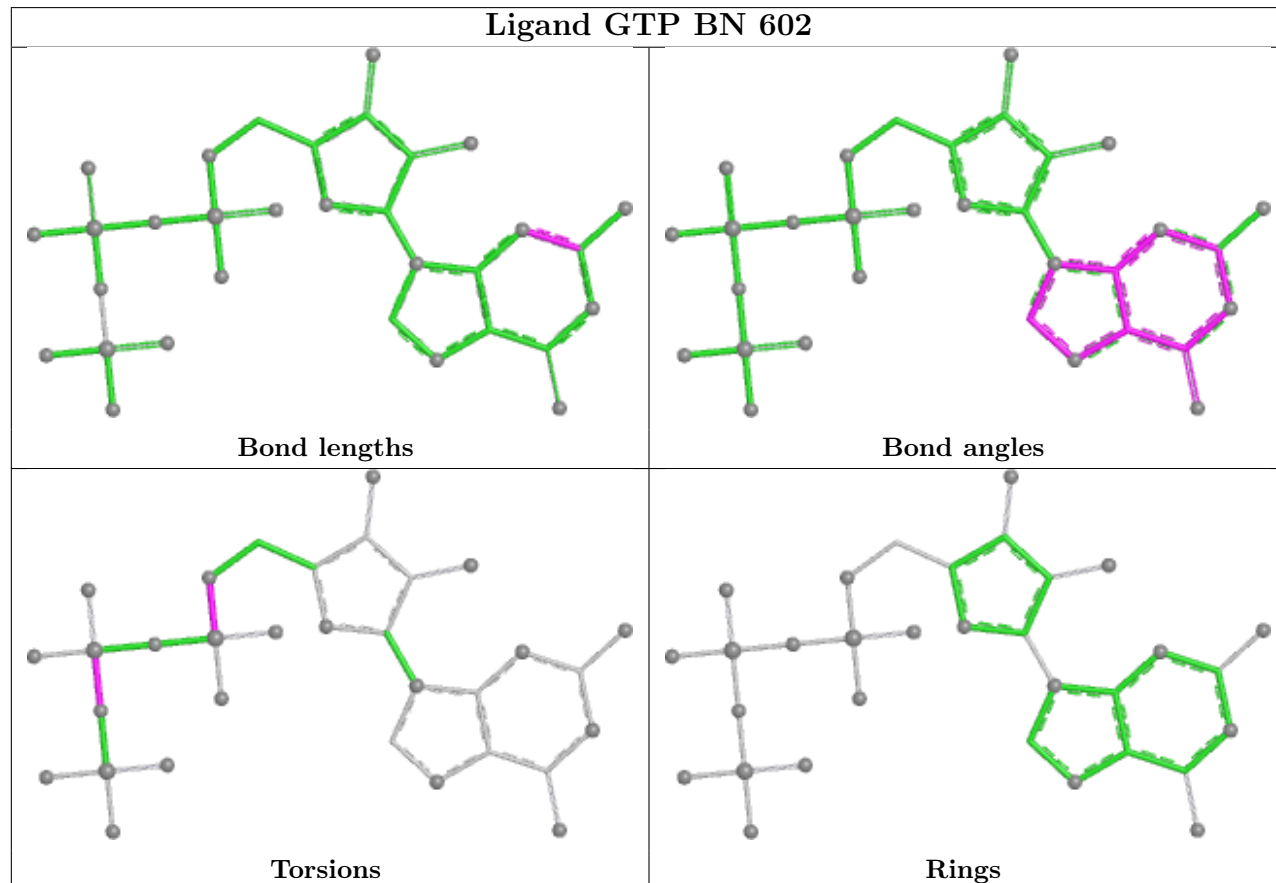
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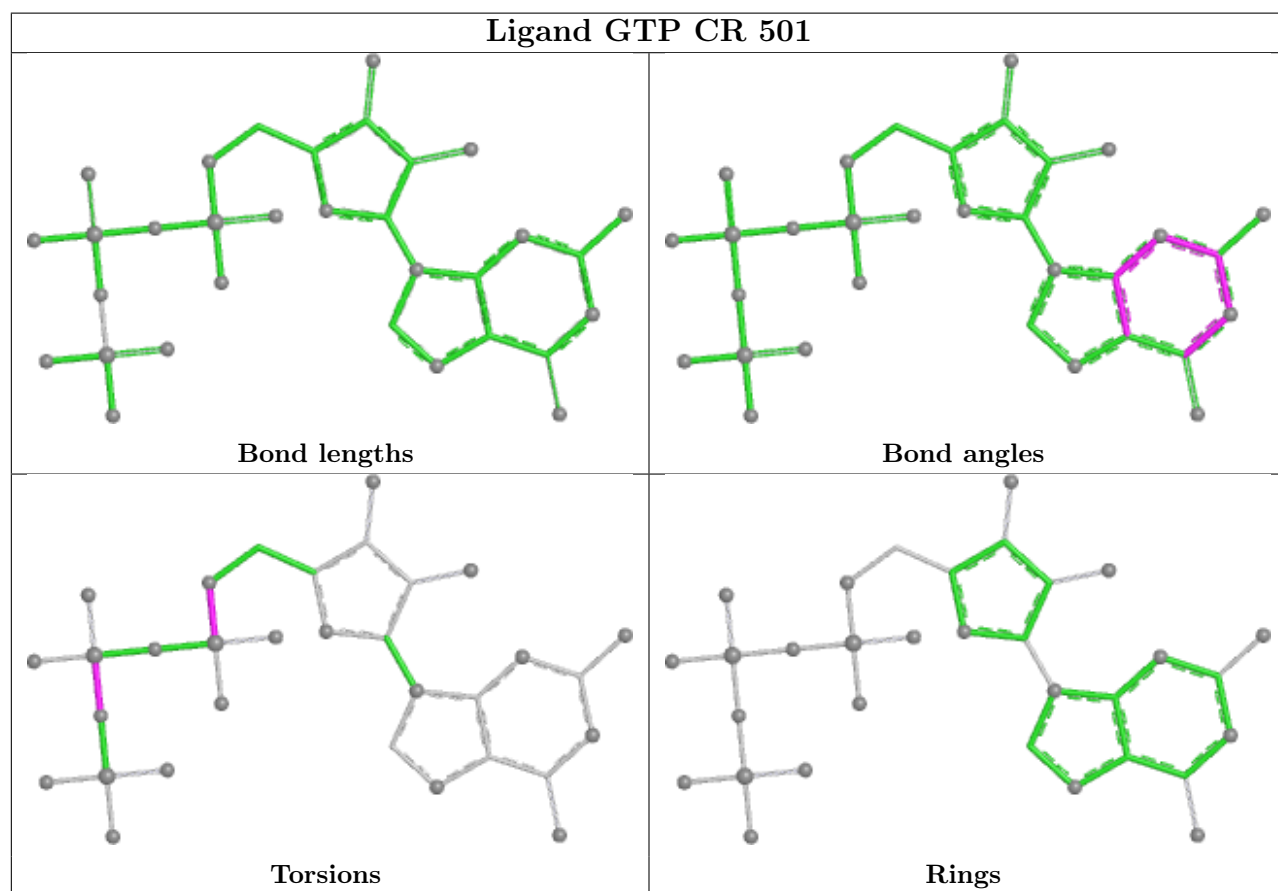
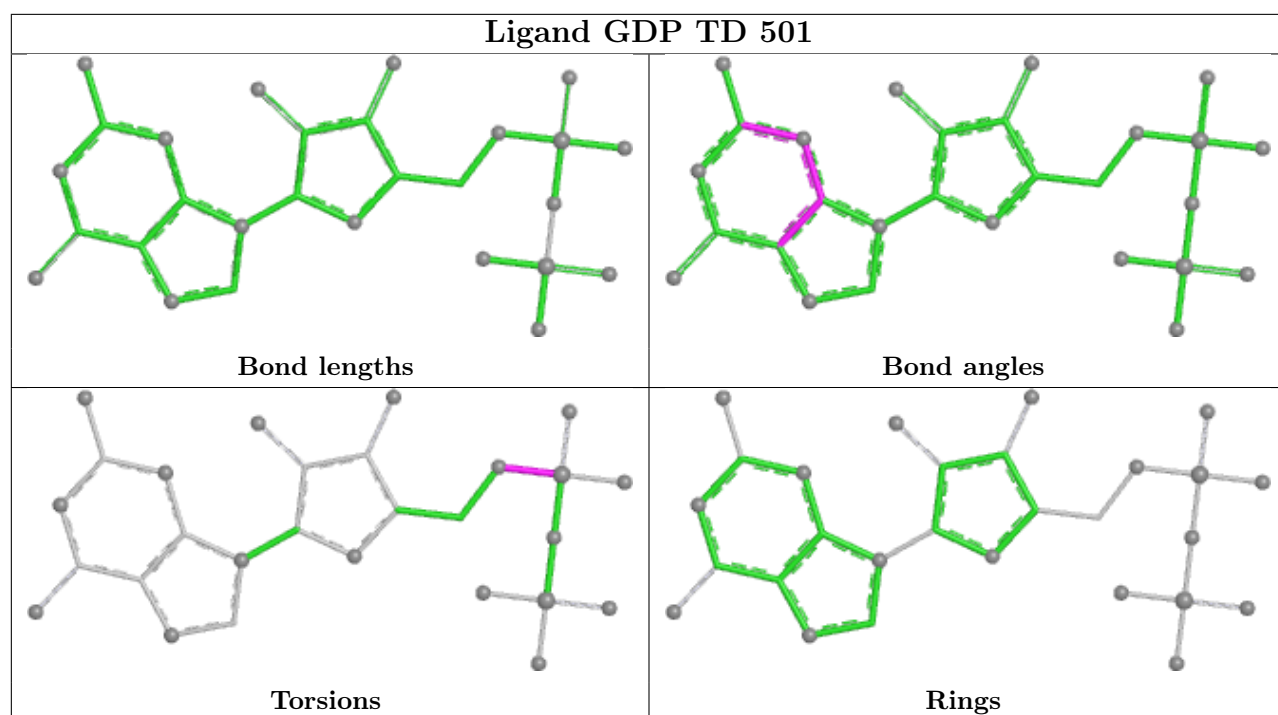


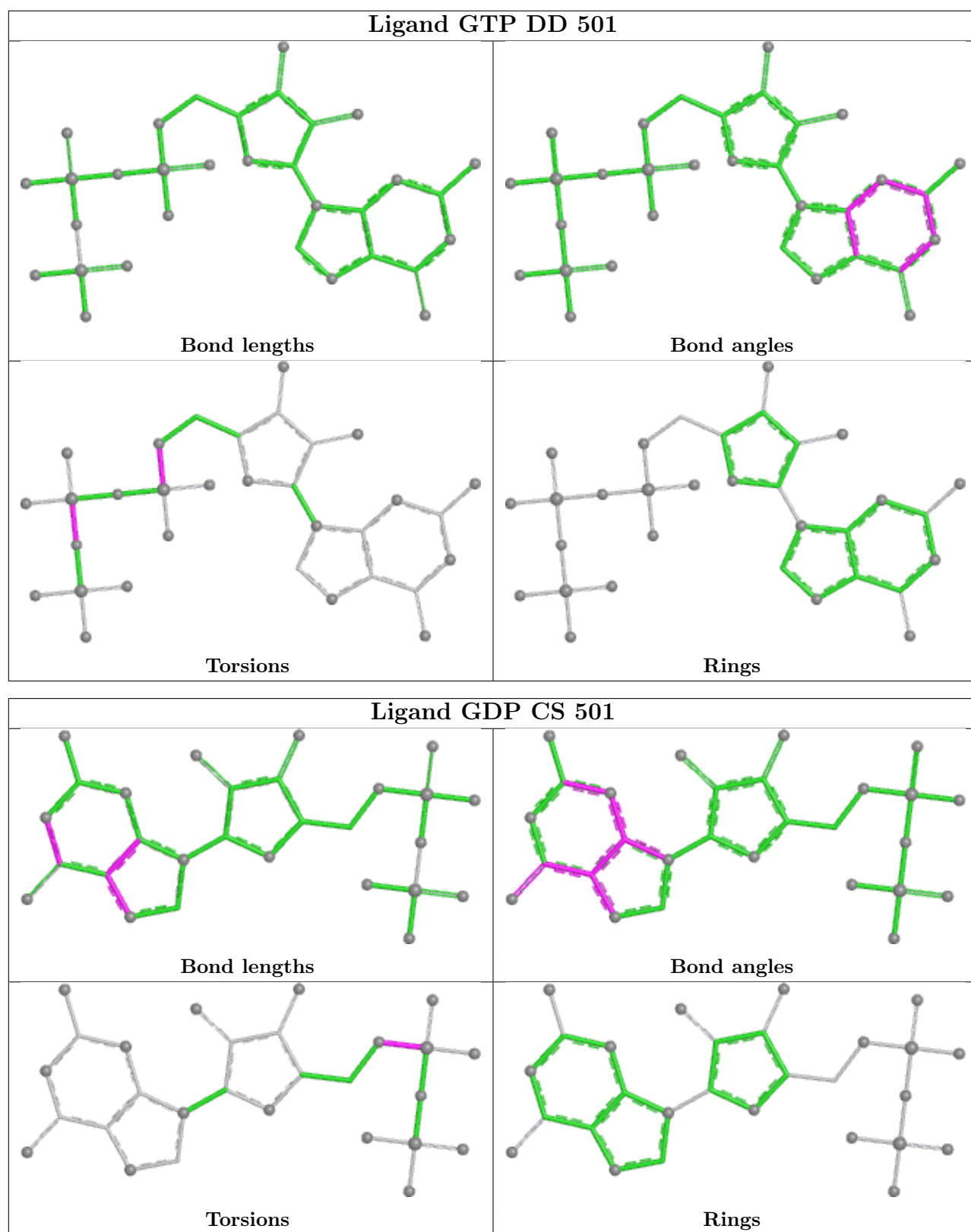
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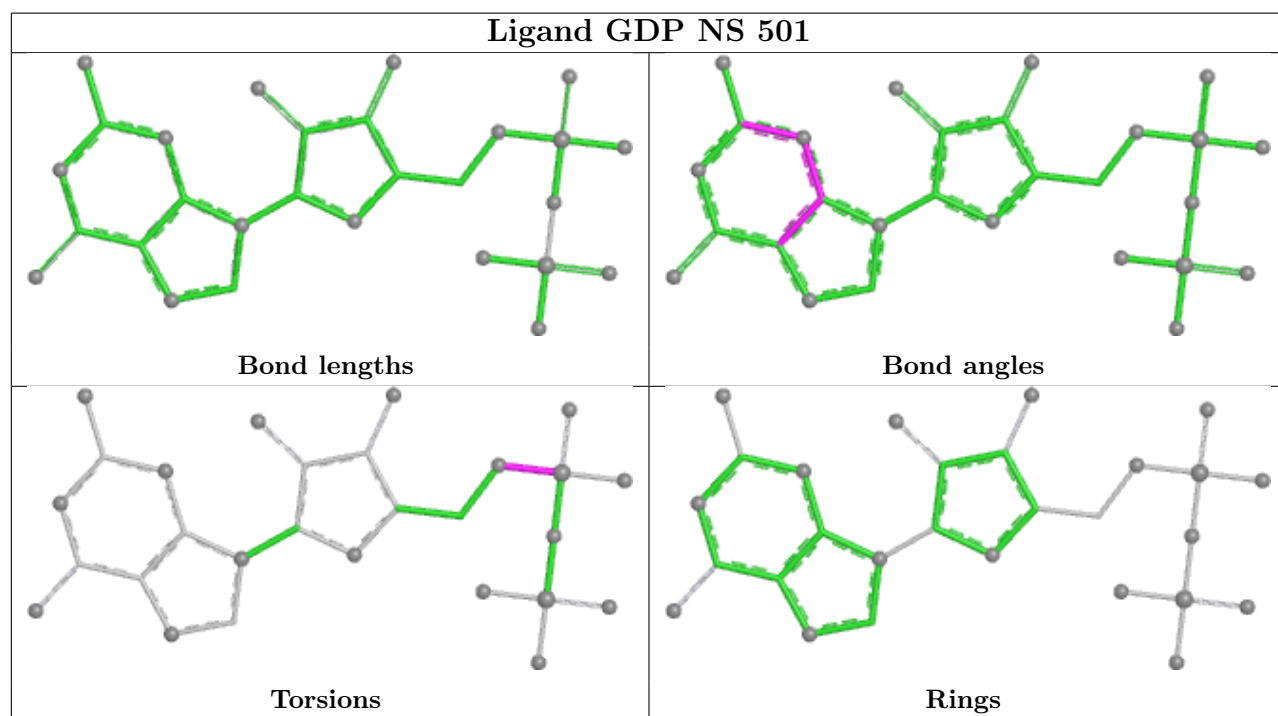
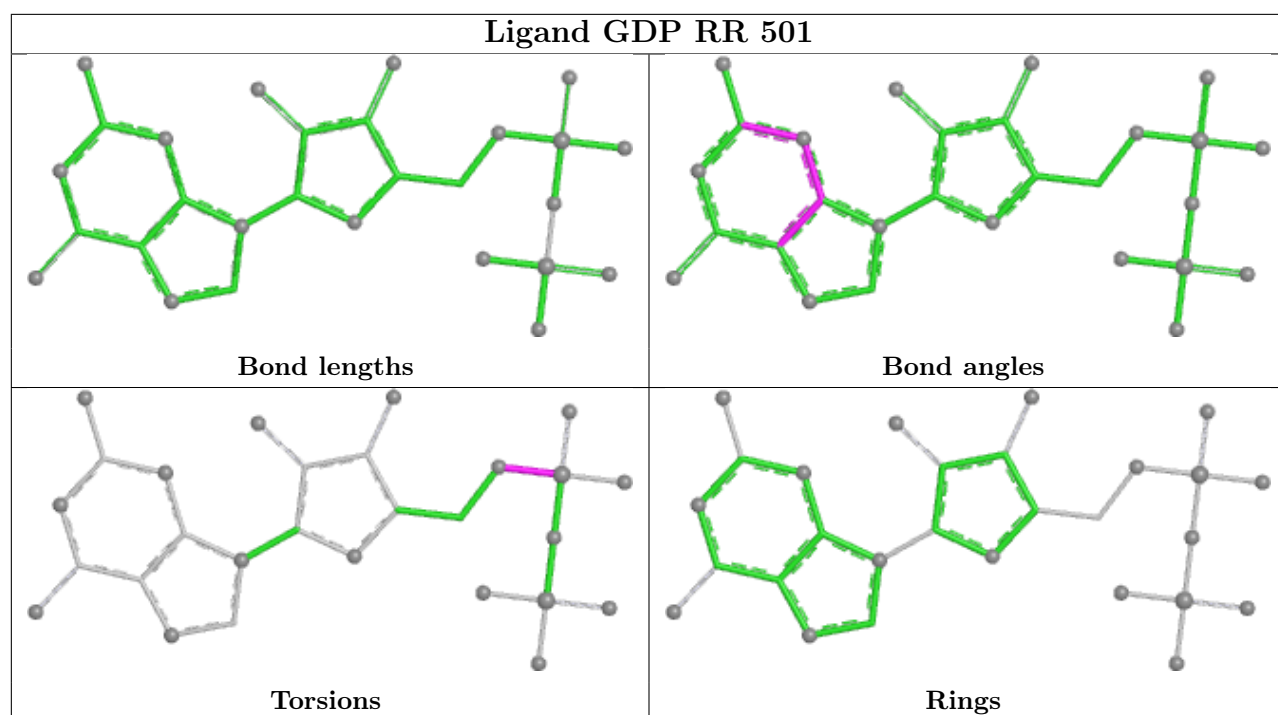


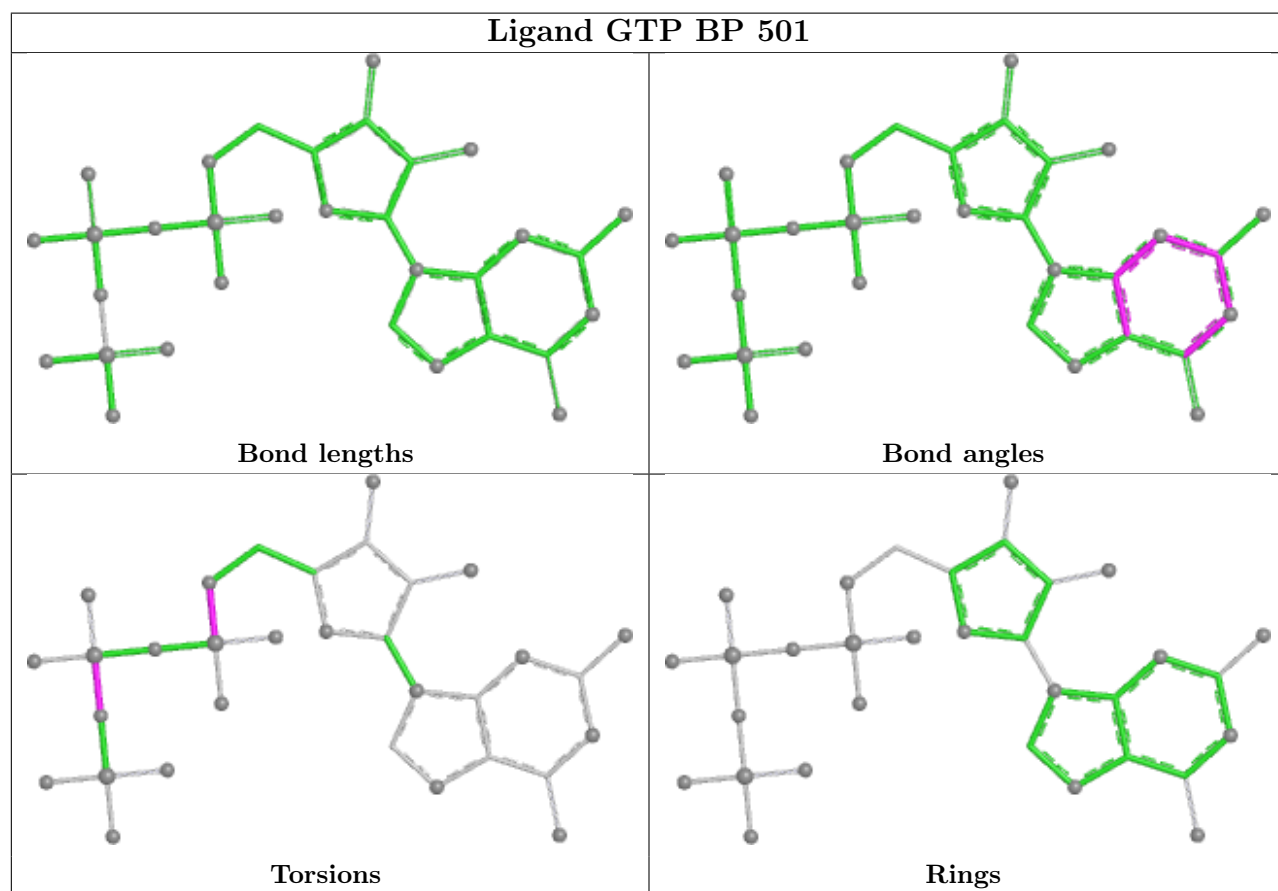
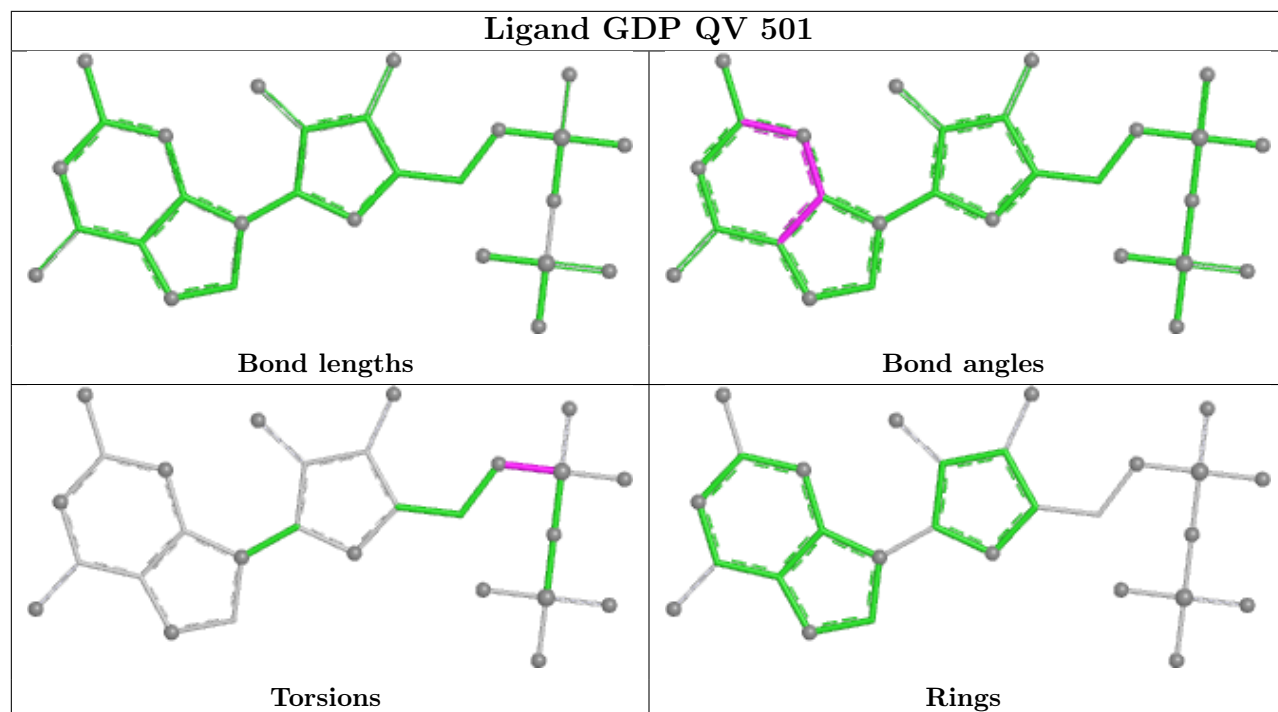
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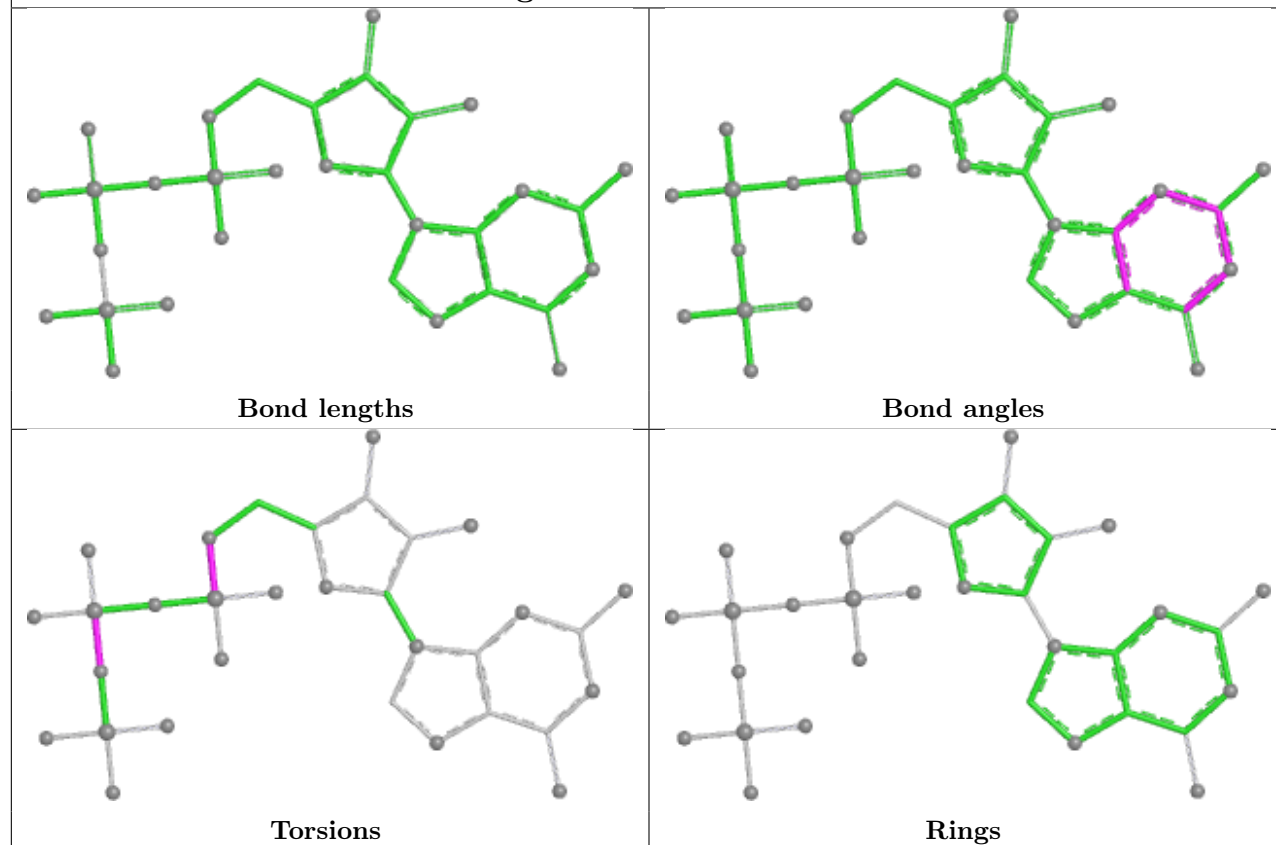




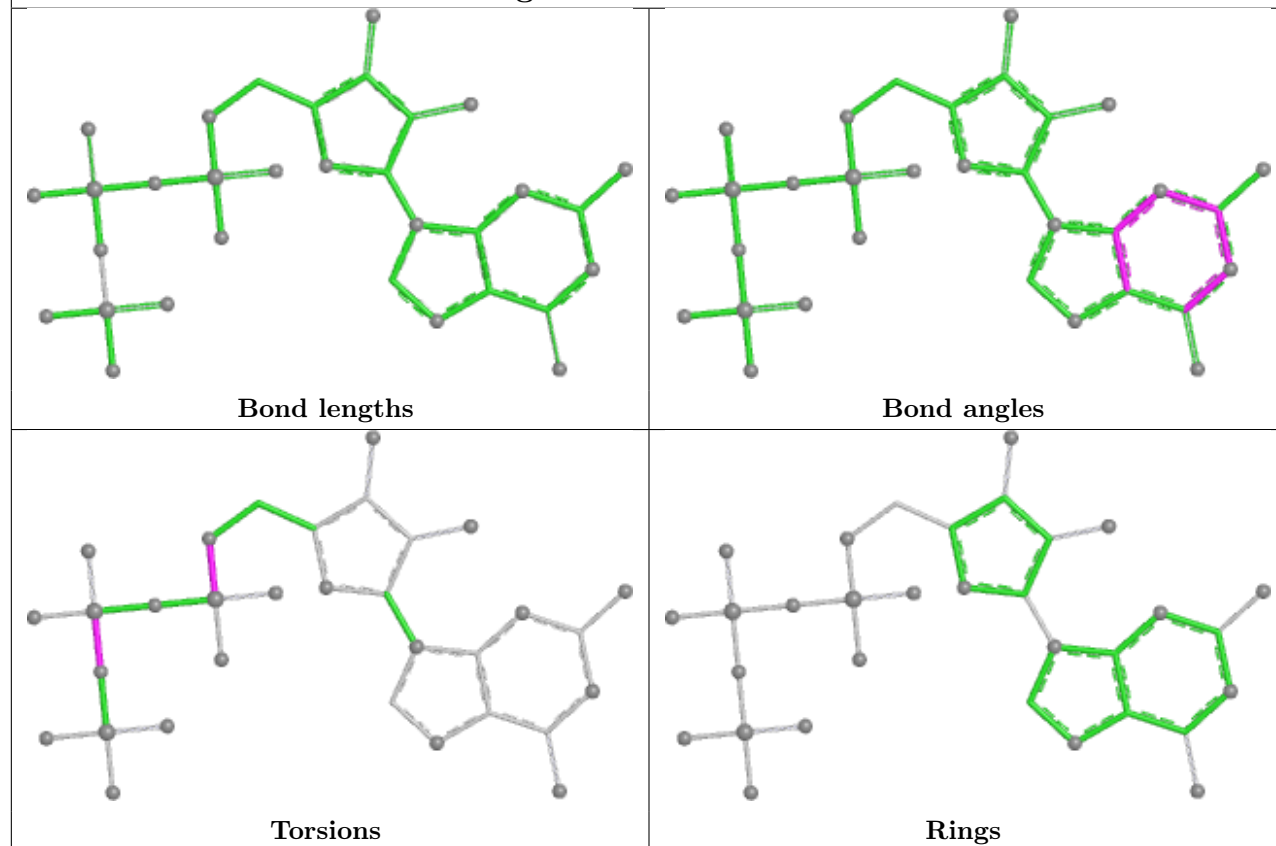




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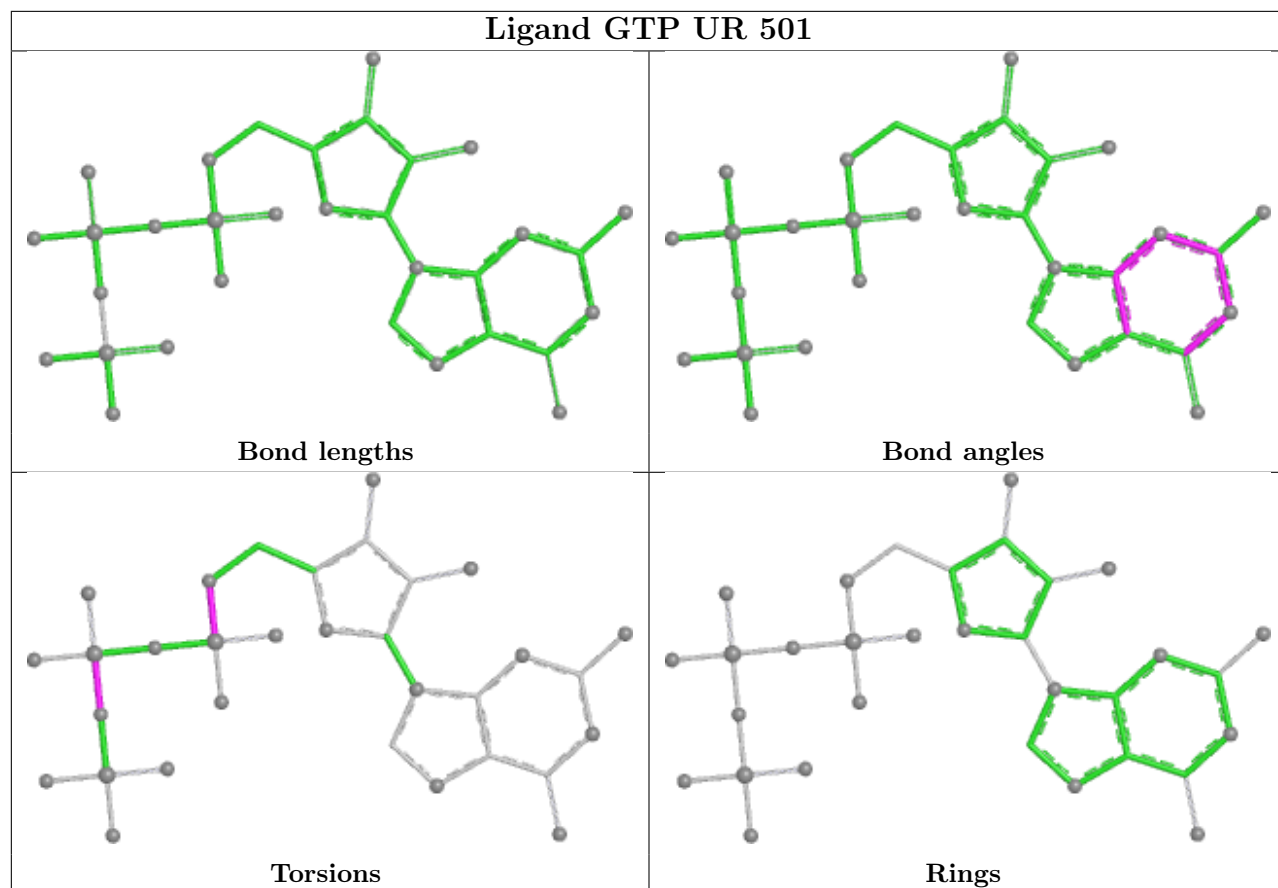


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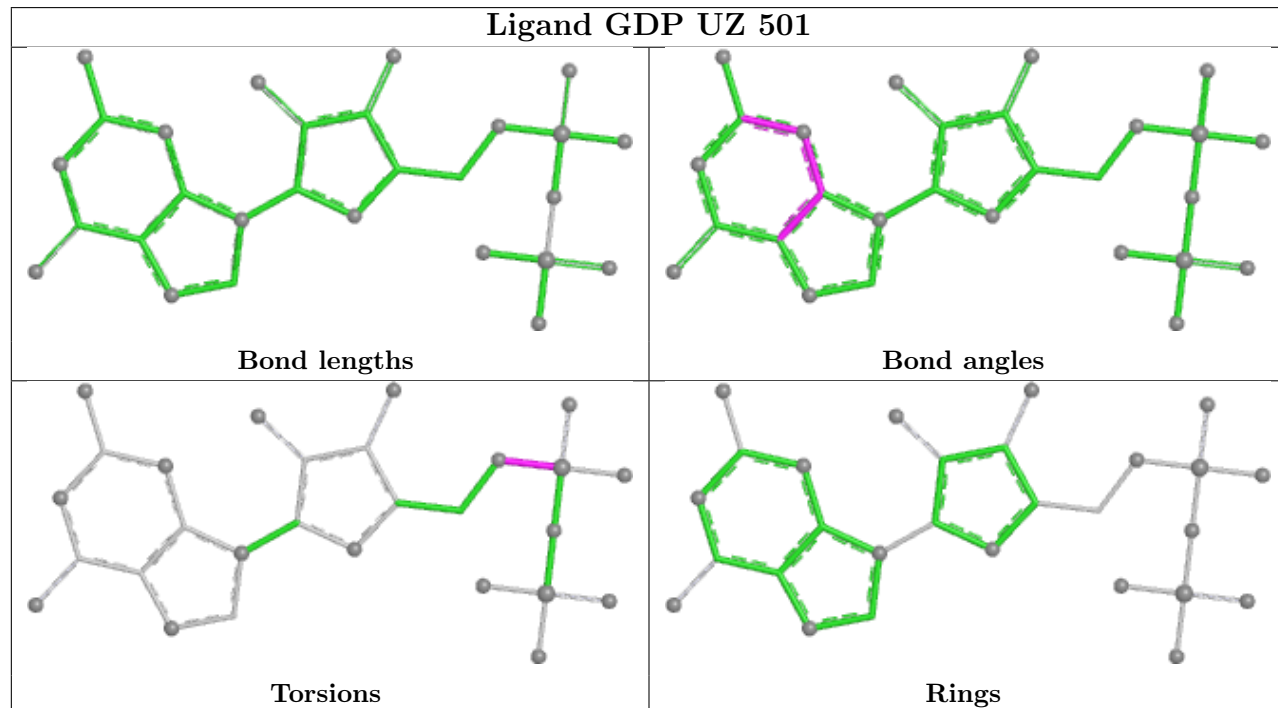




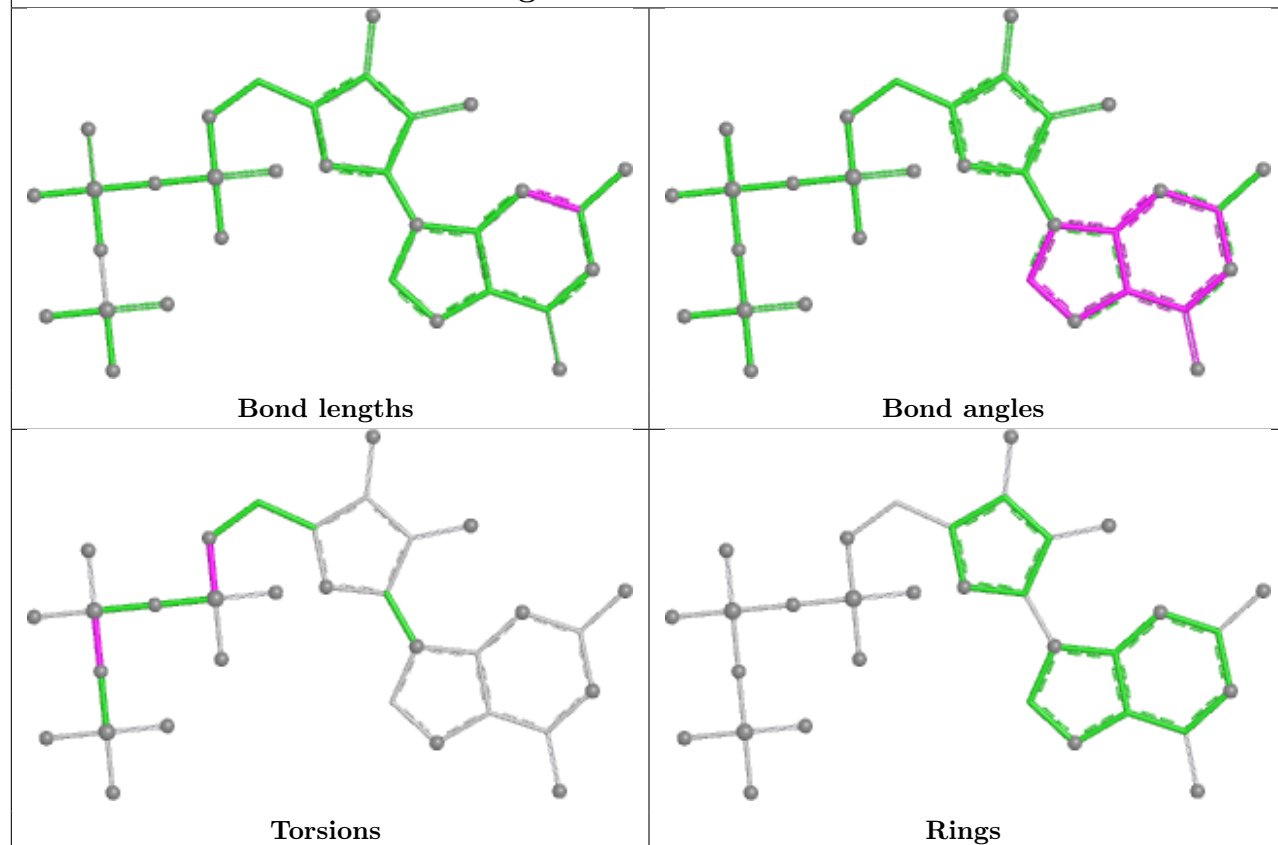
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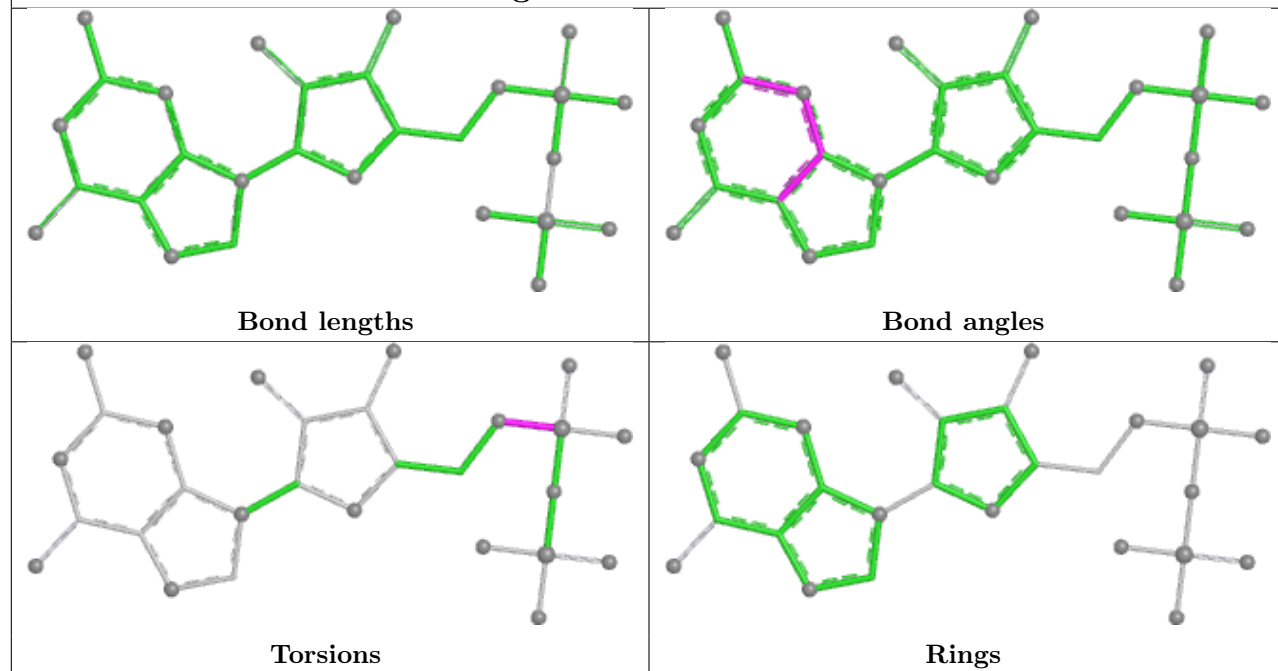
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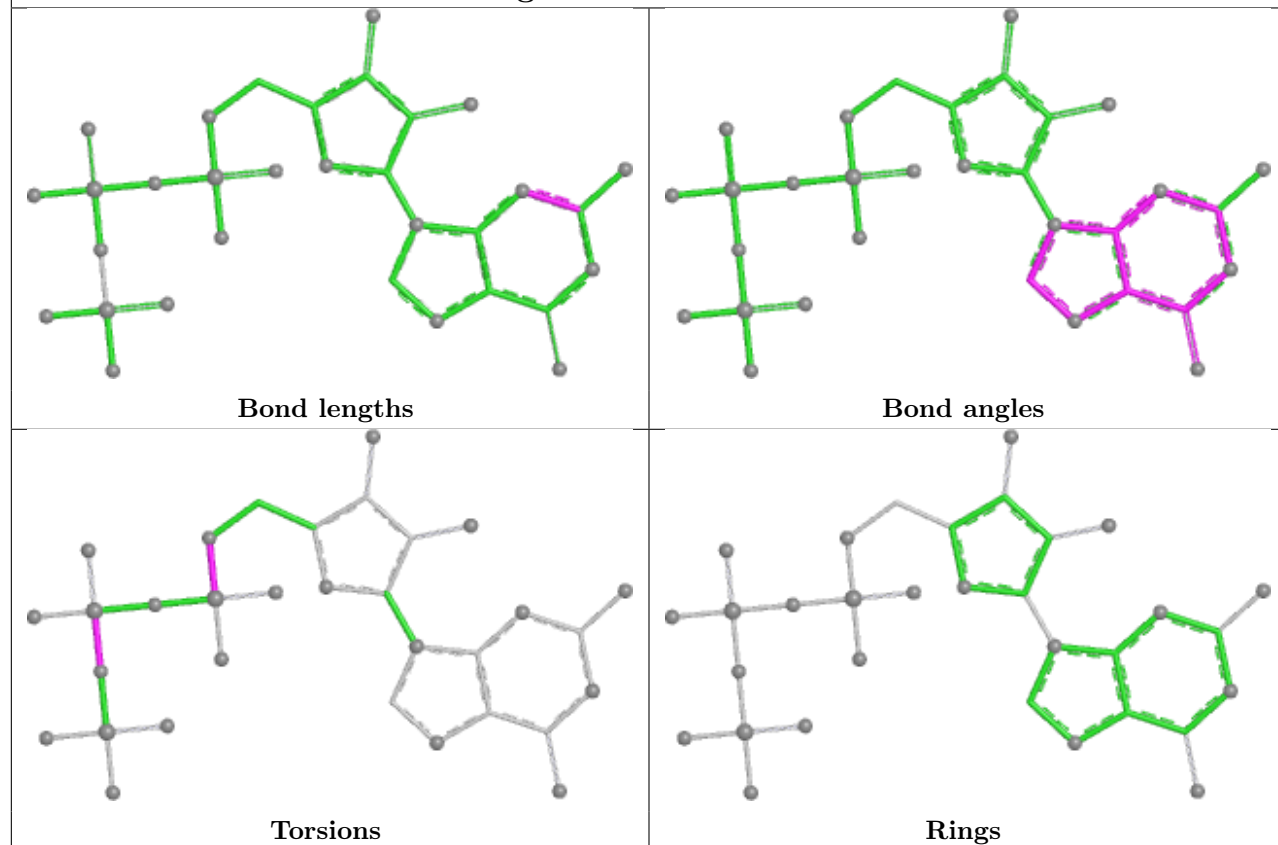
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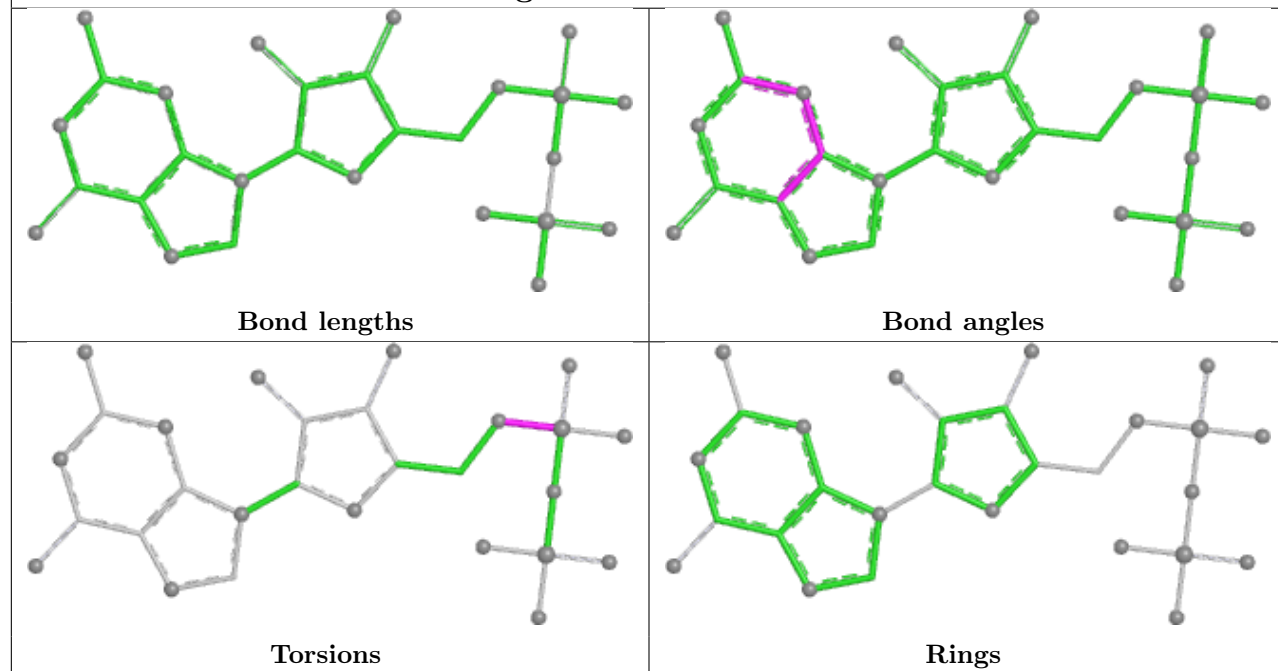
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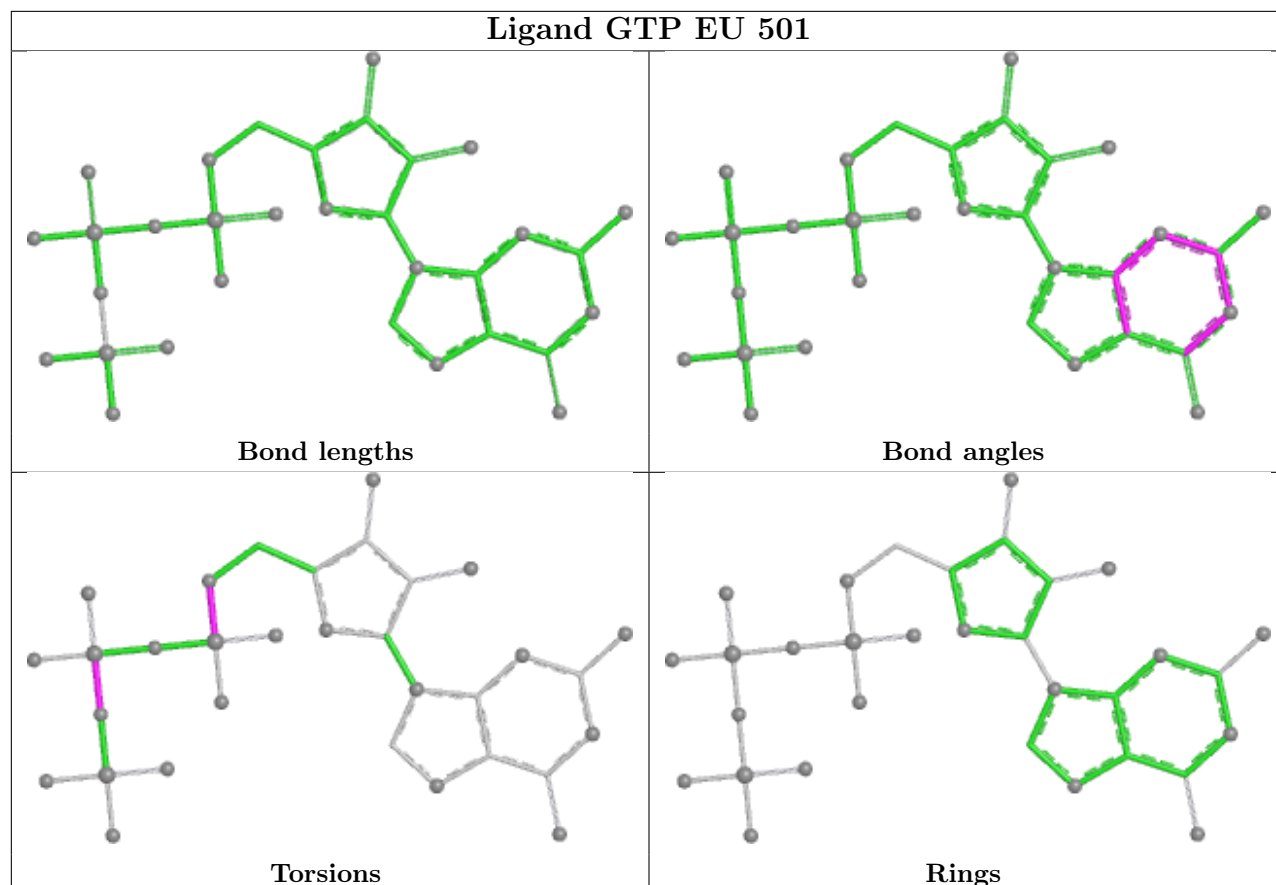
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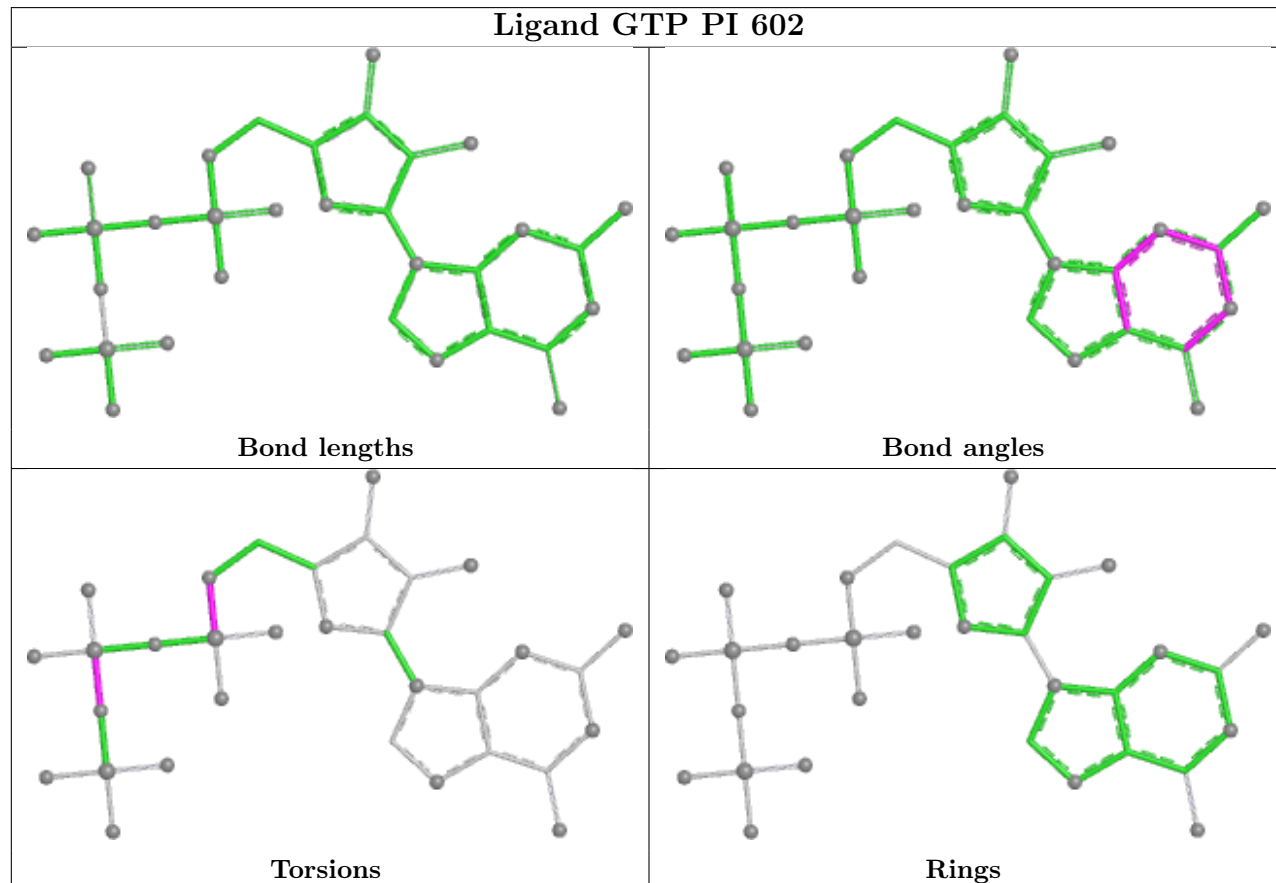
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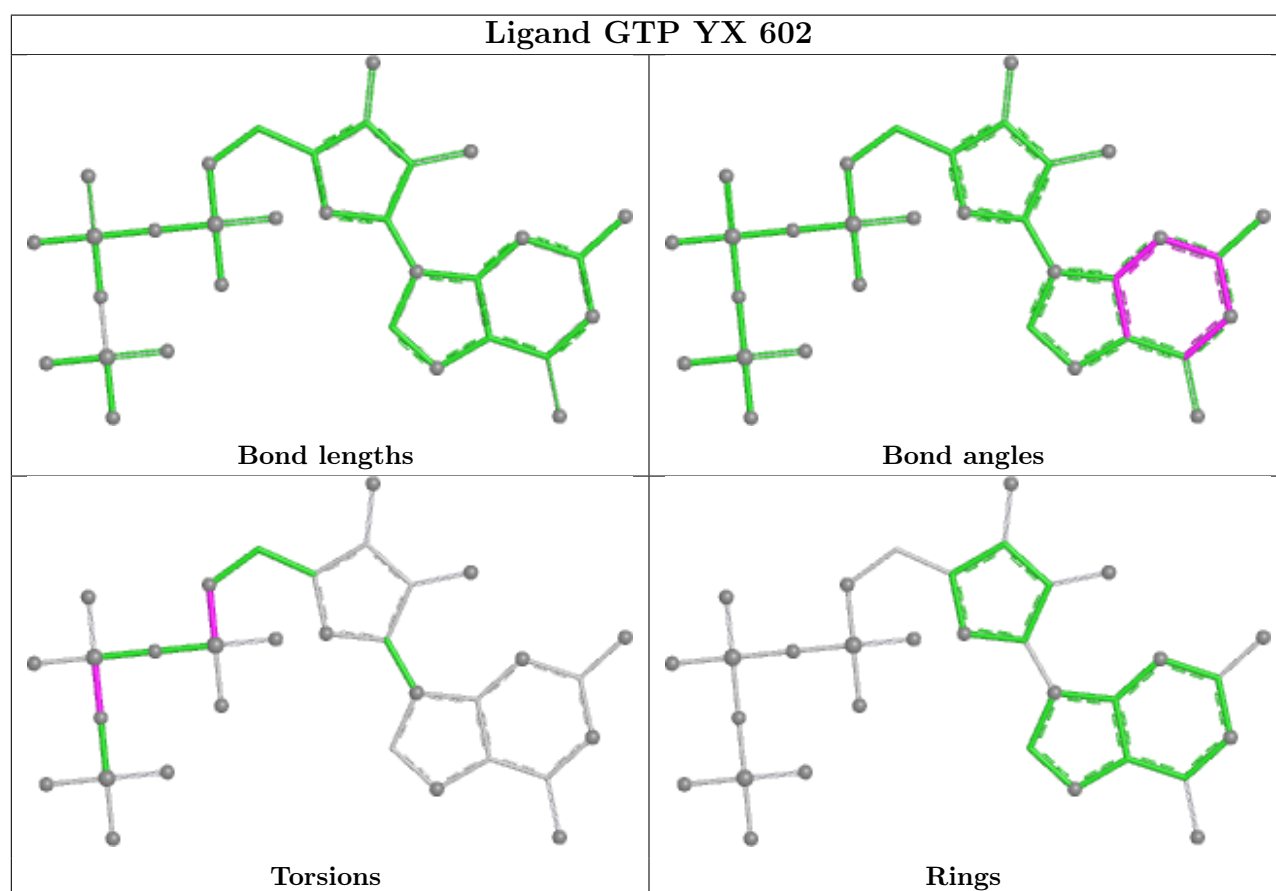
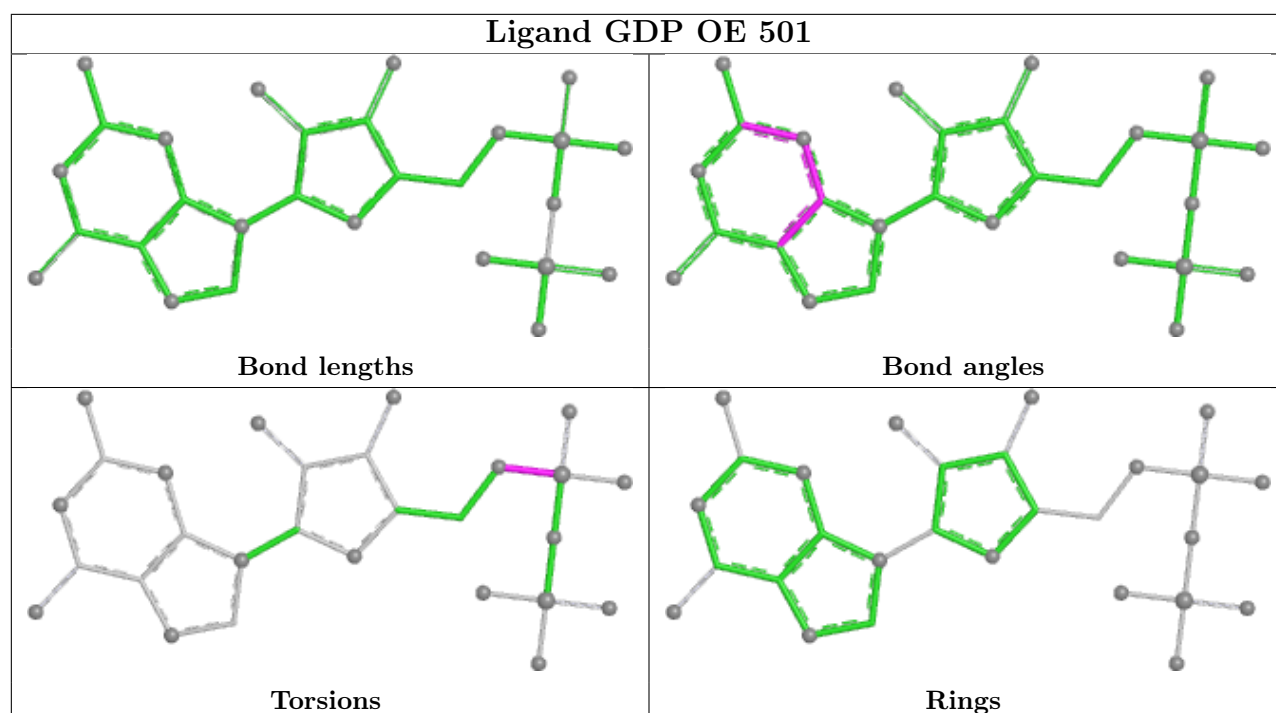


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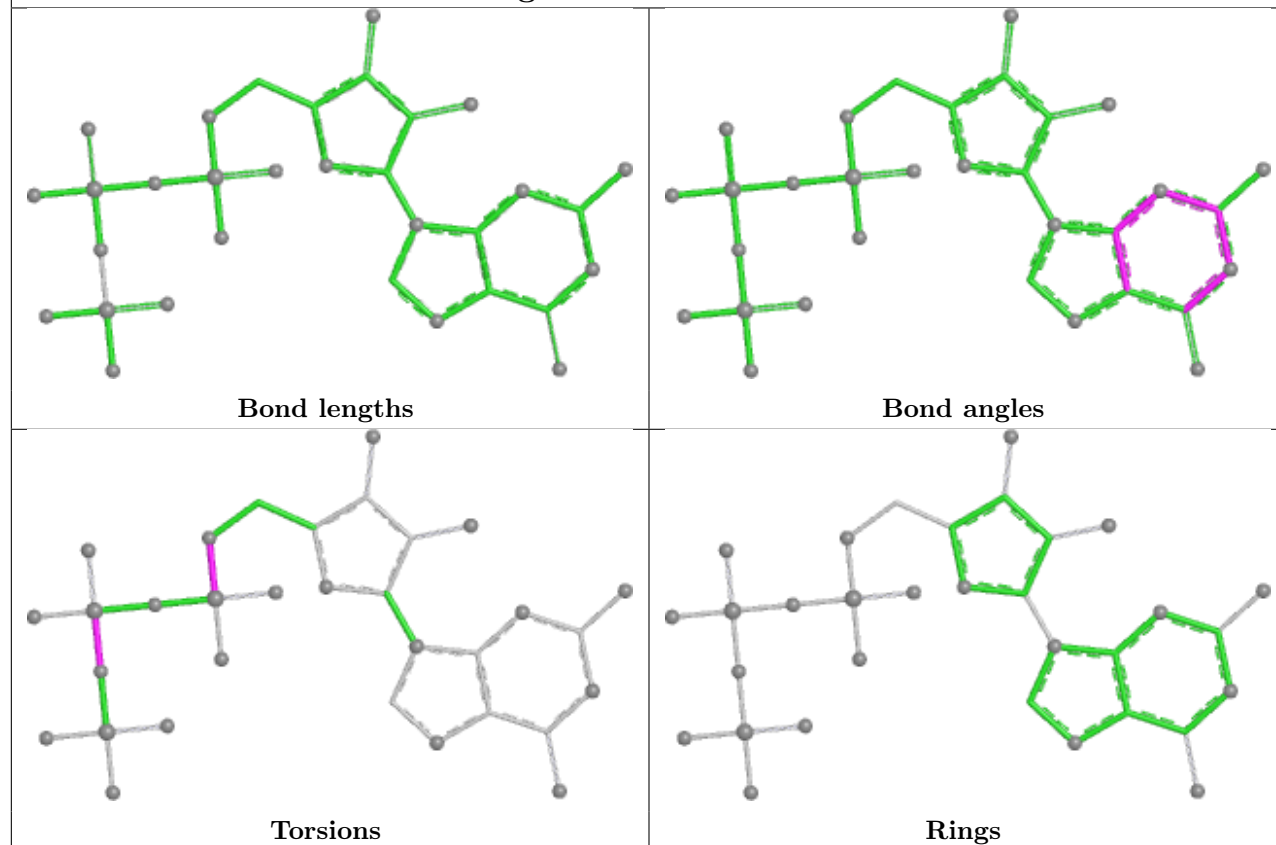


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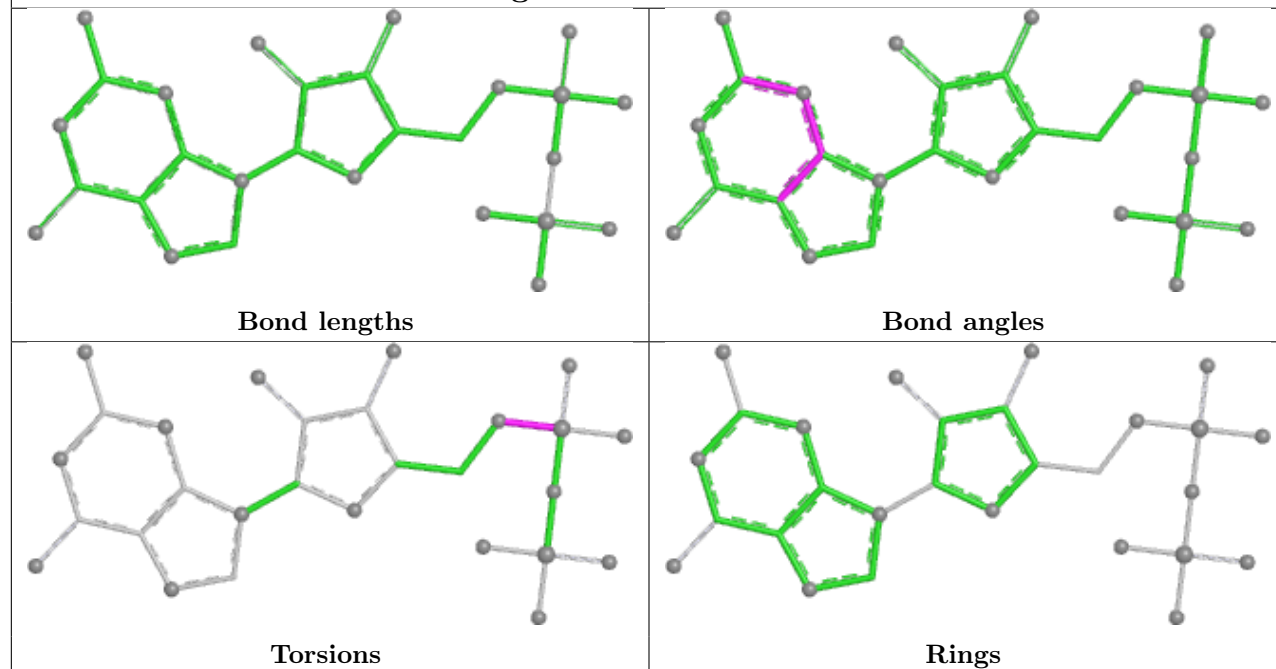


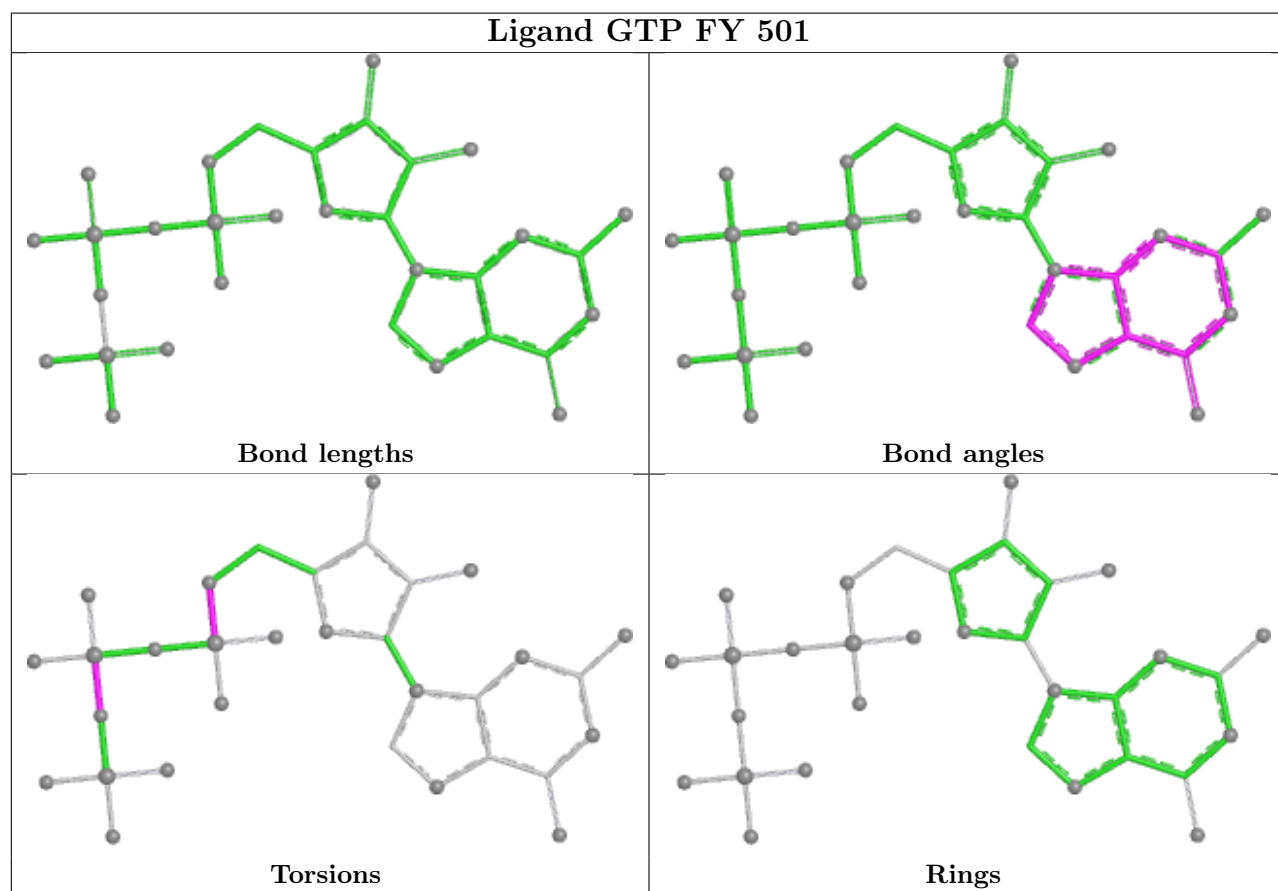
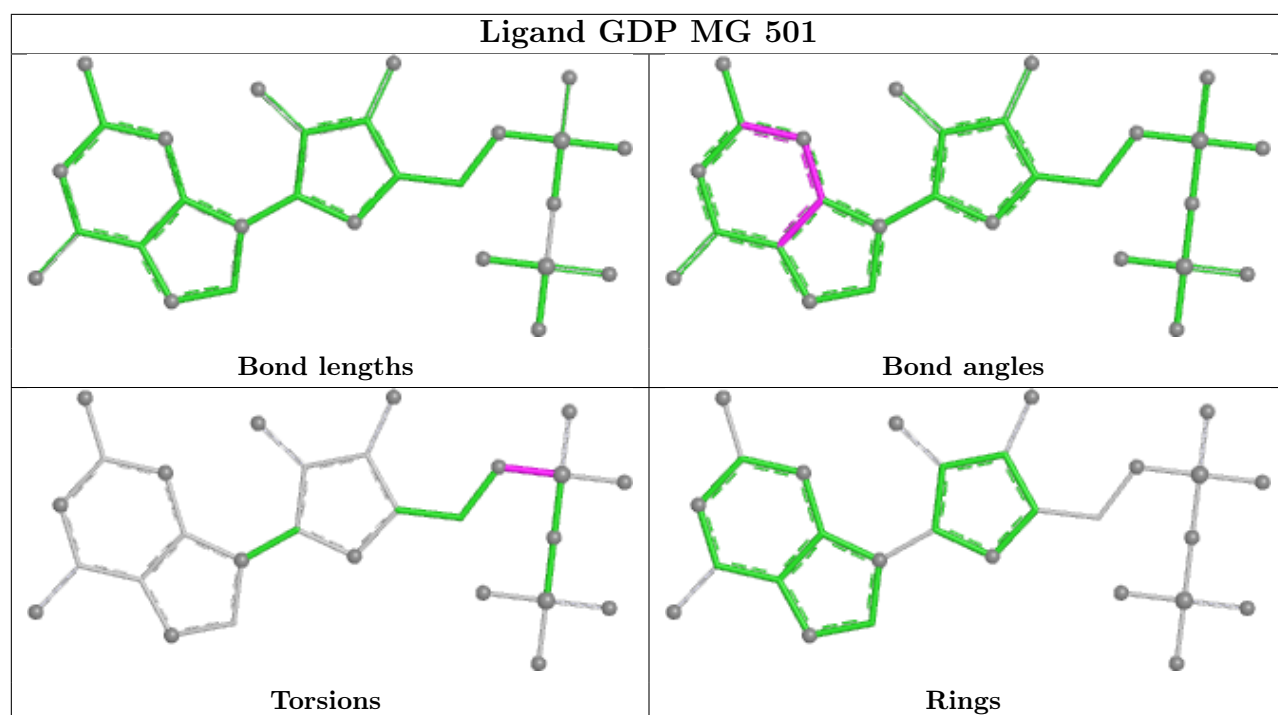


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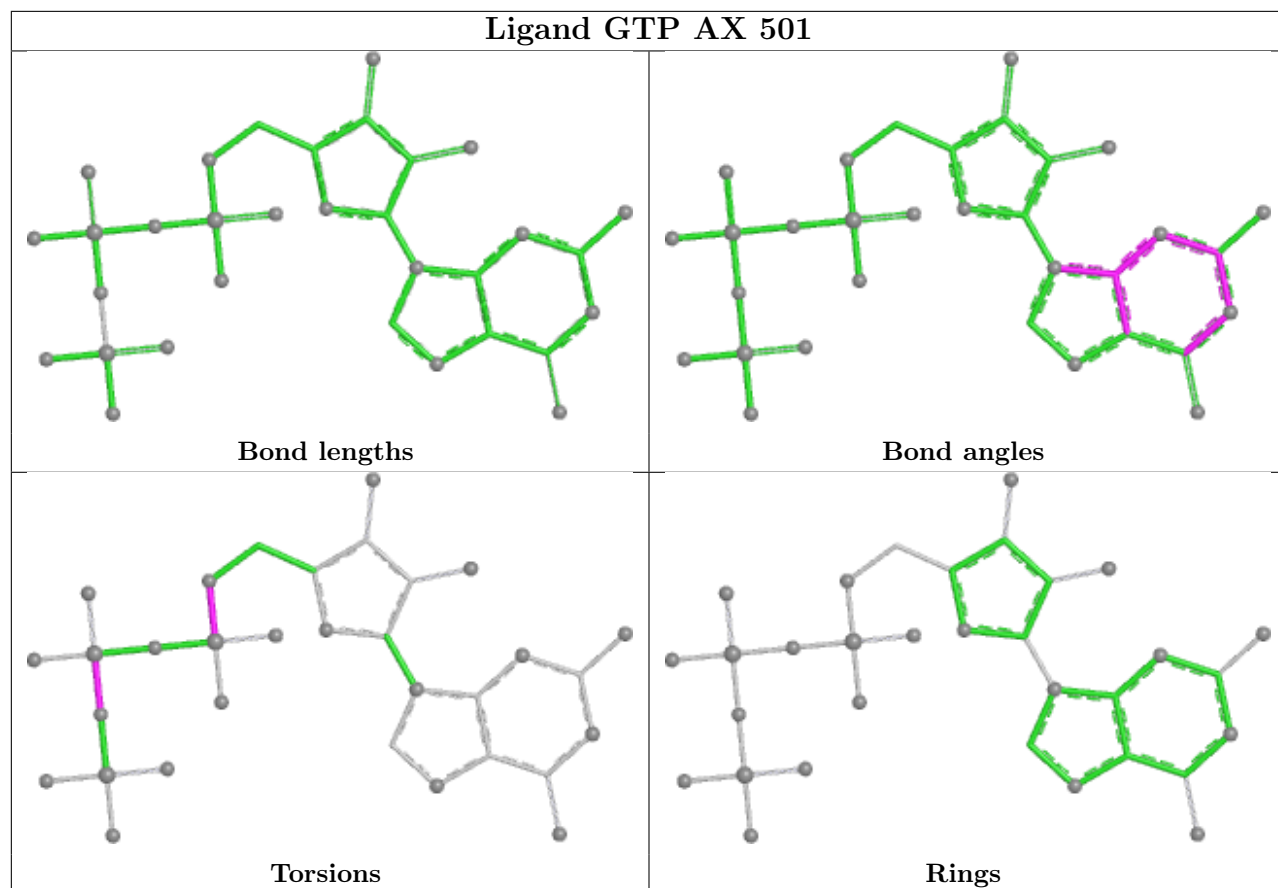


## Ligand GDP WT 501

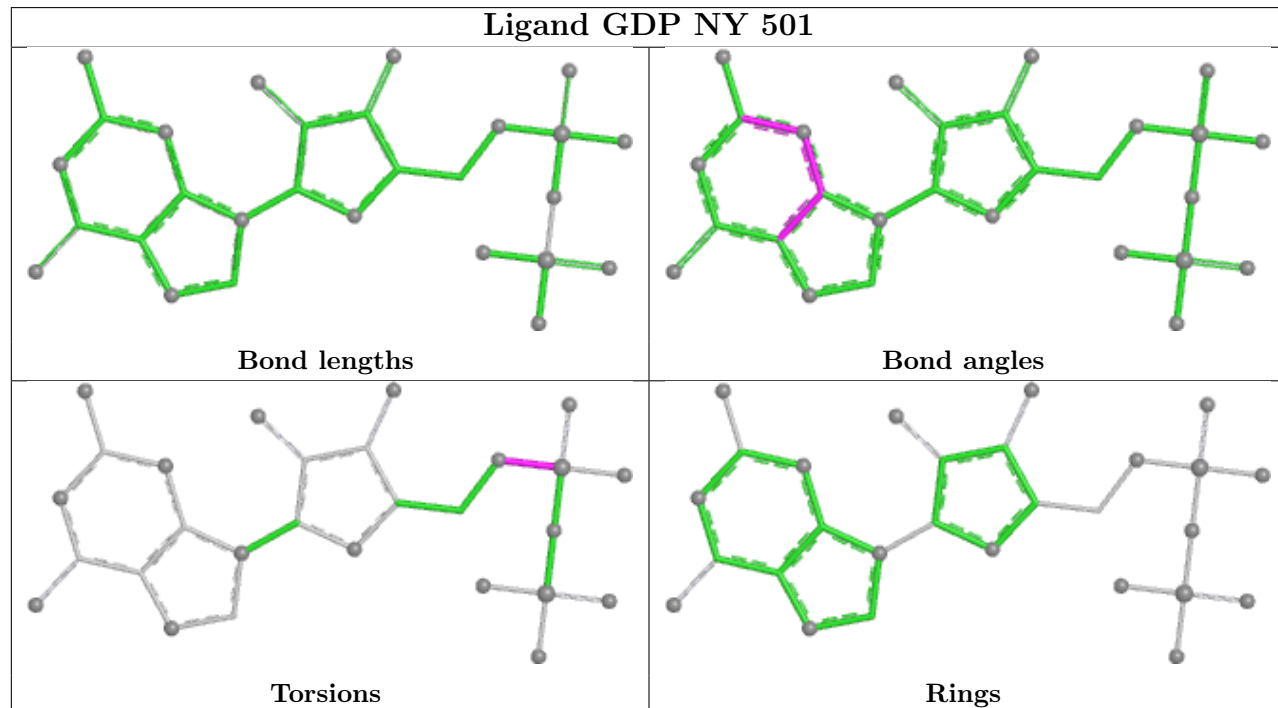




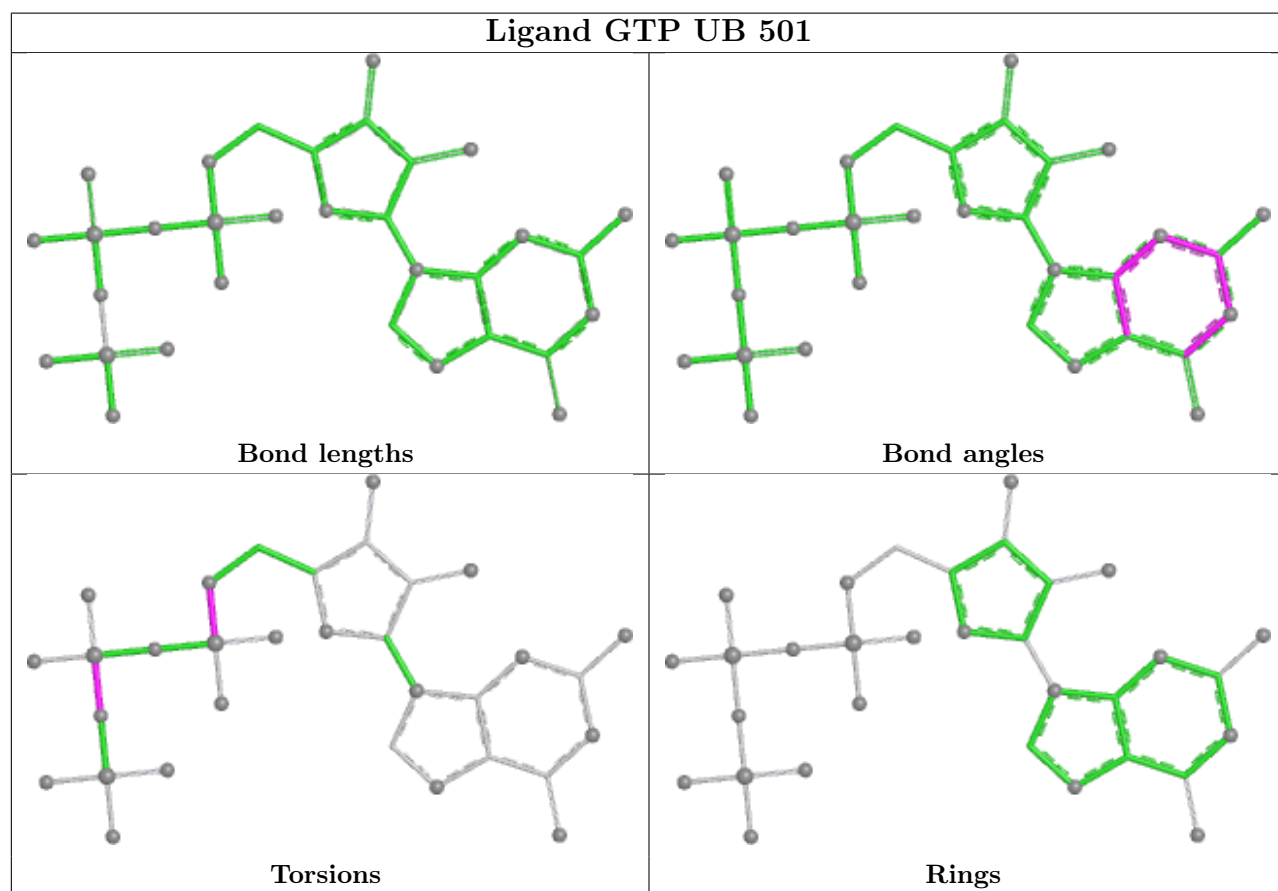
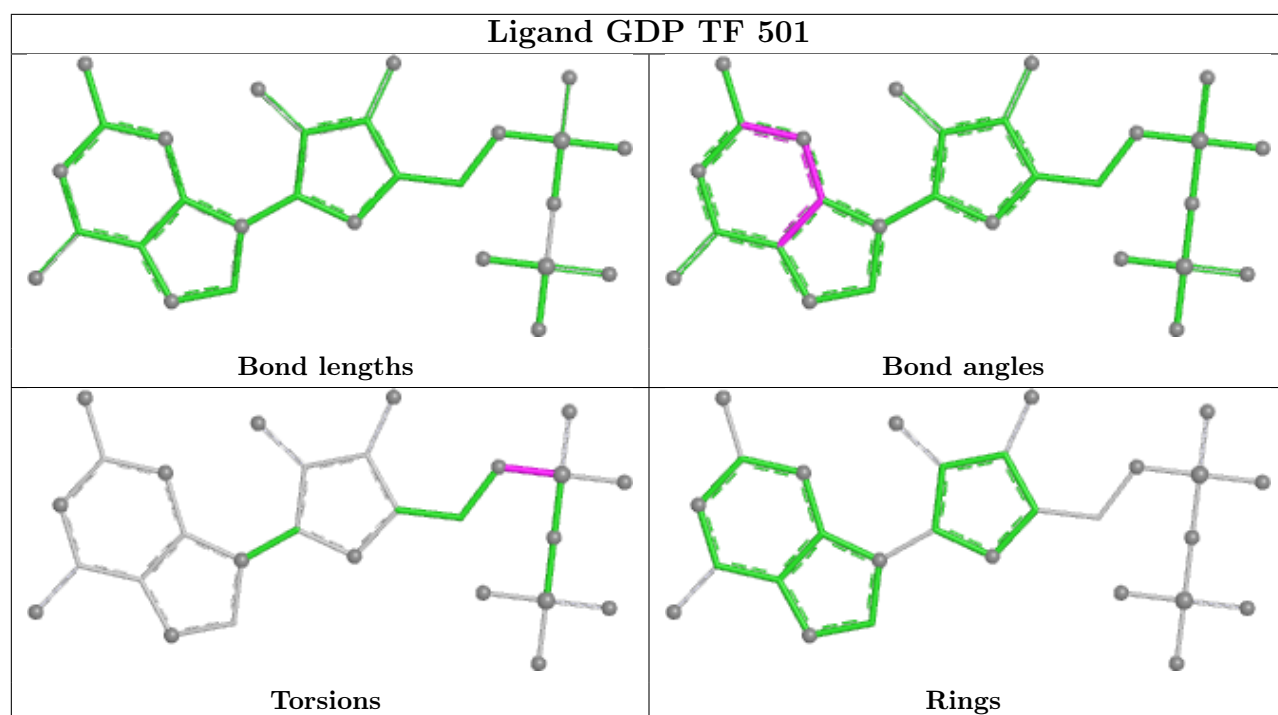
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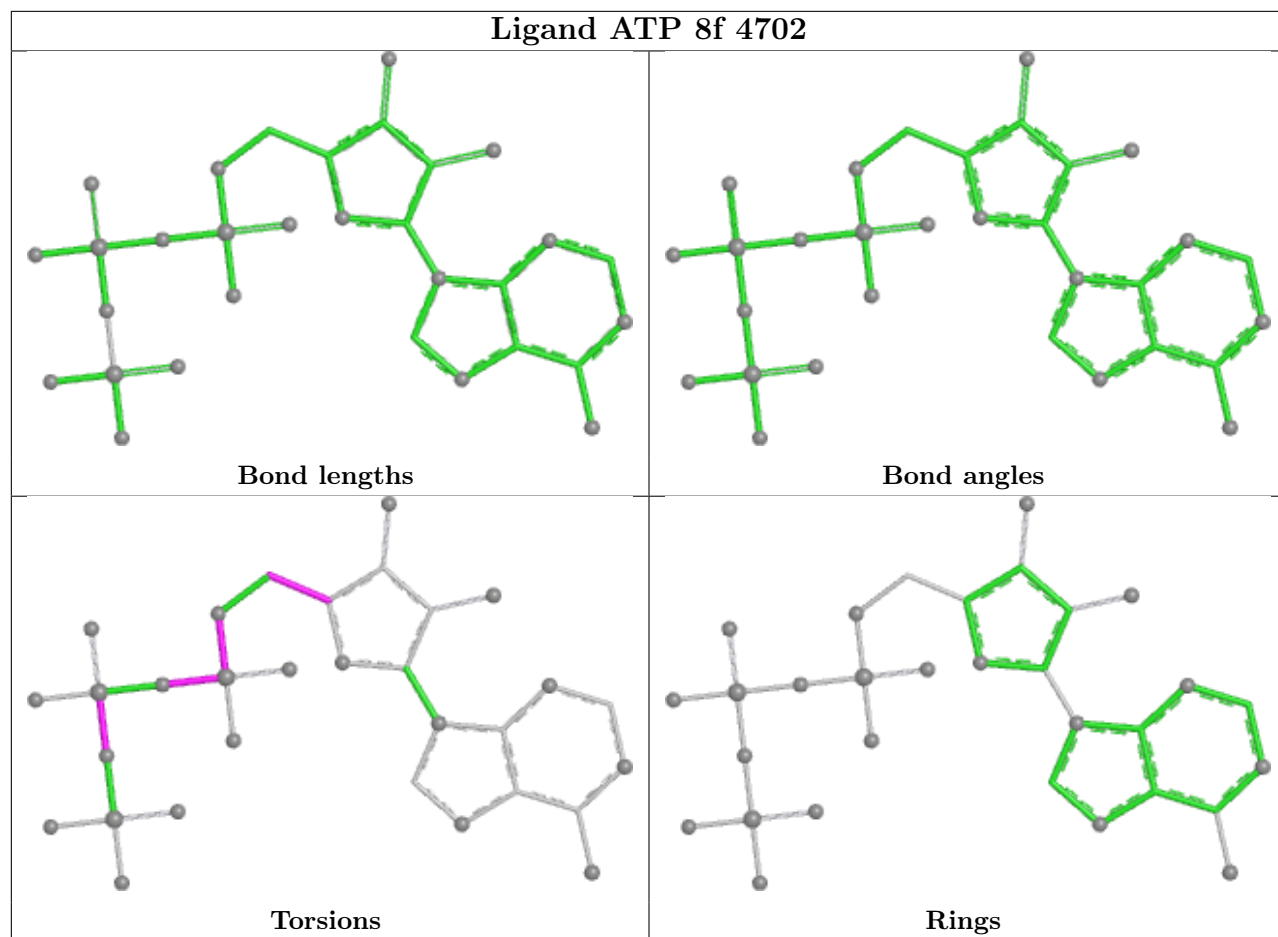


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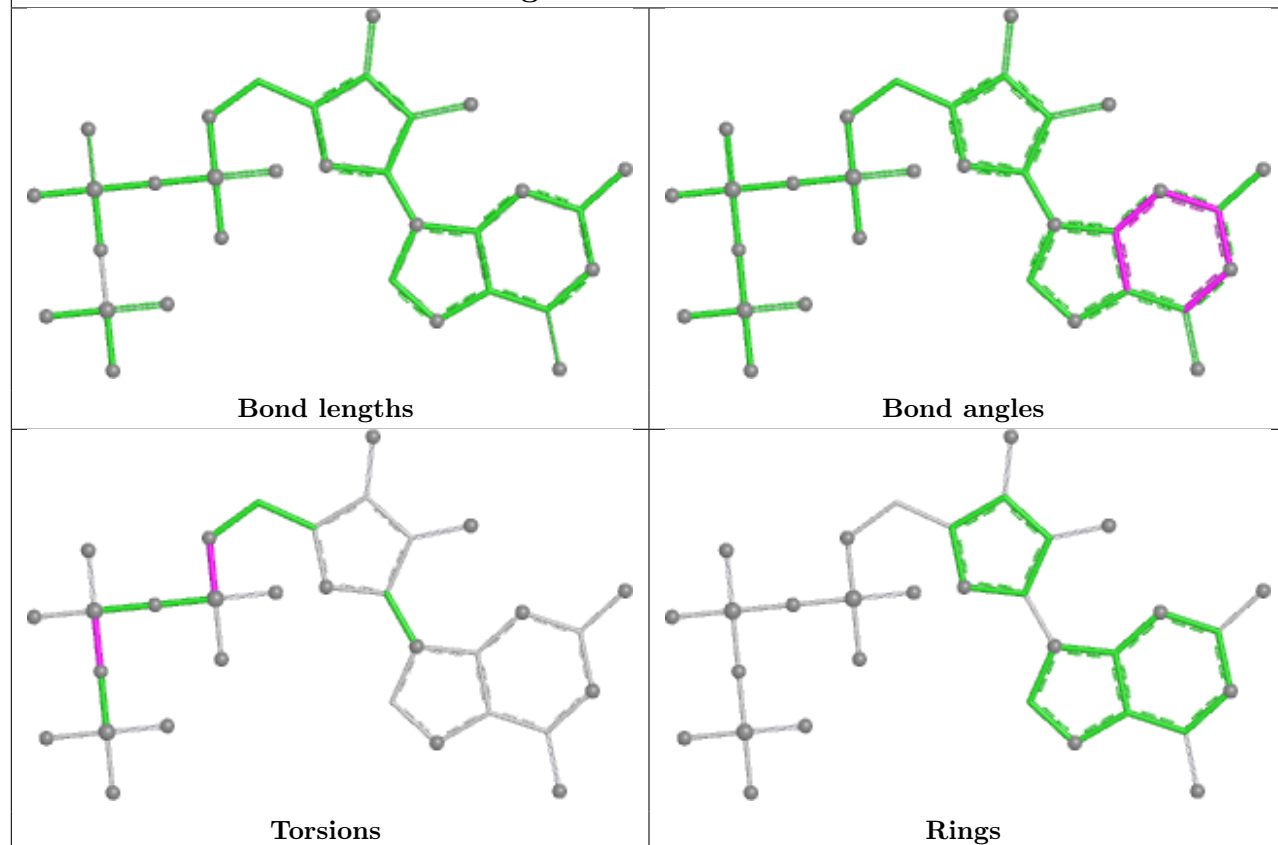




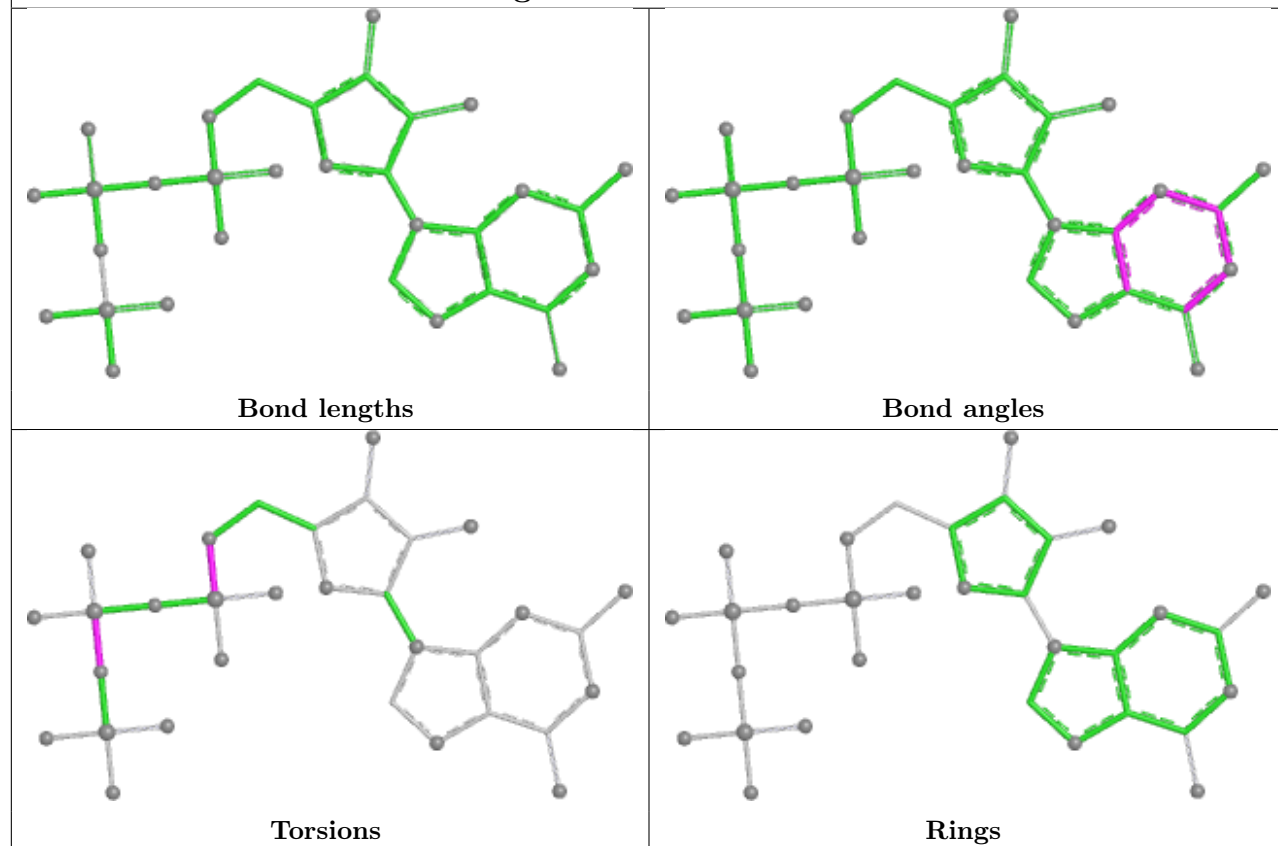


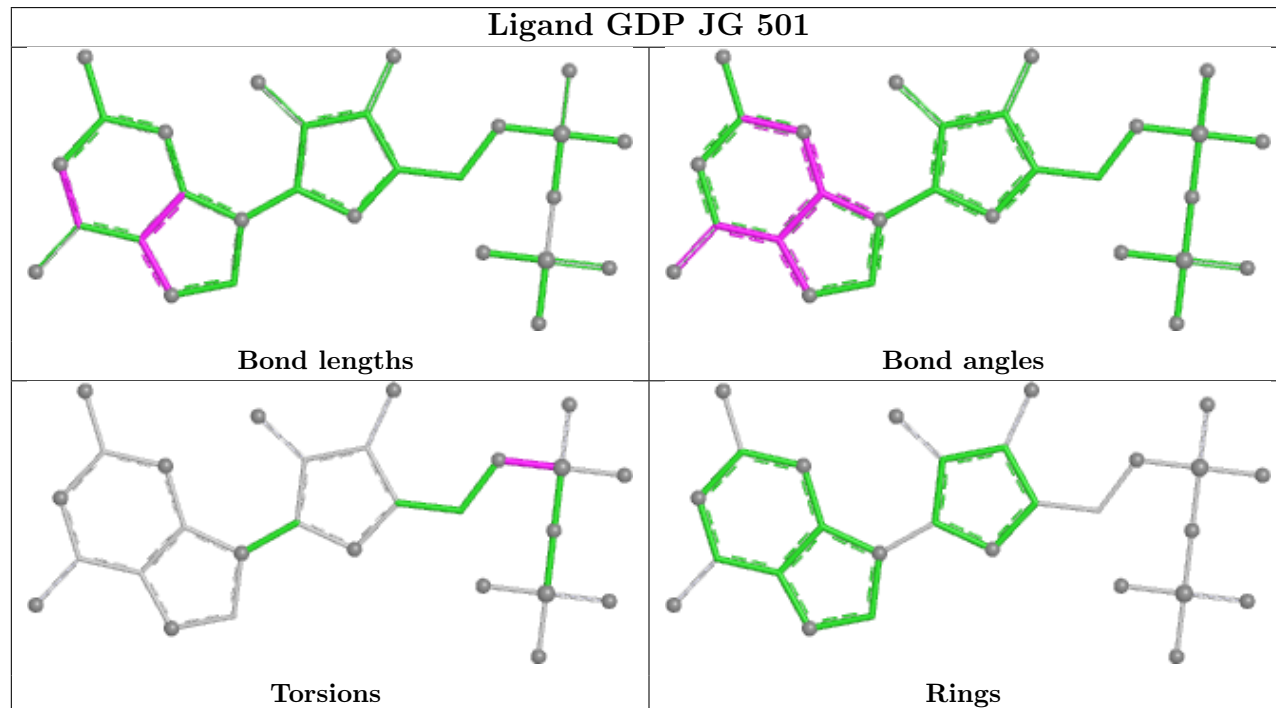
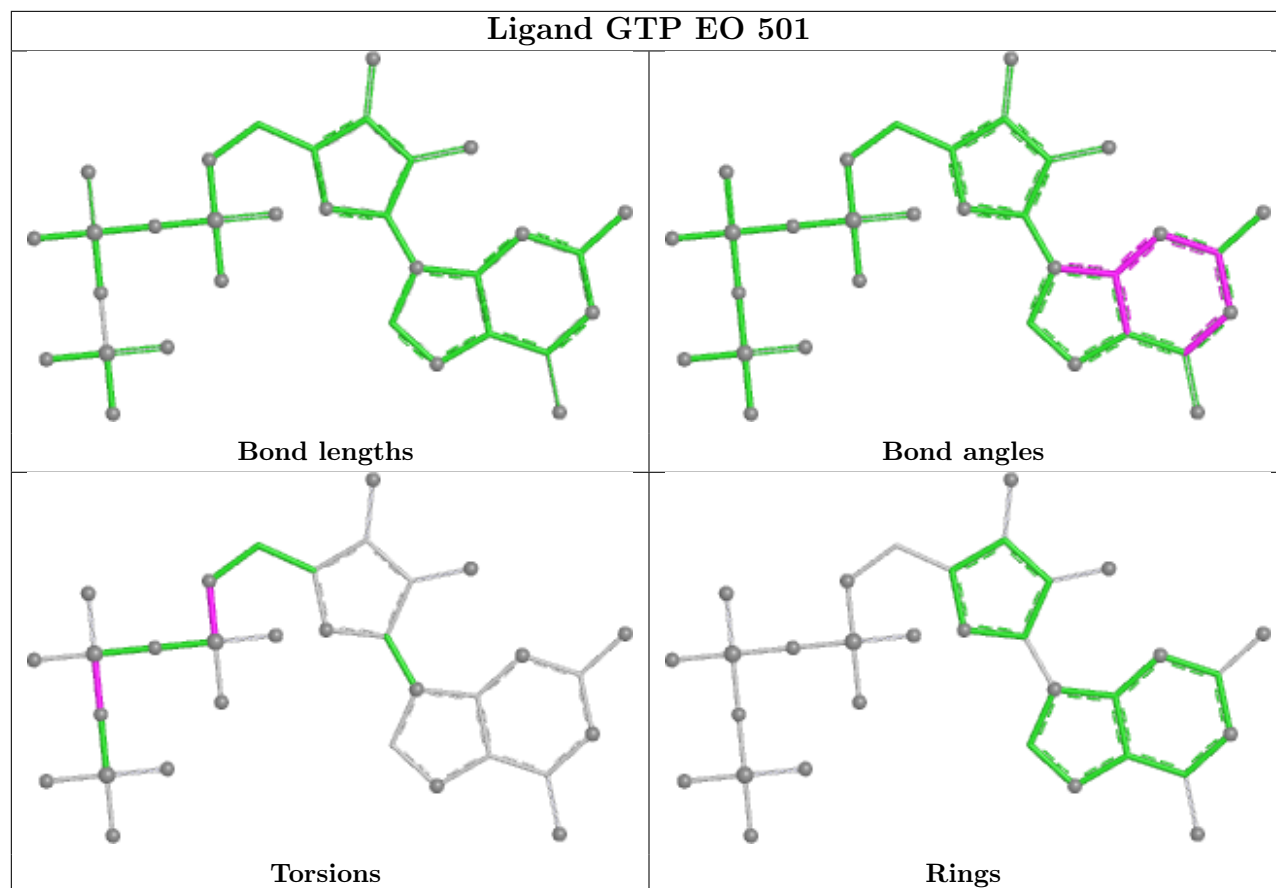


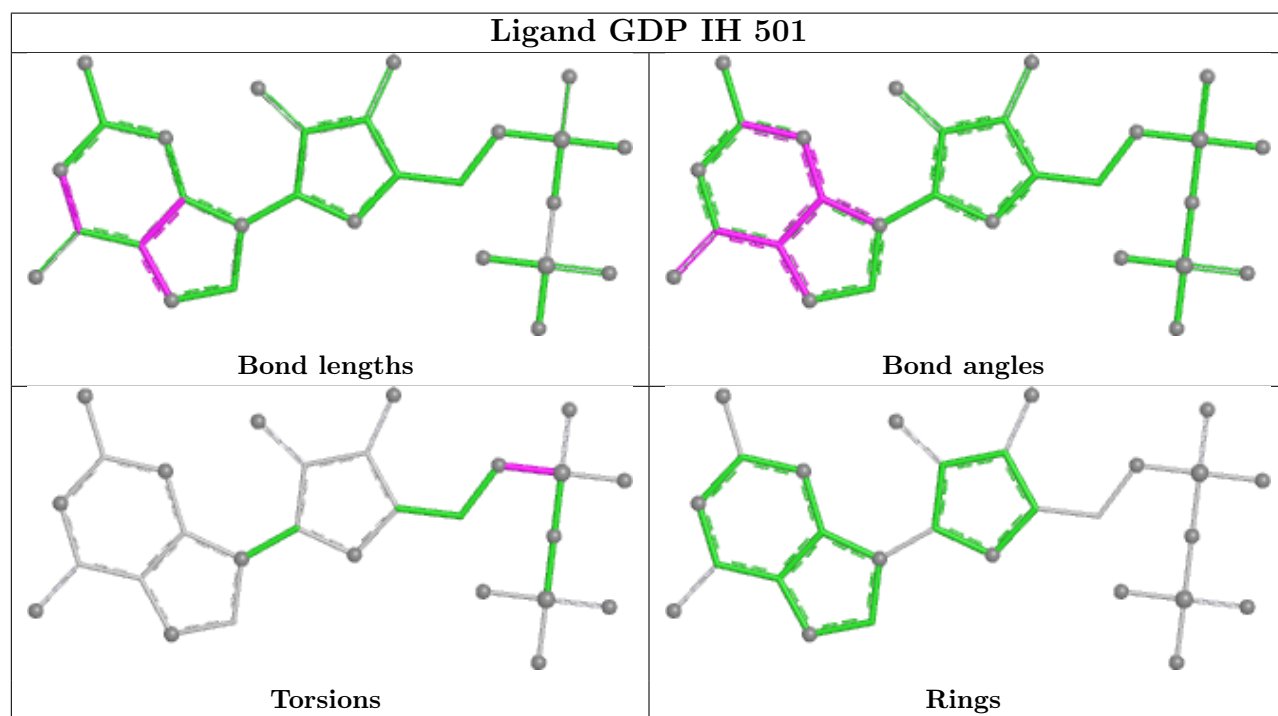
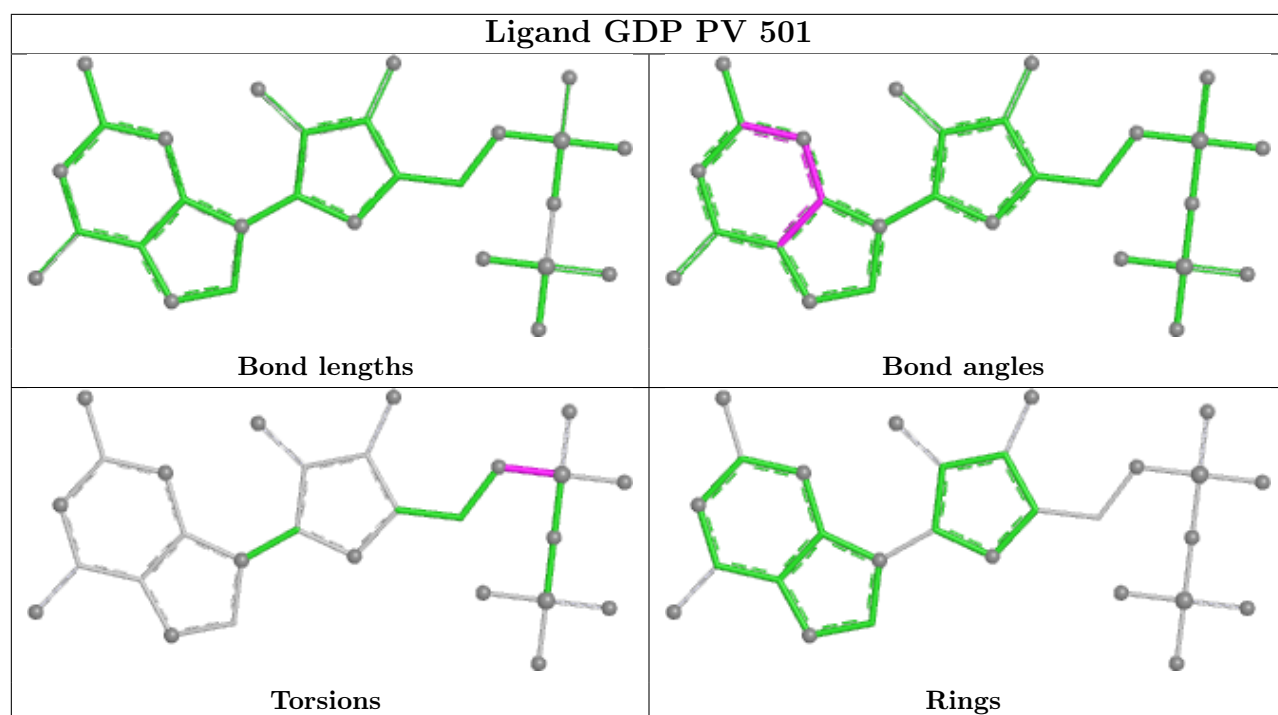
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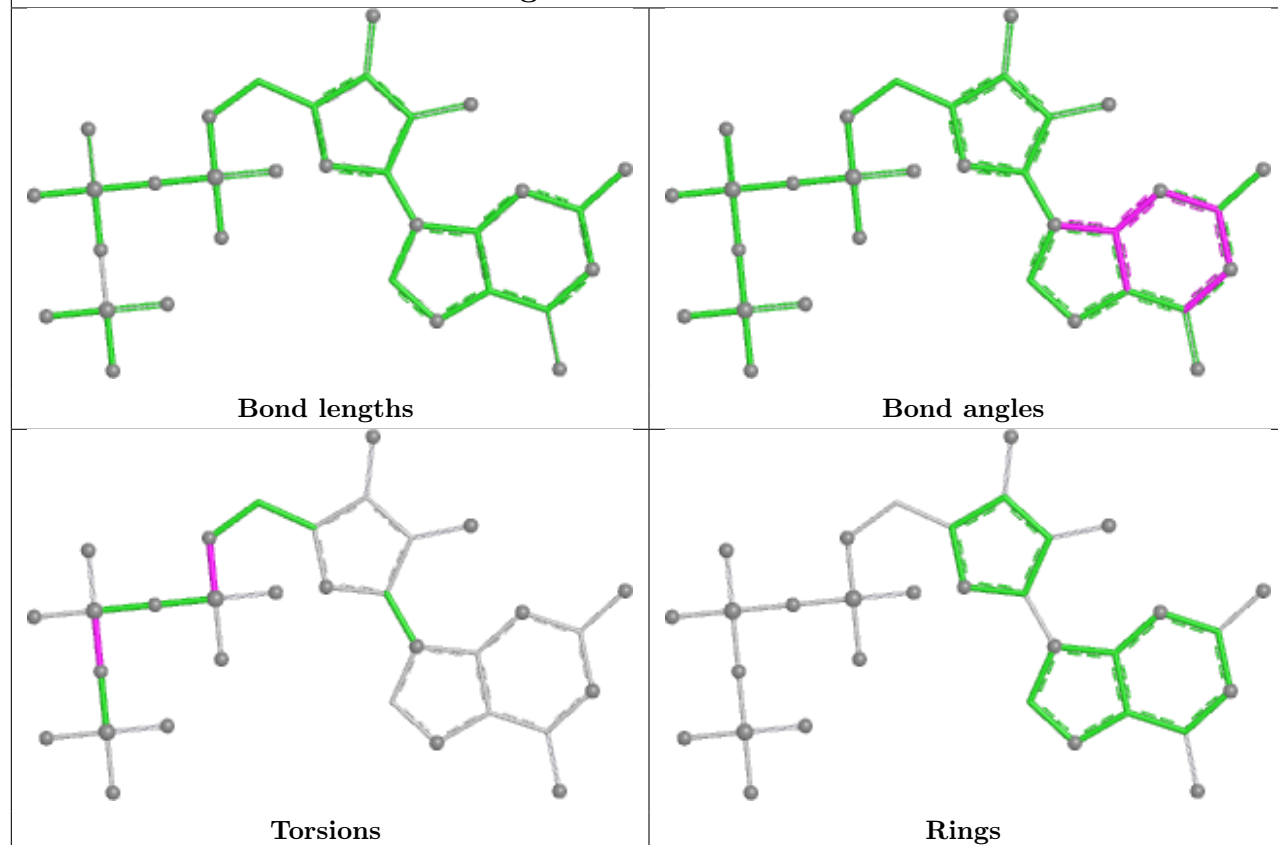
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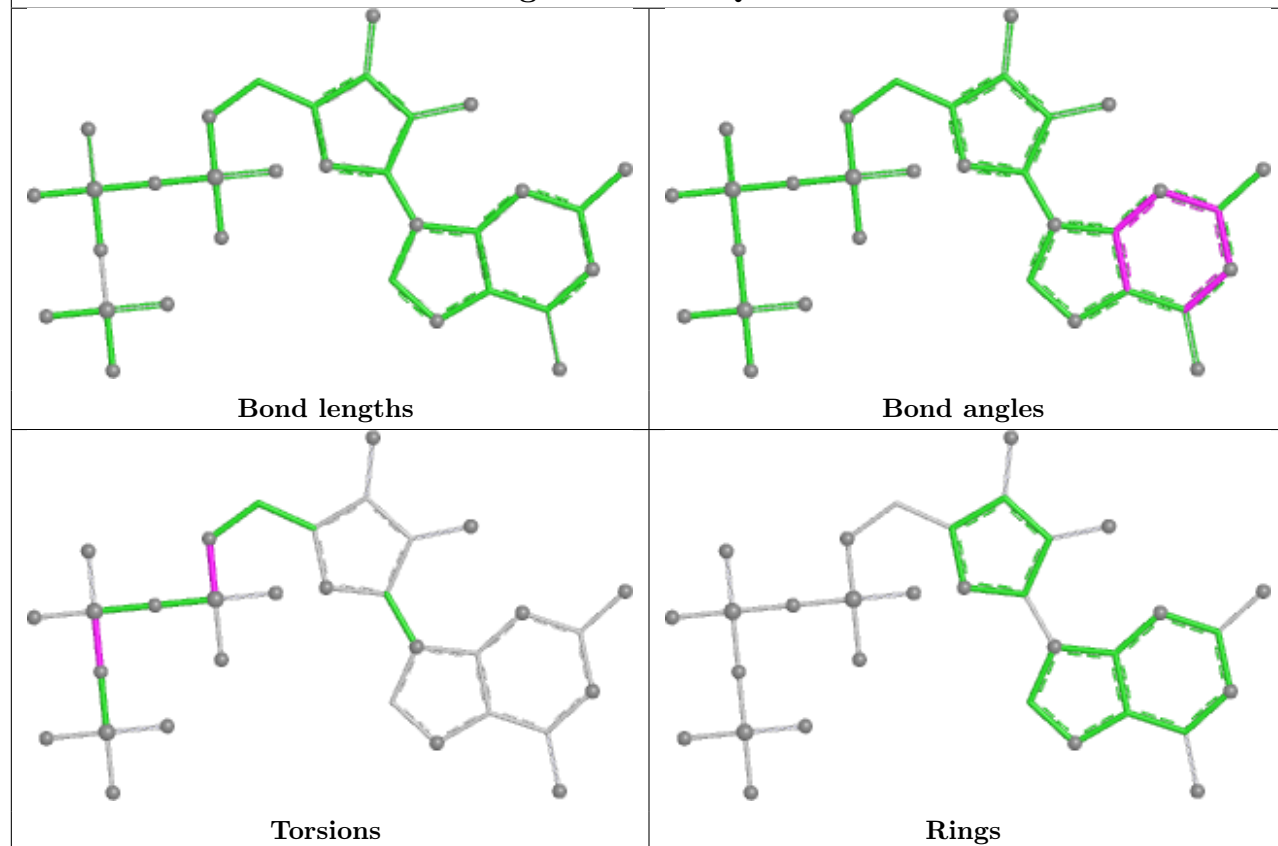


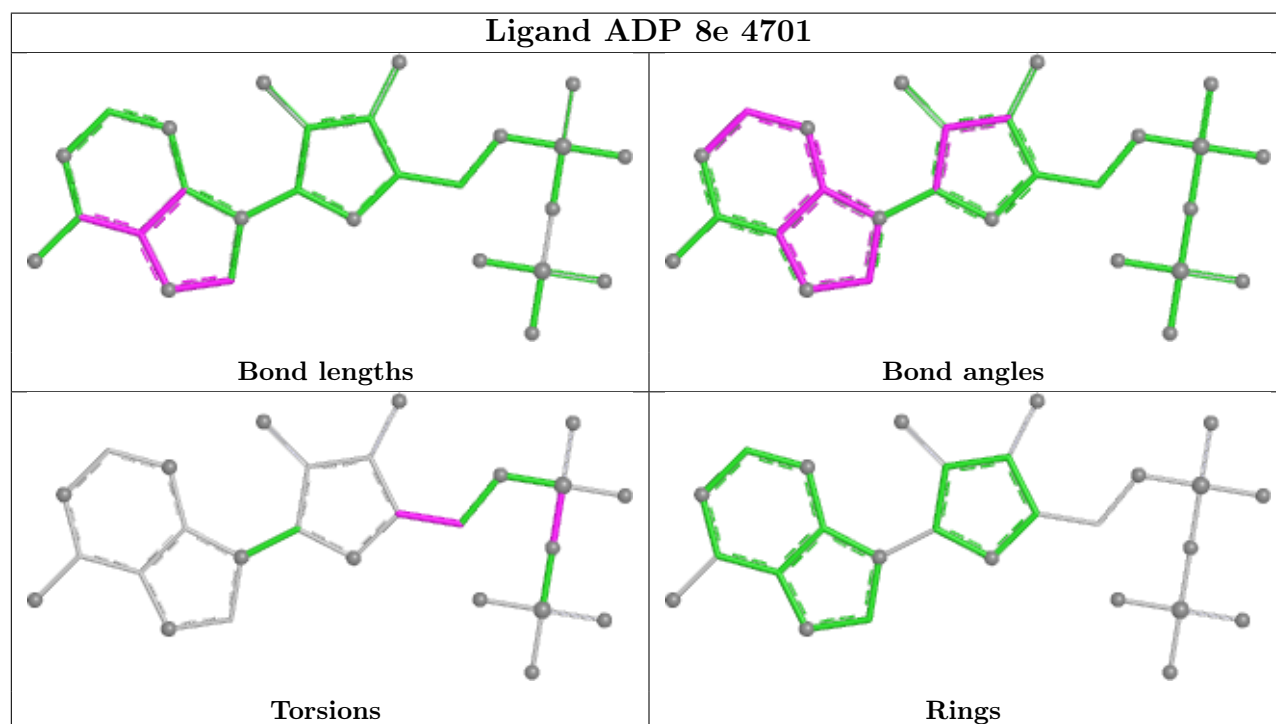
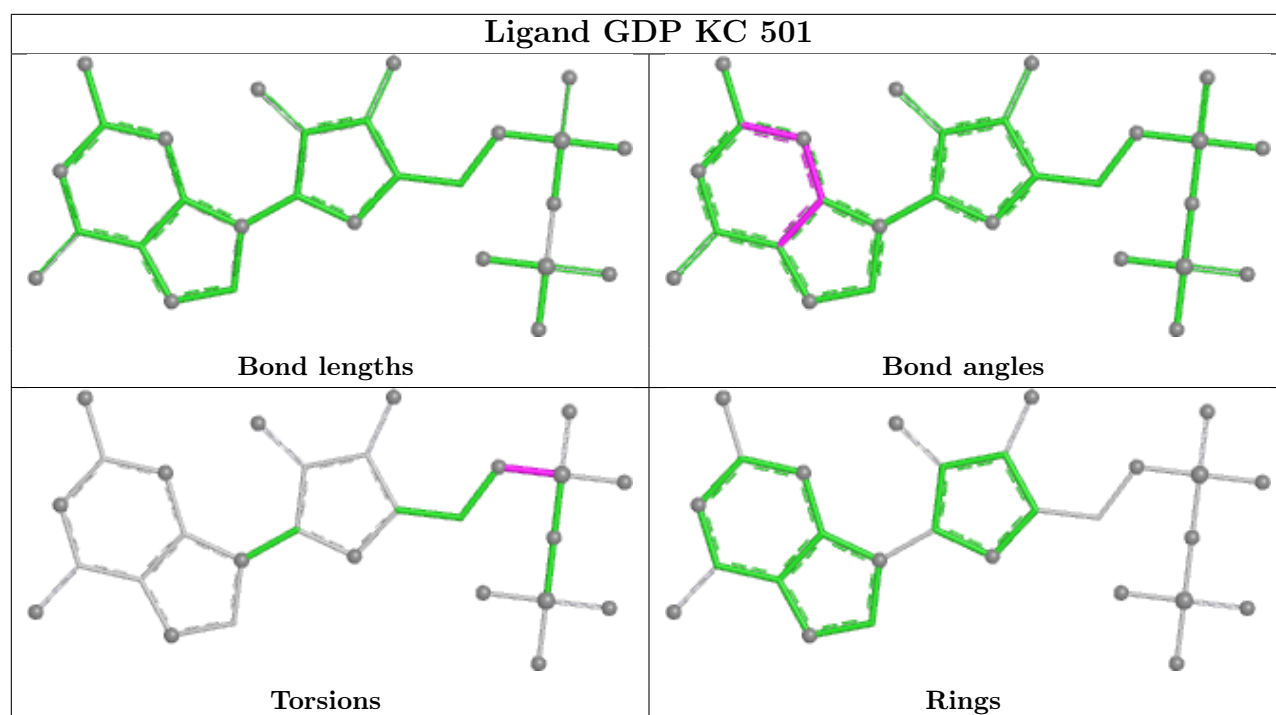


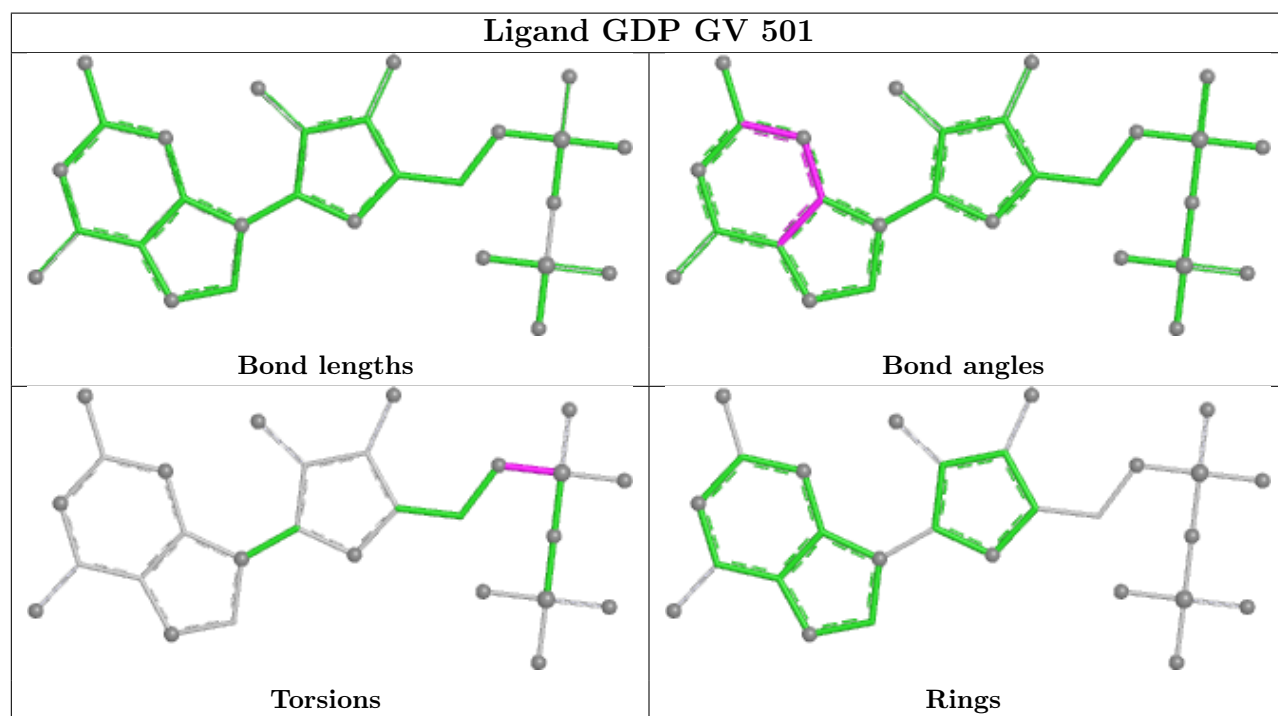
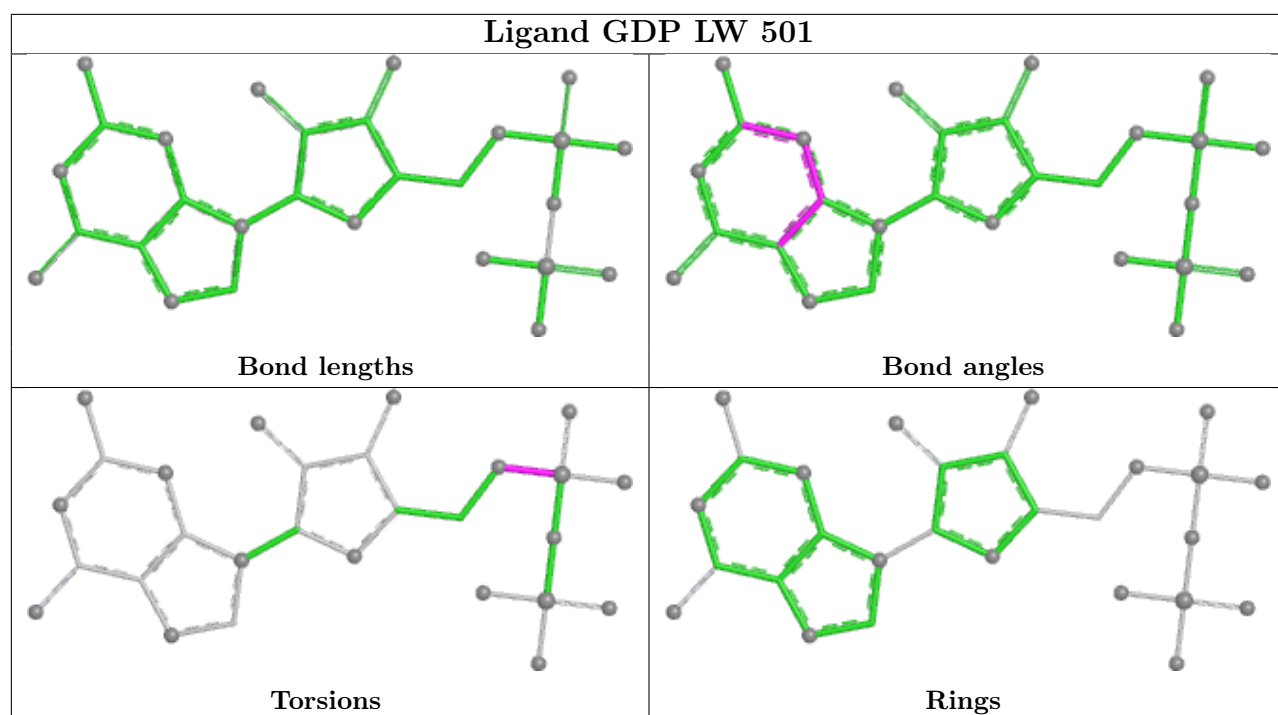
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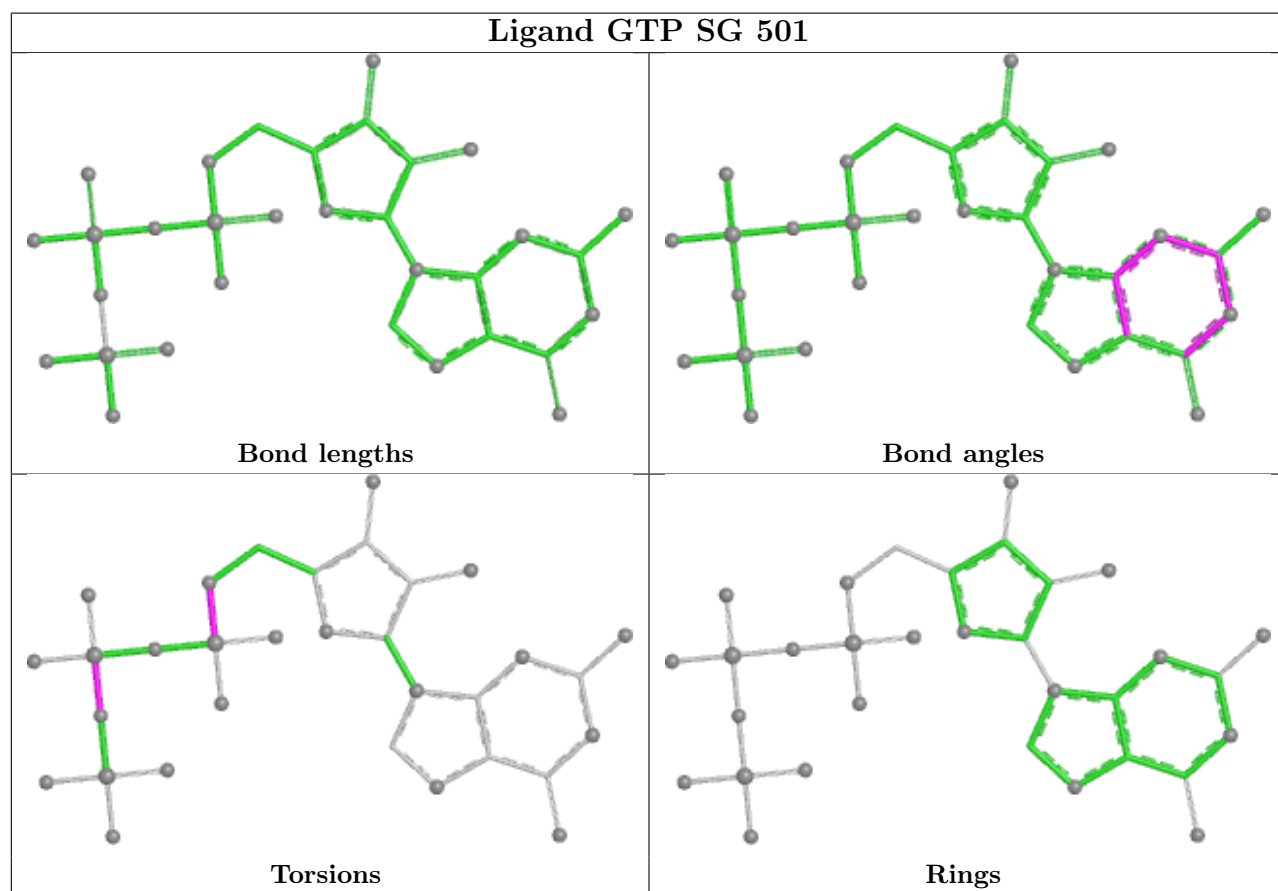
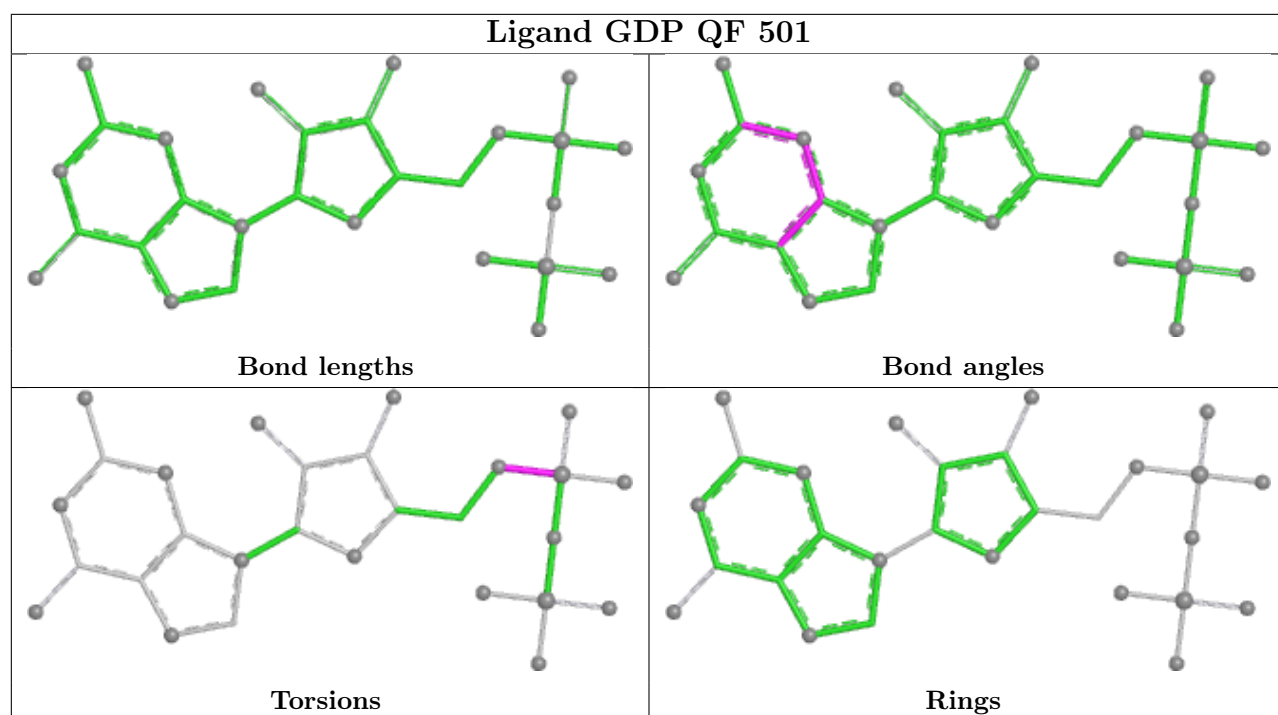
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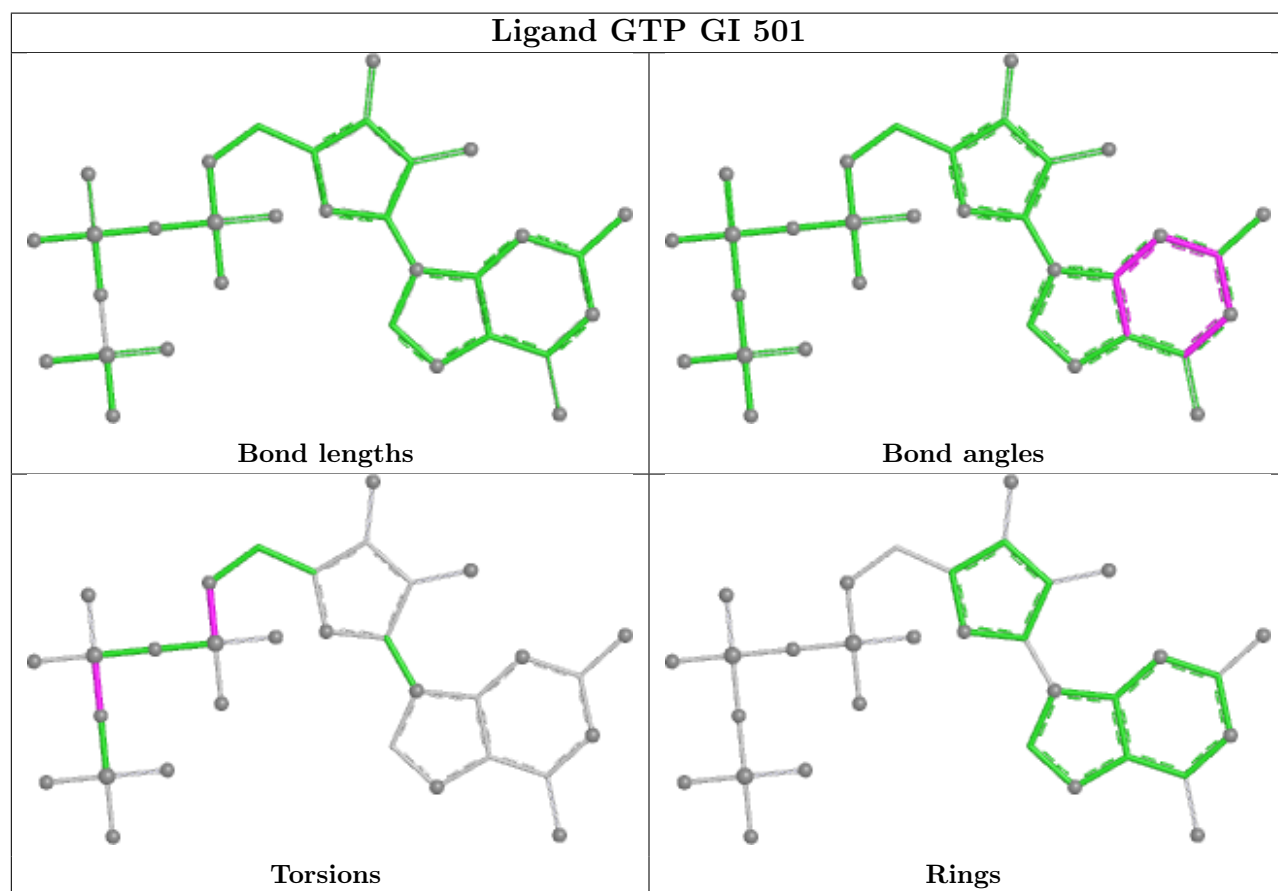
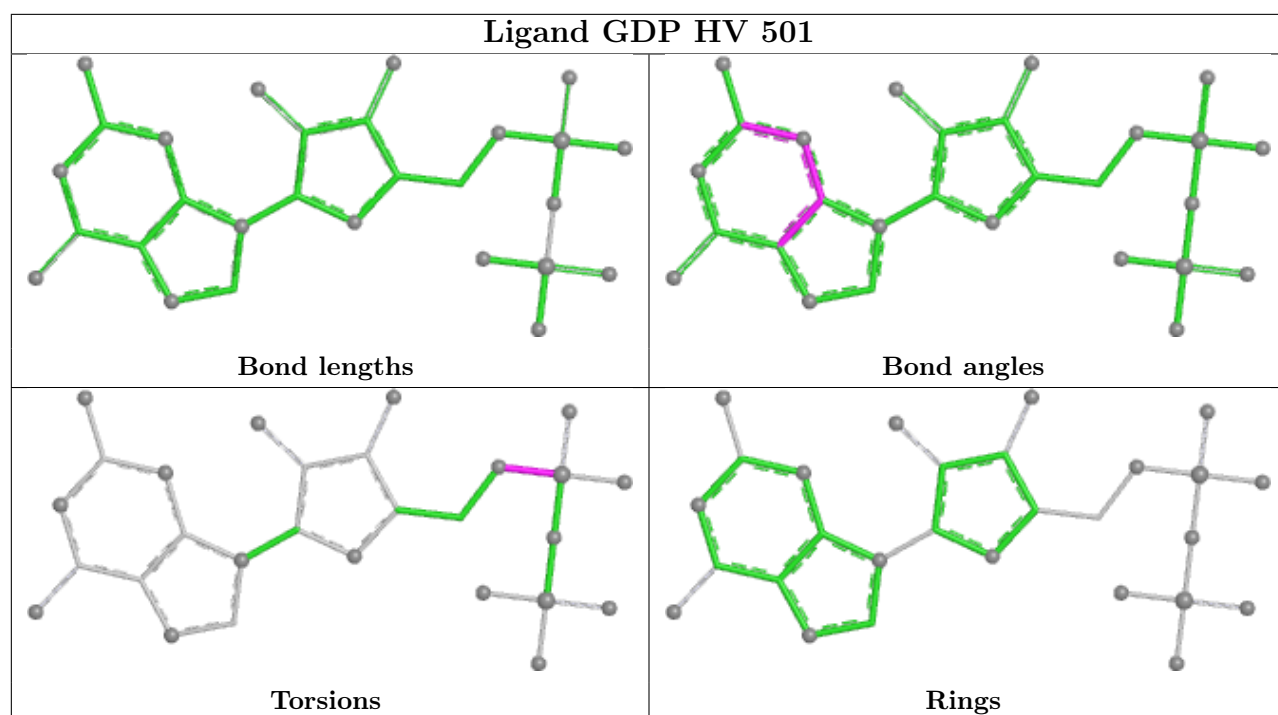




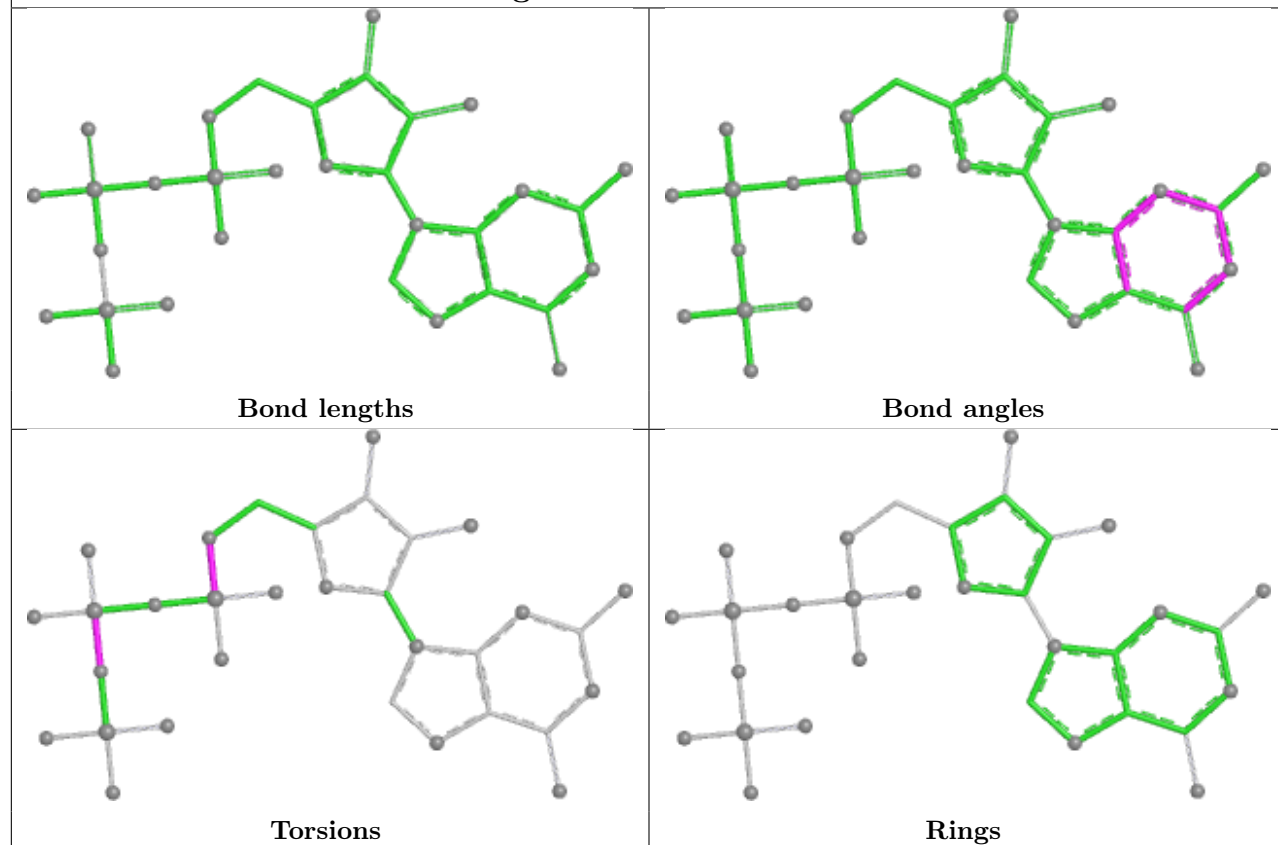




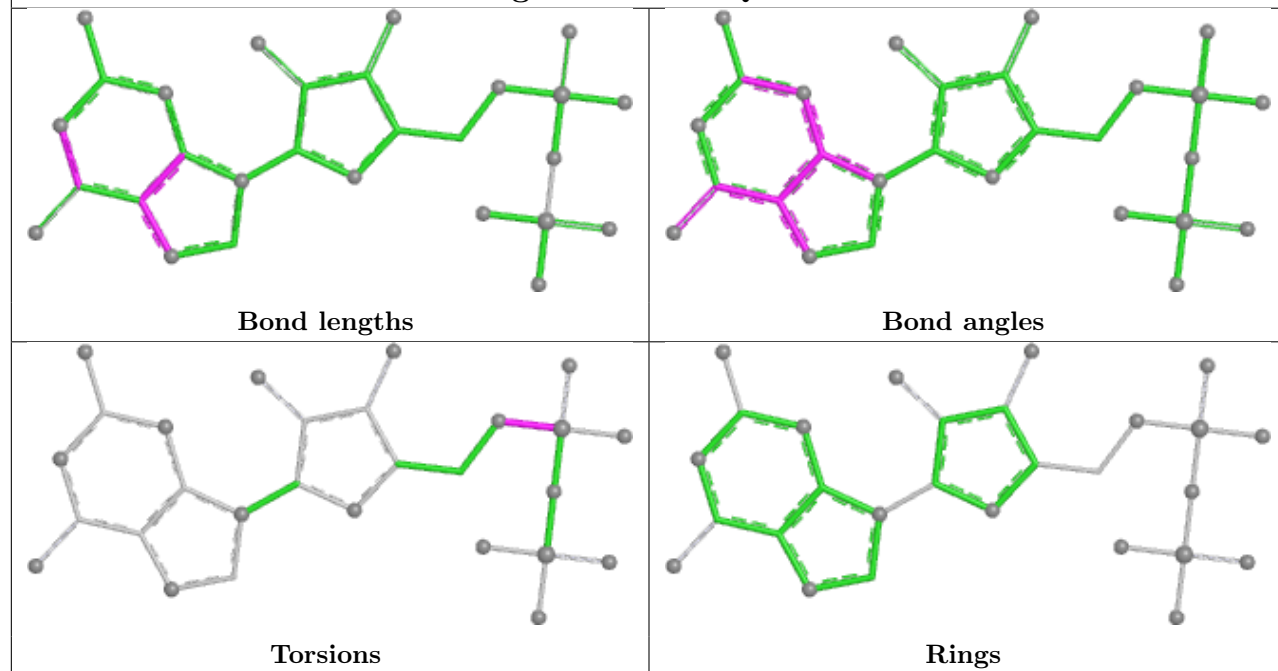


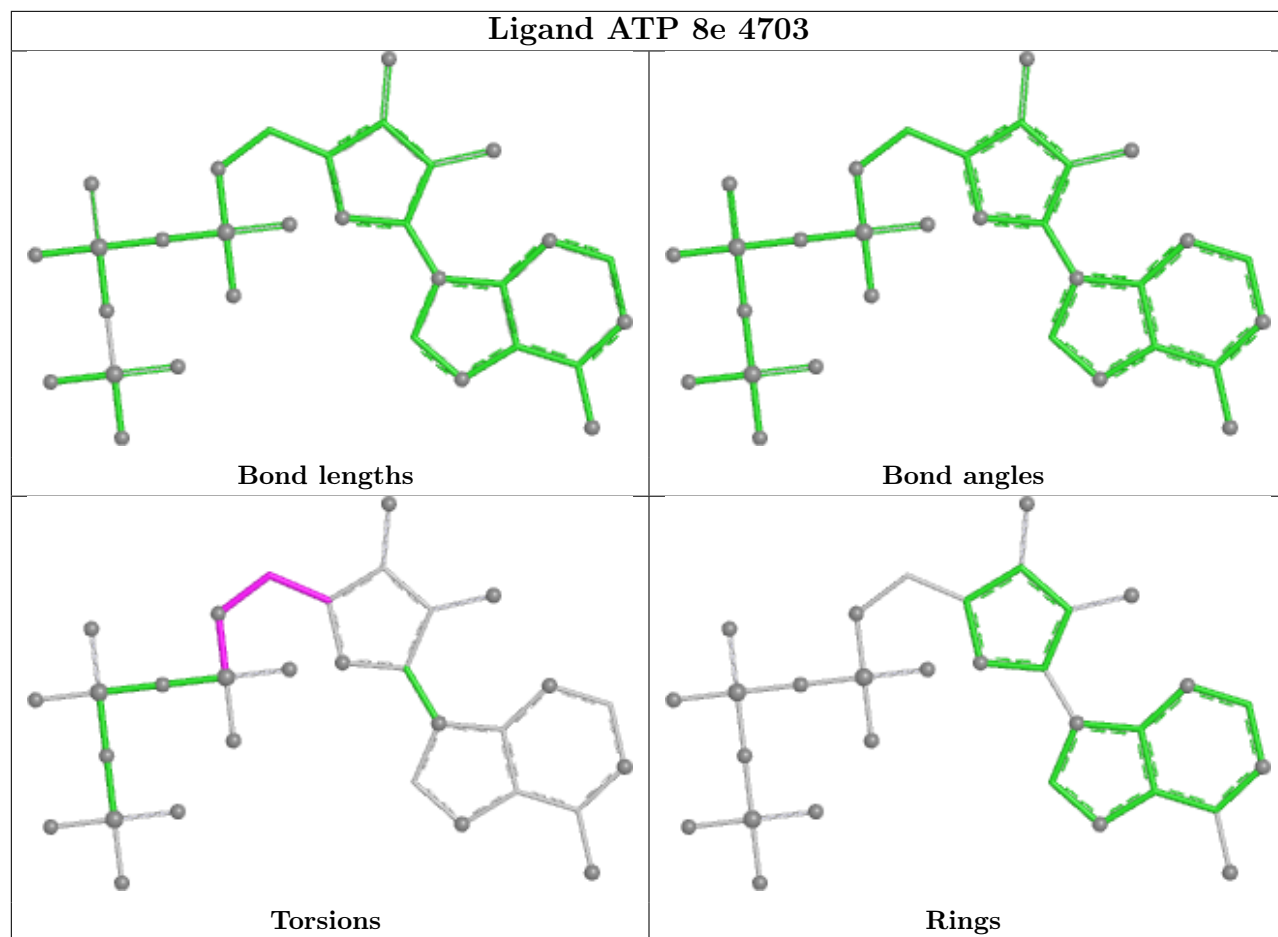


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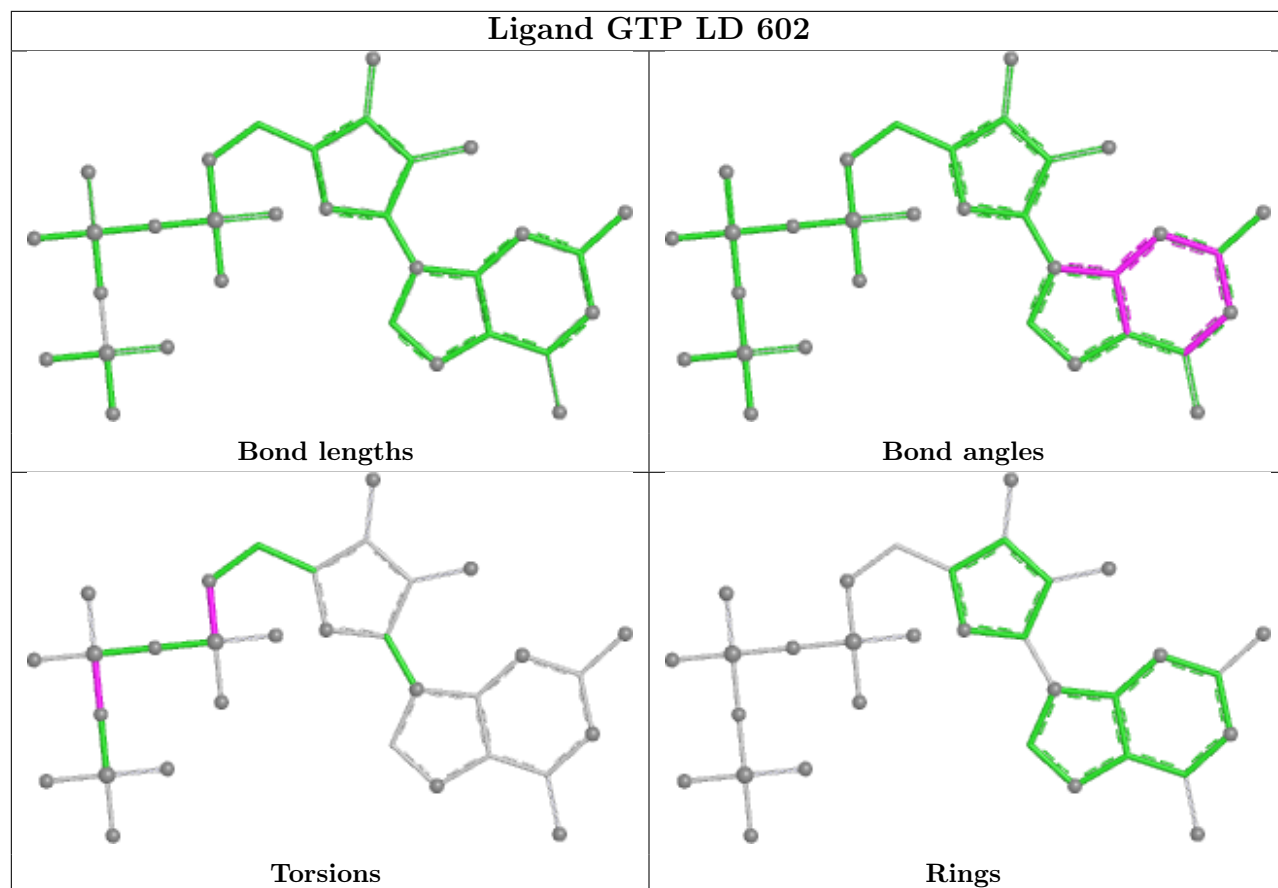


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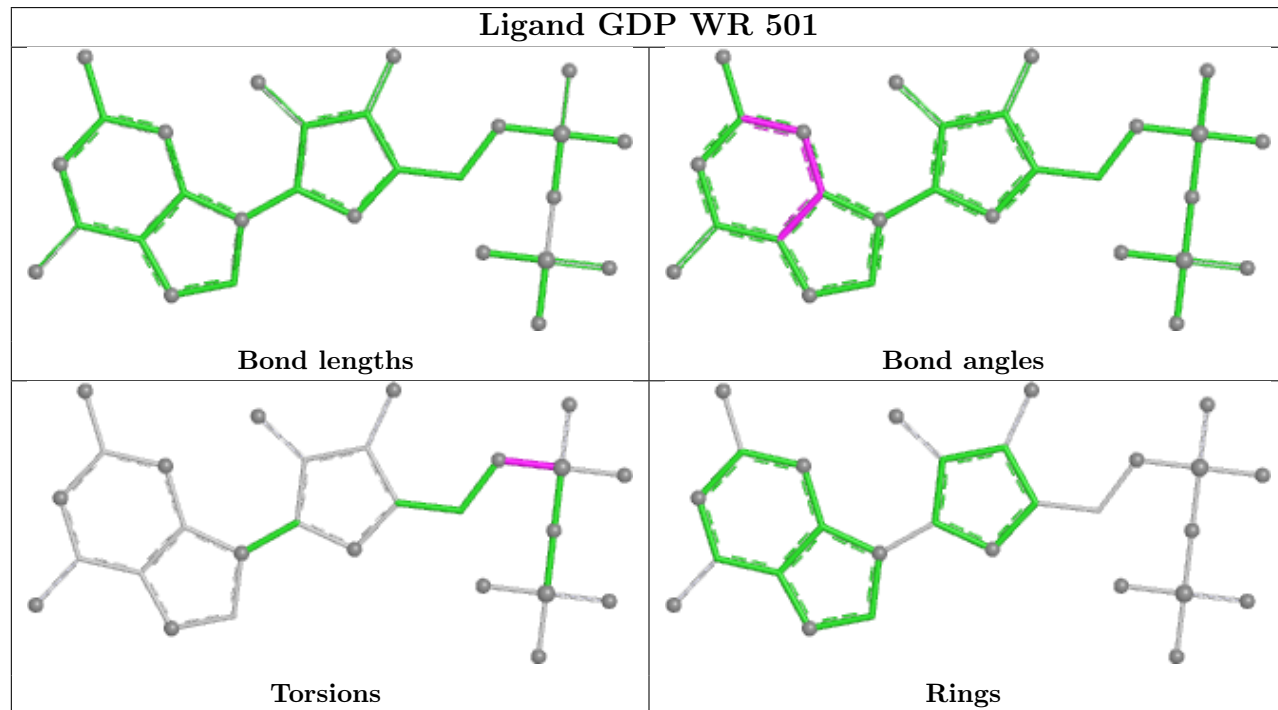




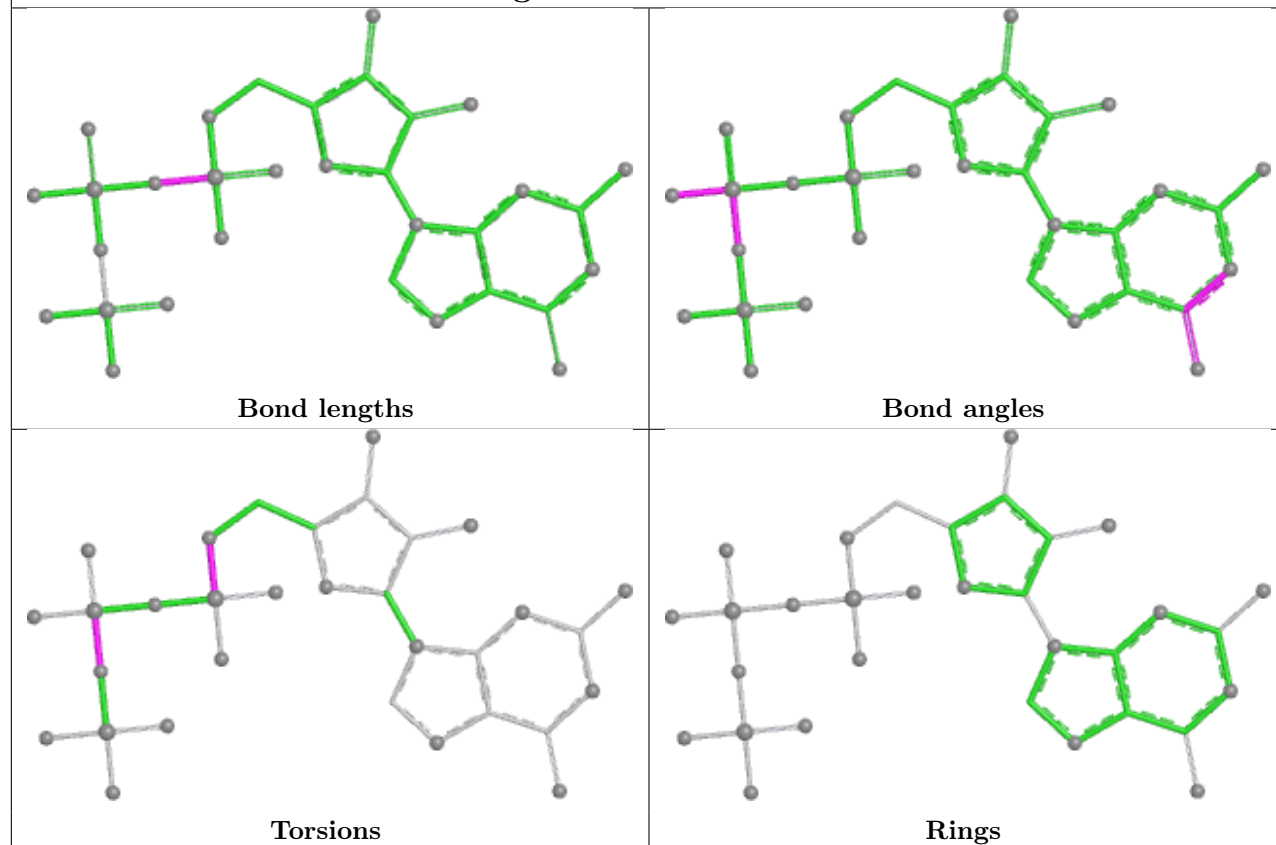
## Ligand GTP LD 602



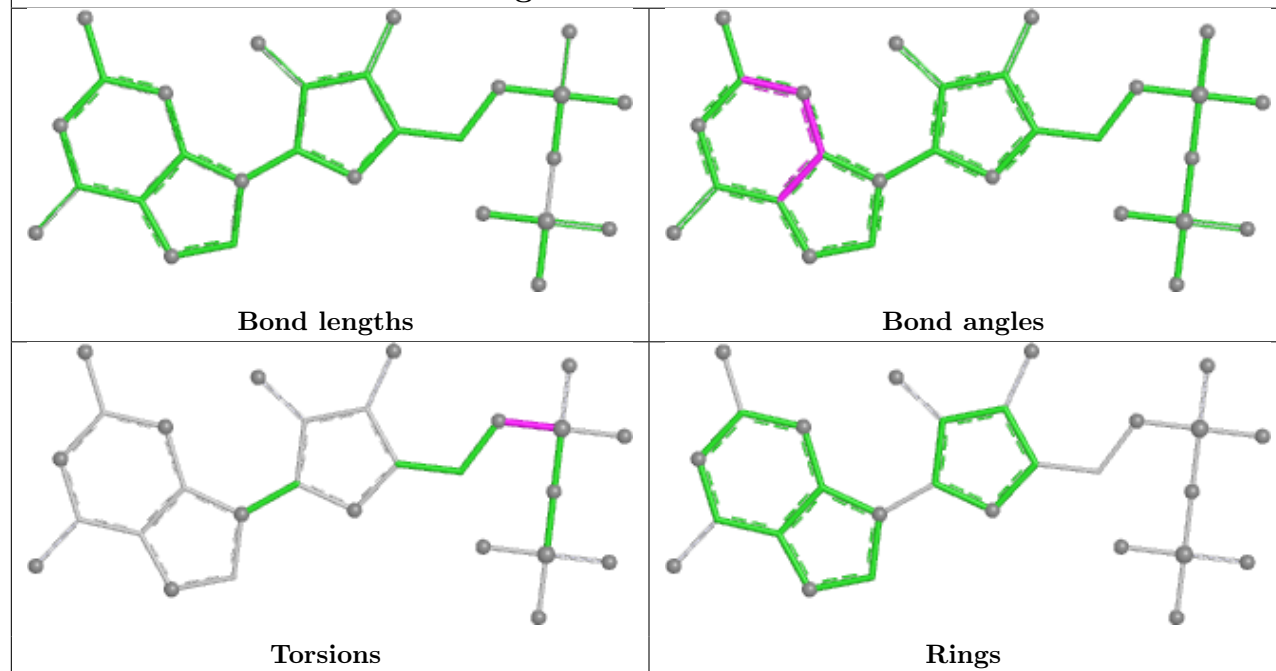
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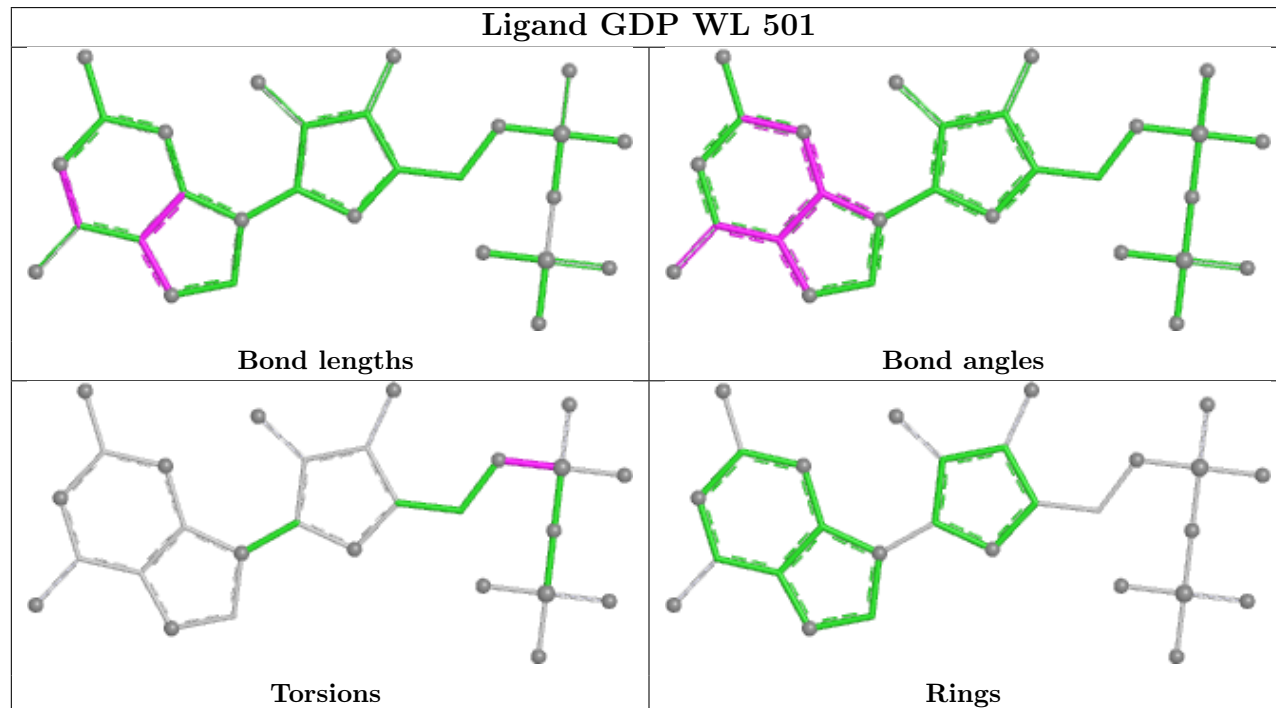
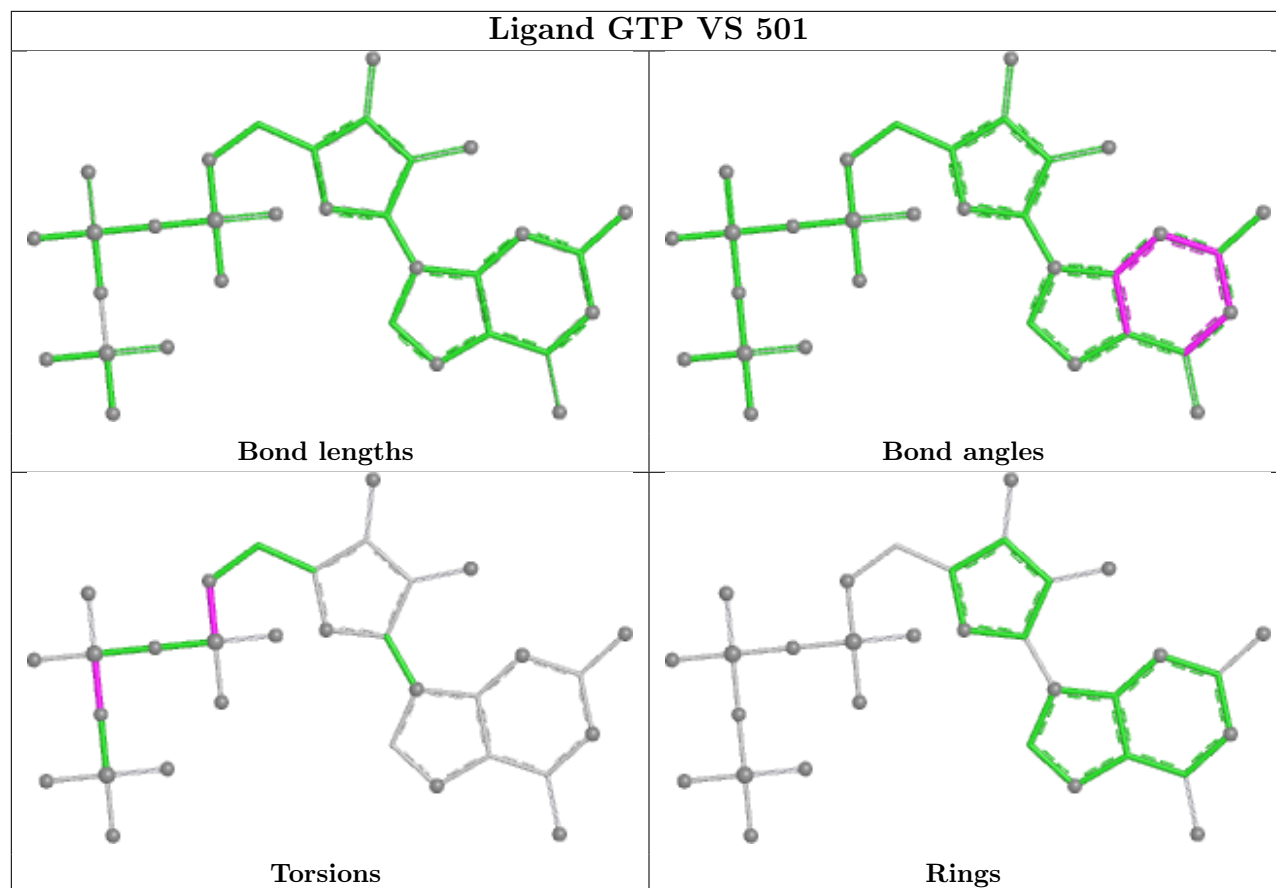


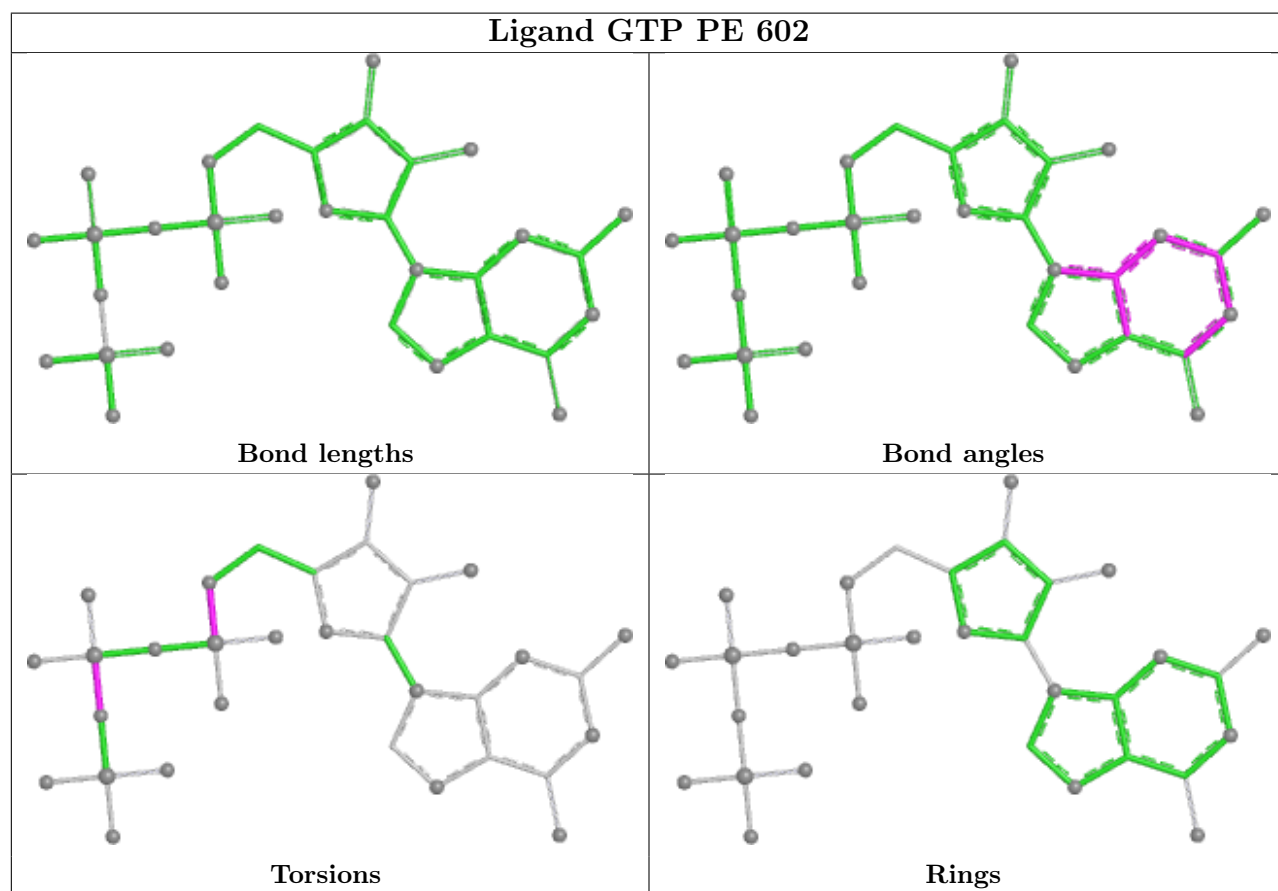
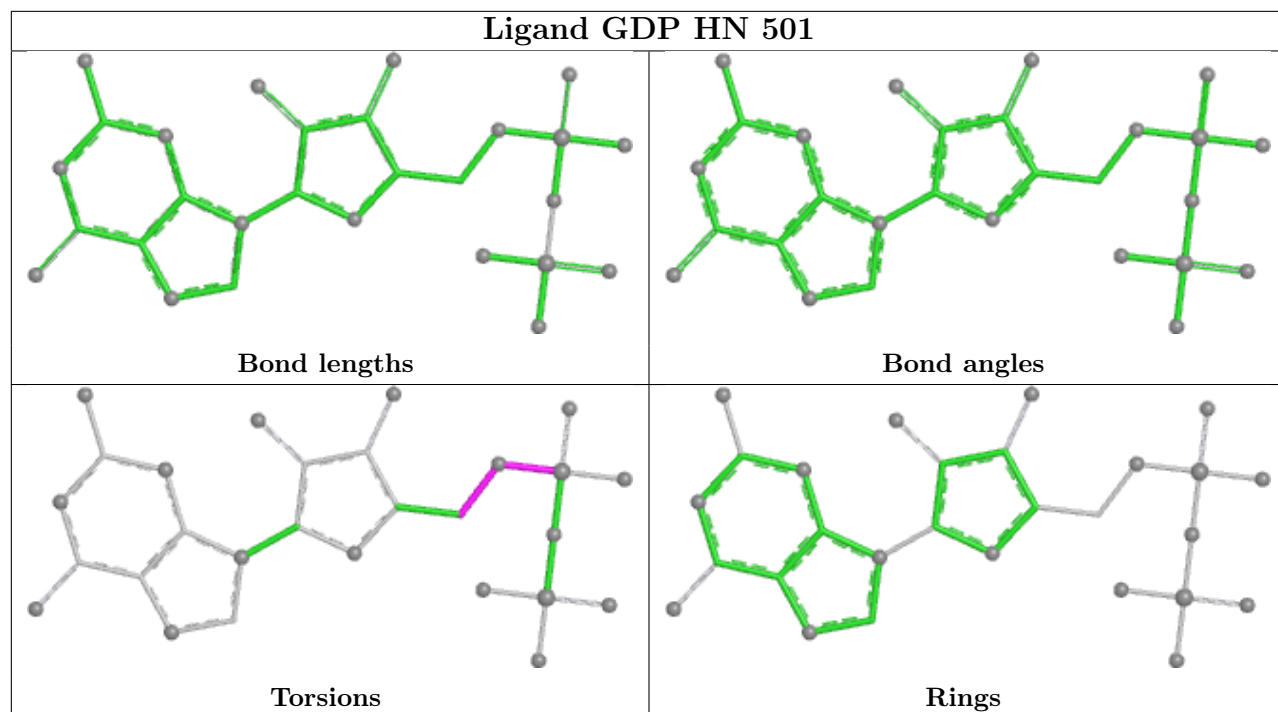
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## Ligand GDP GR 501

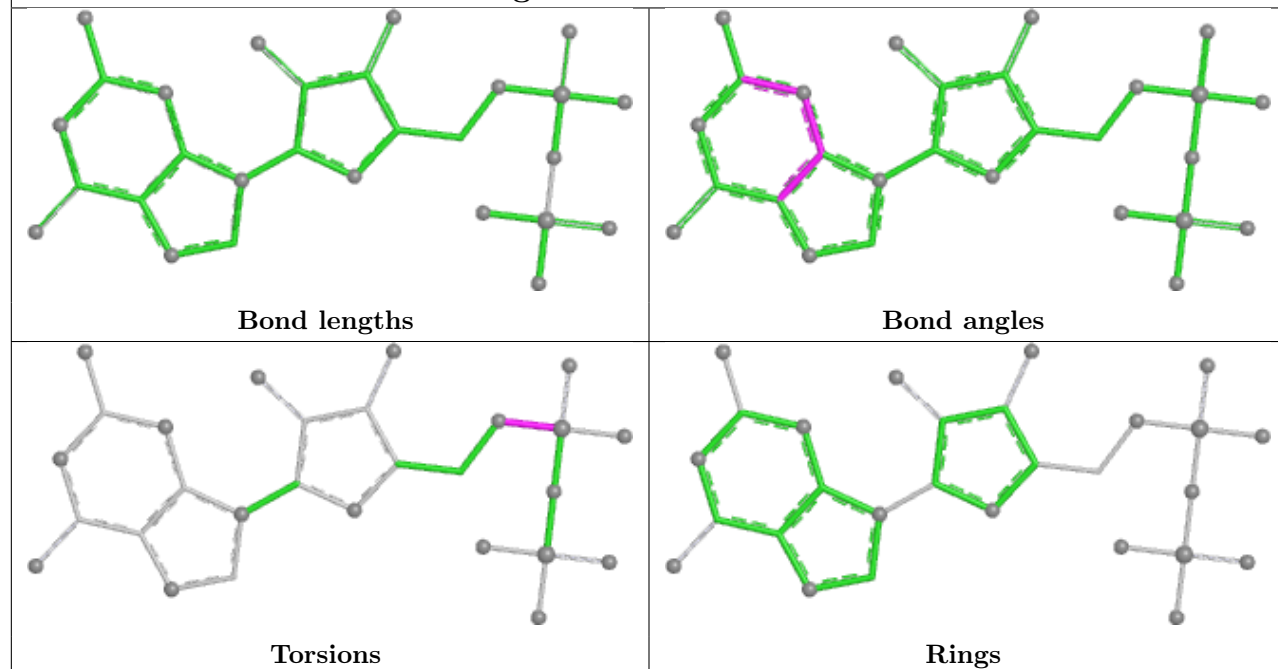




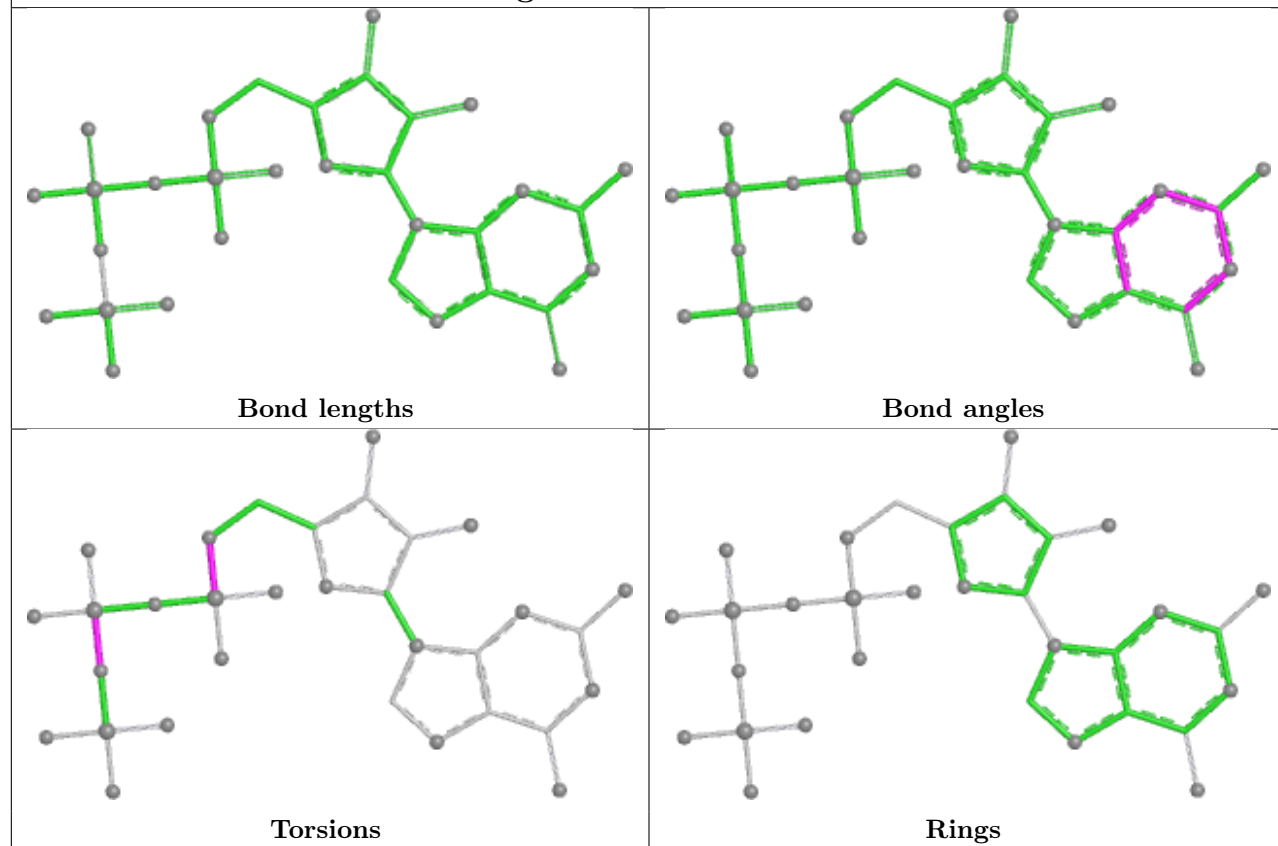


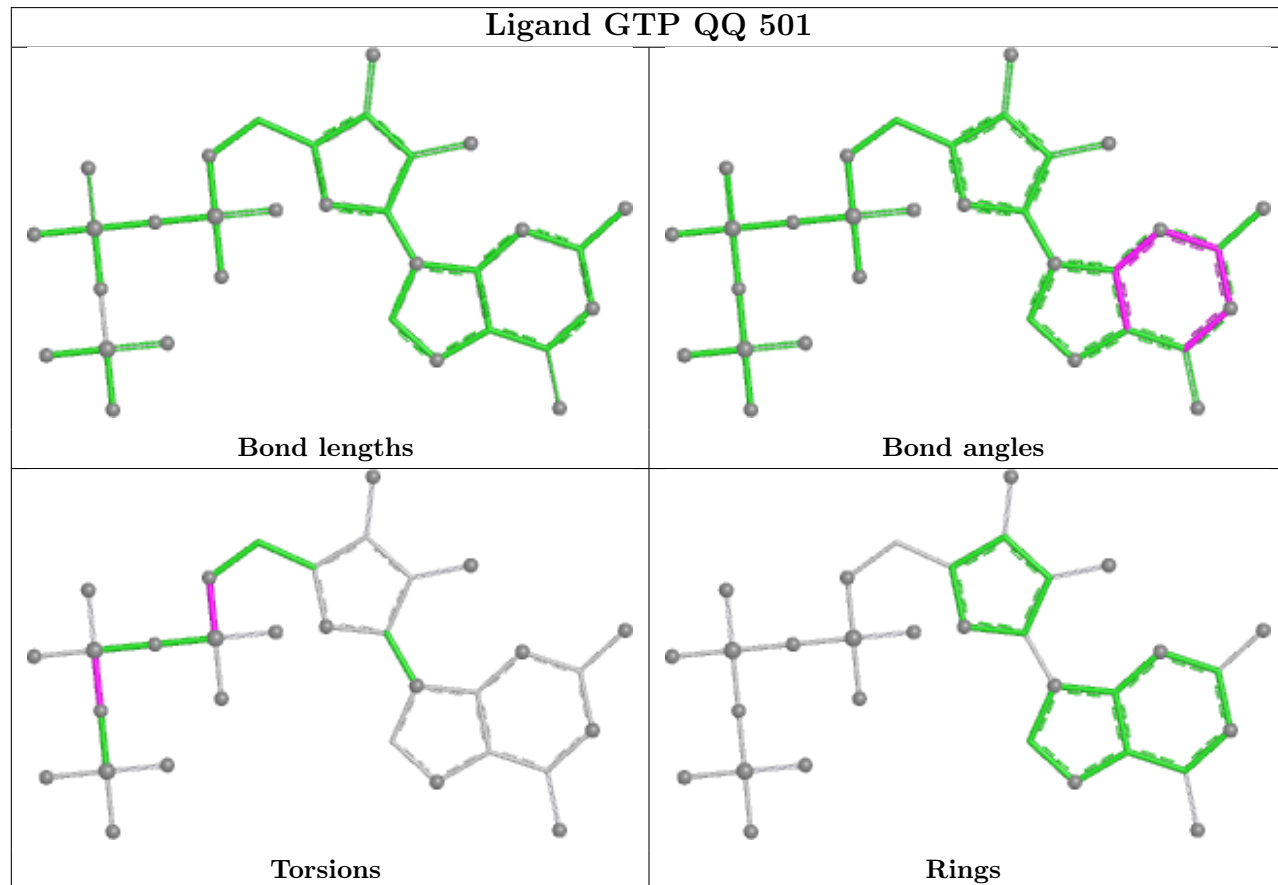
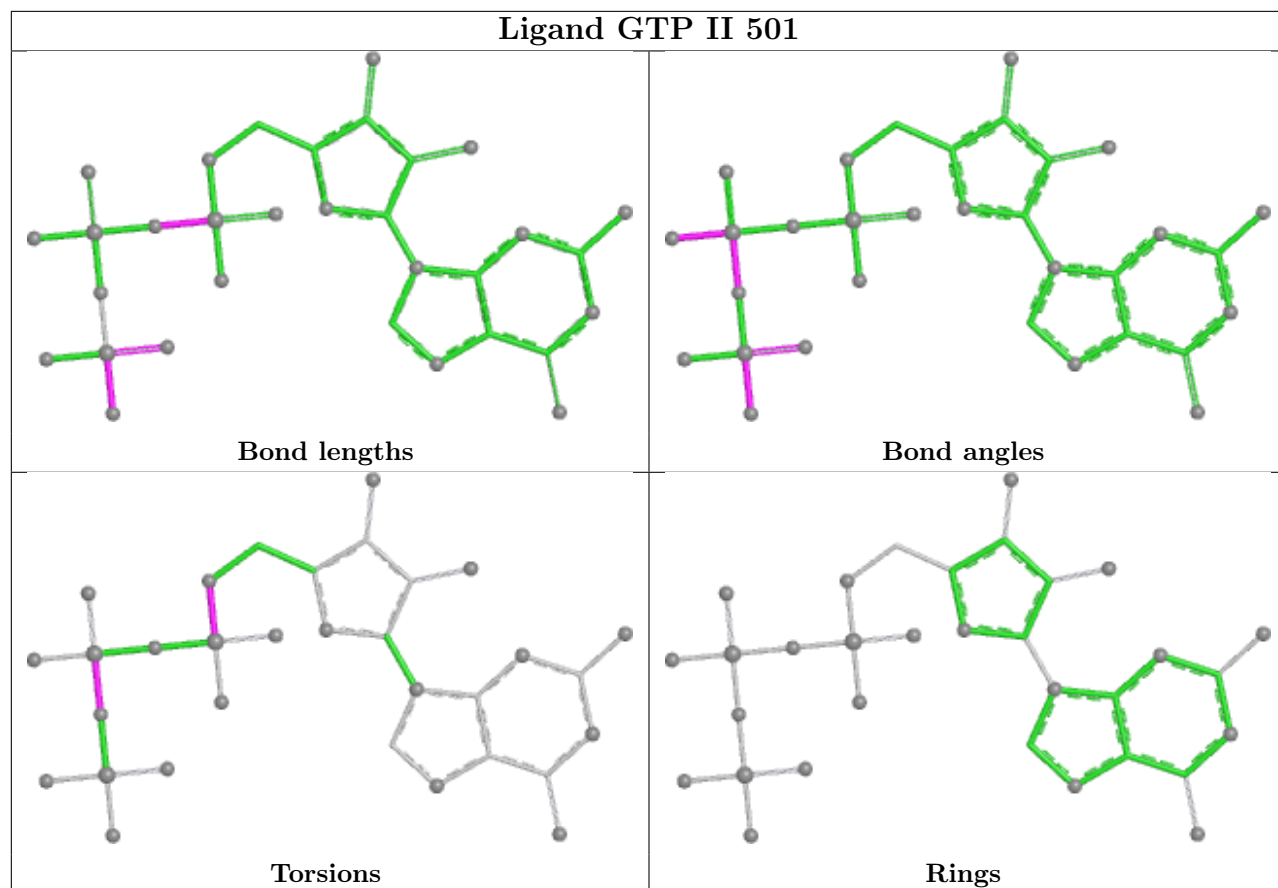


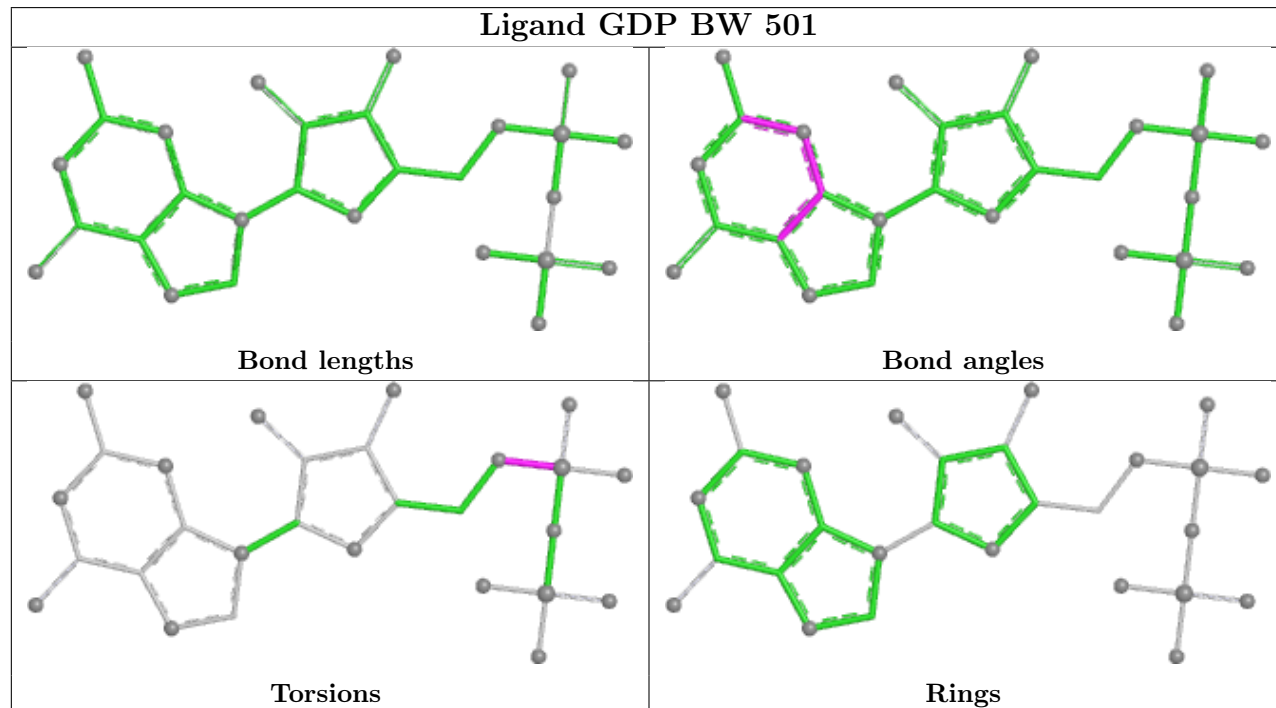
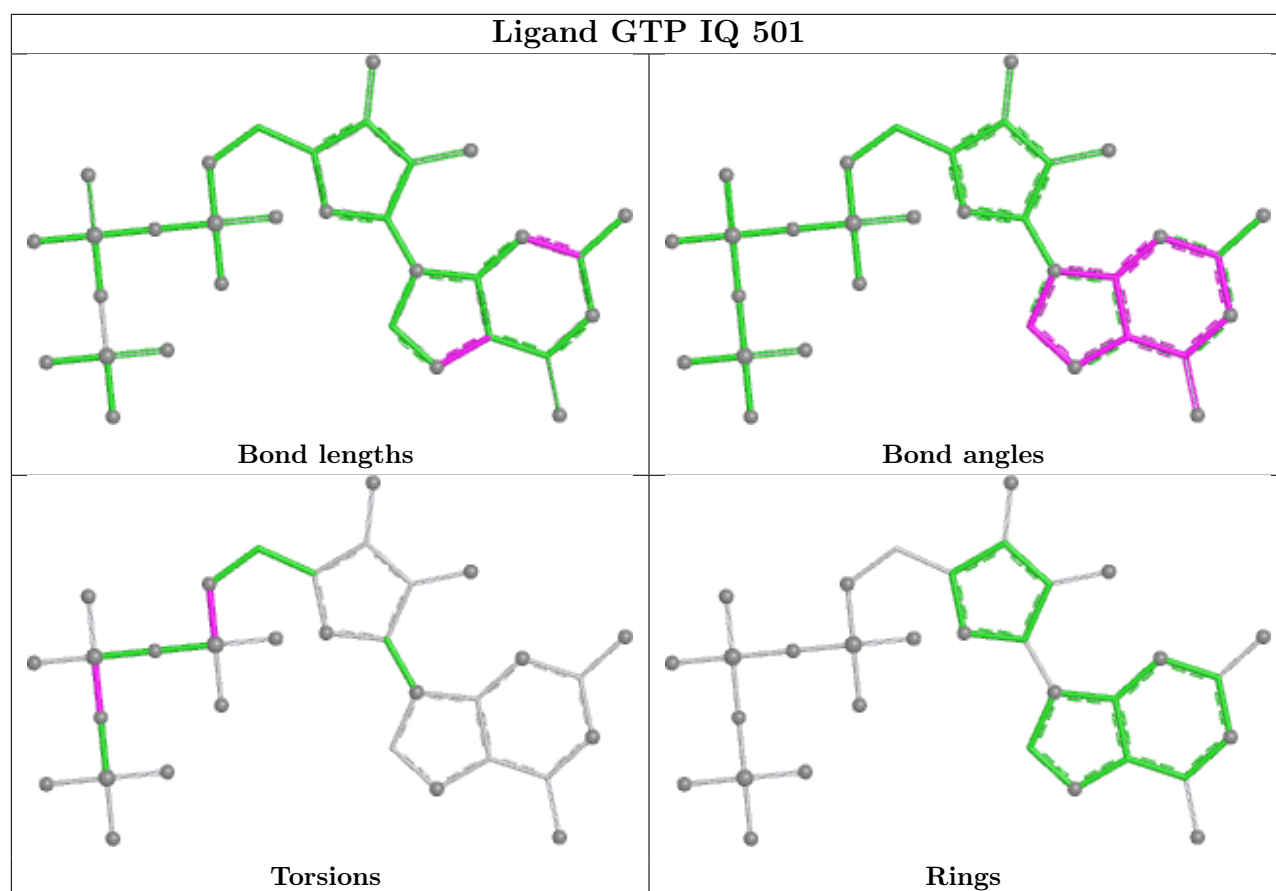
## Ligand GDP ZW 501

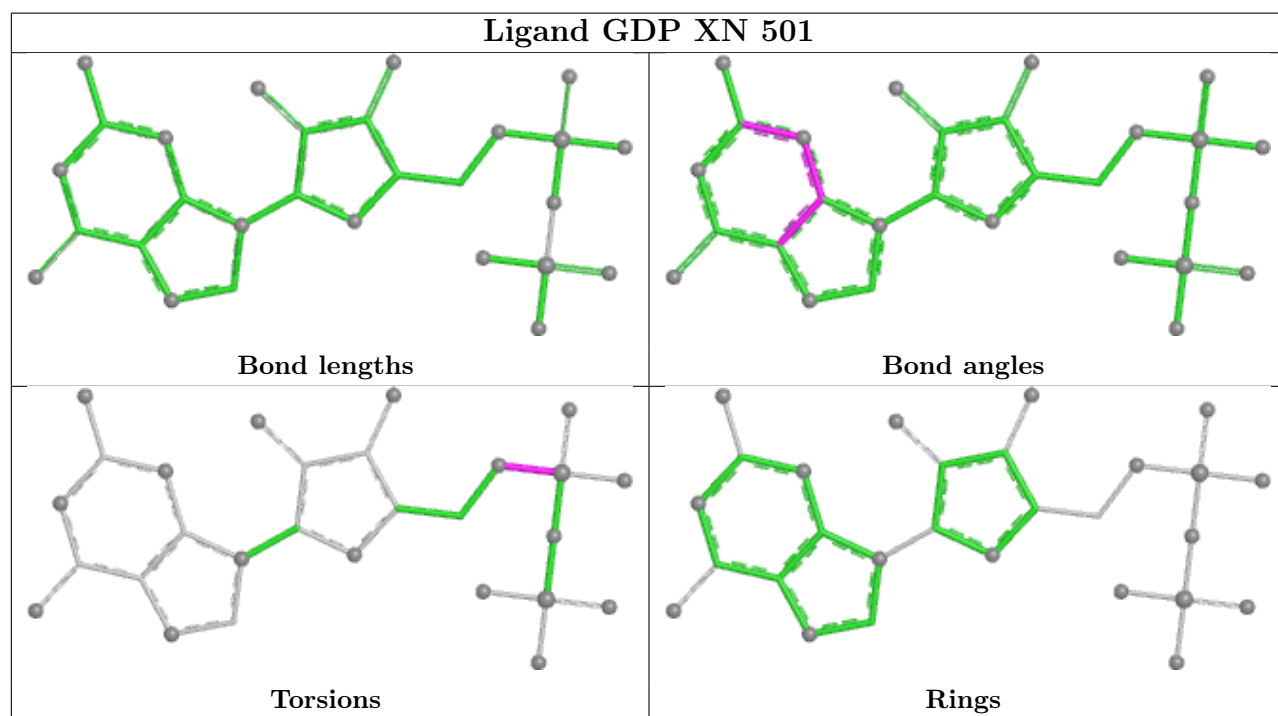
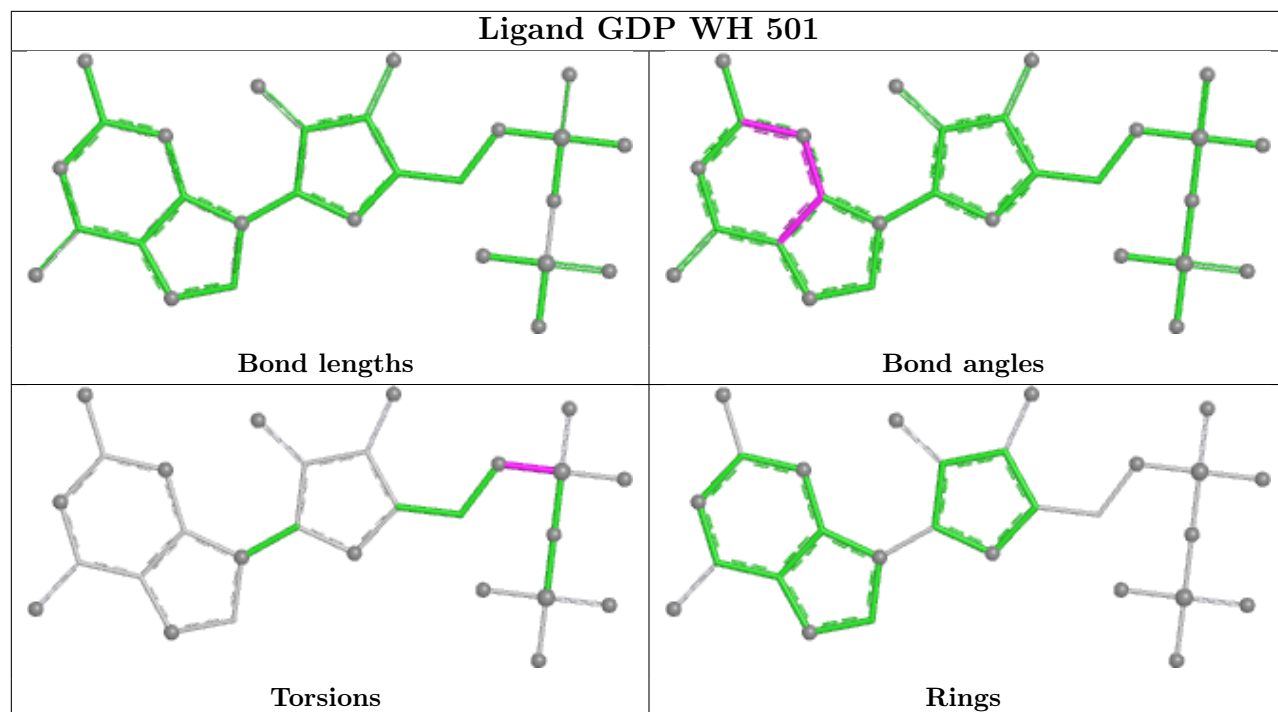


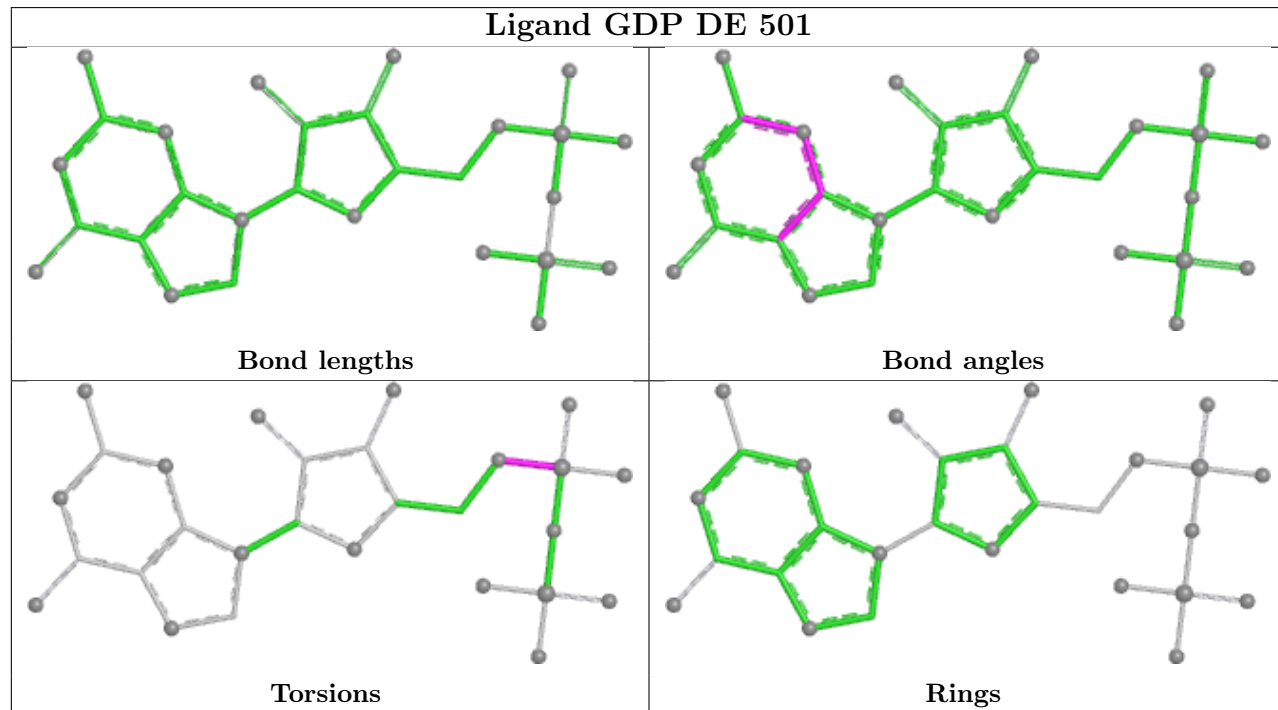
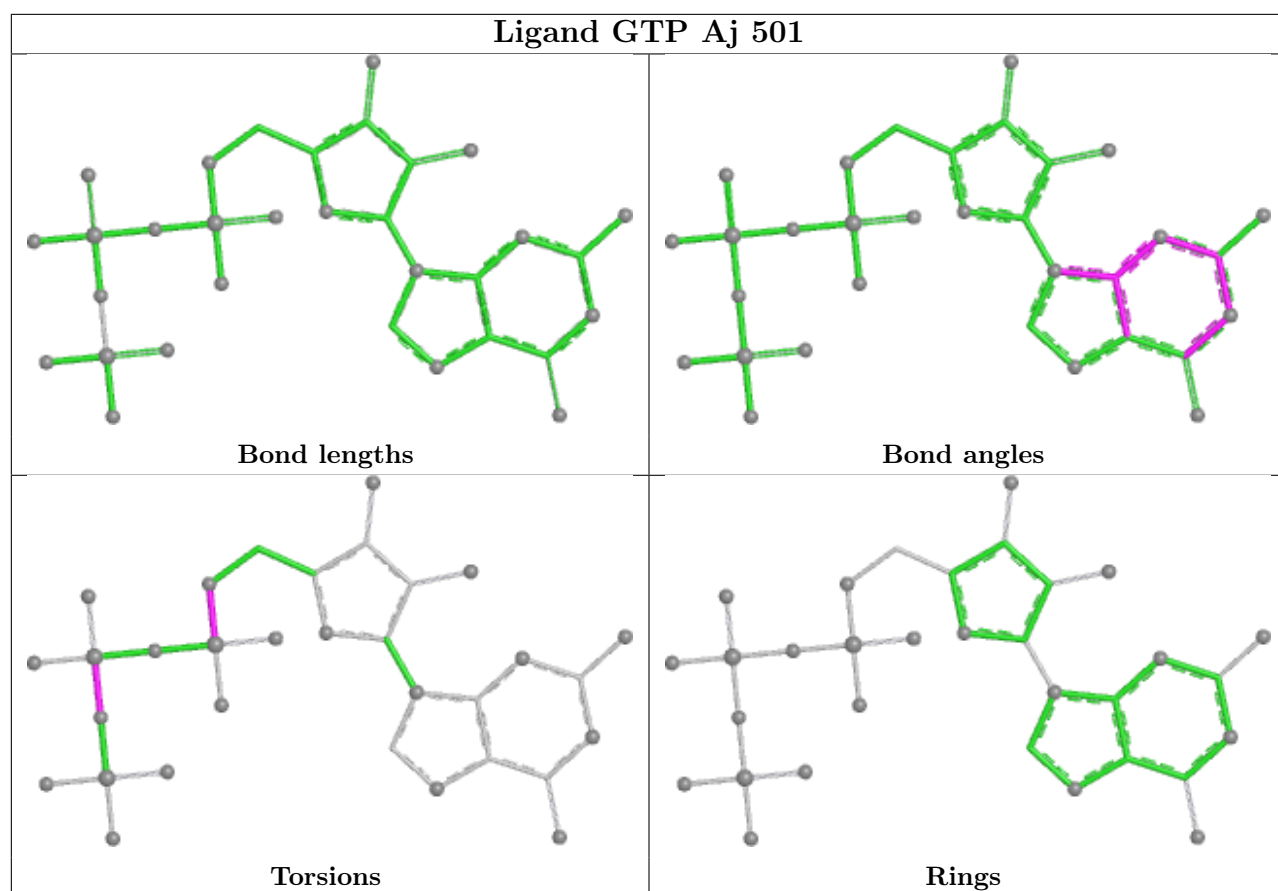
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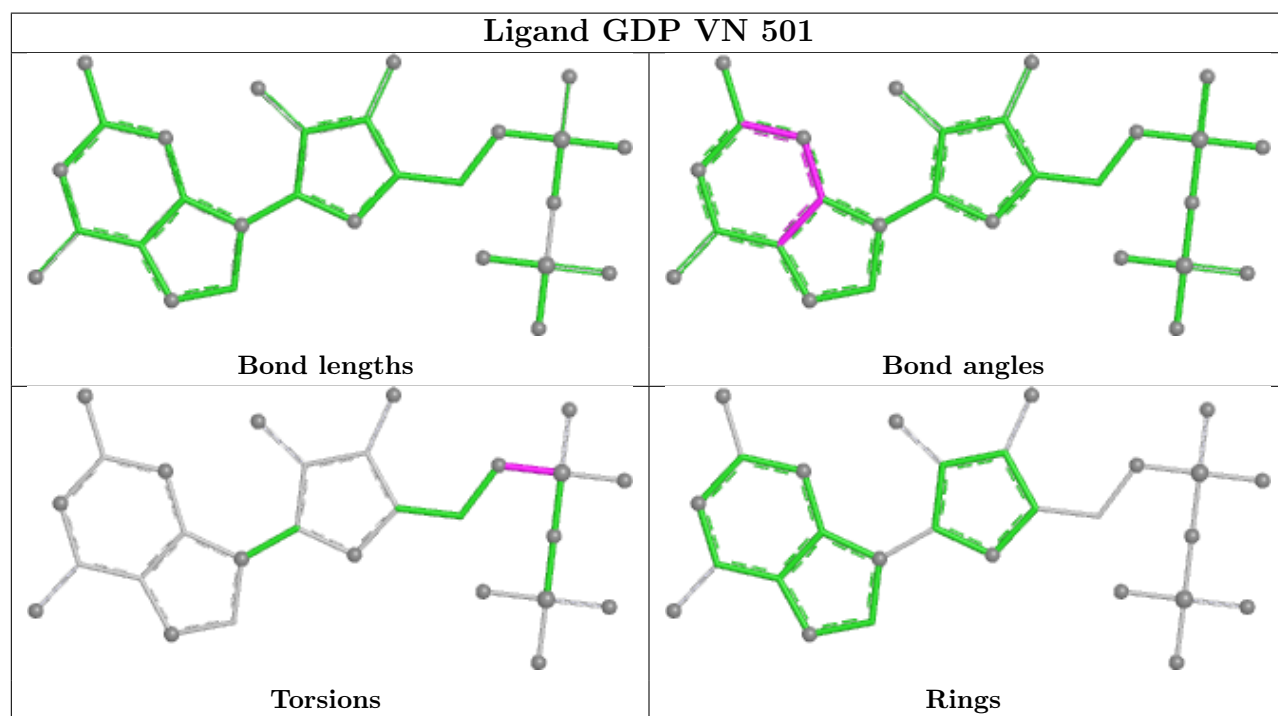
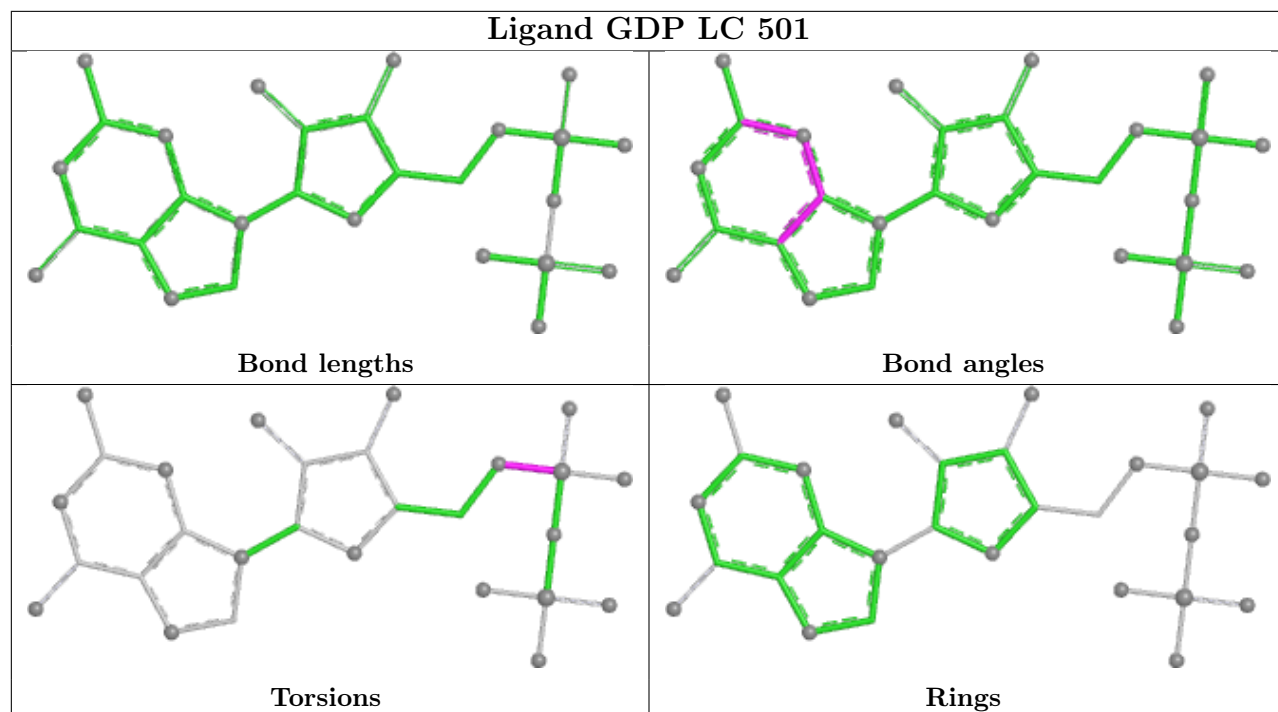




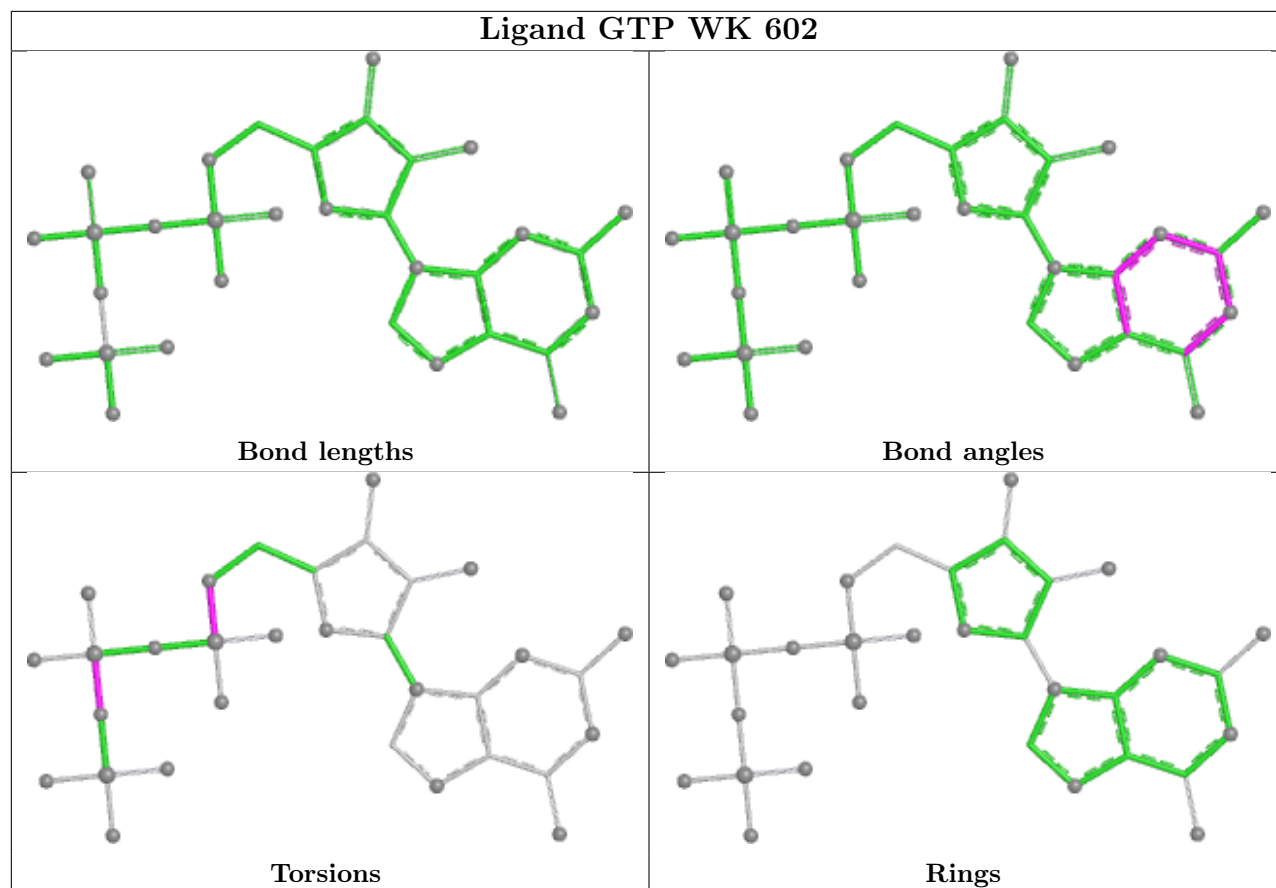




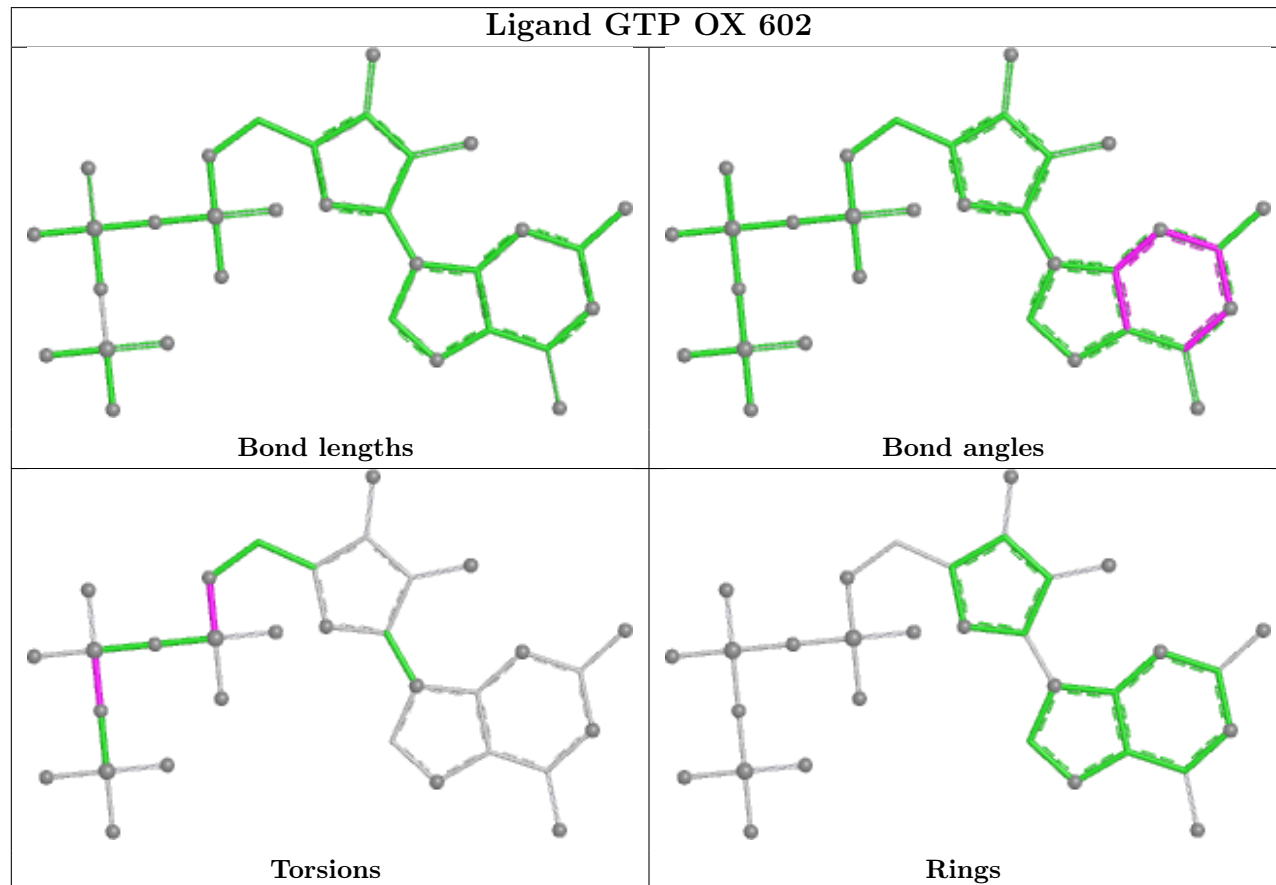


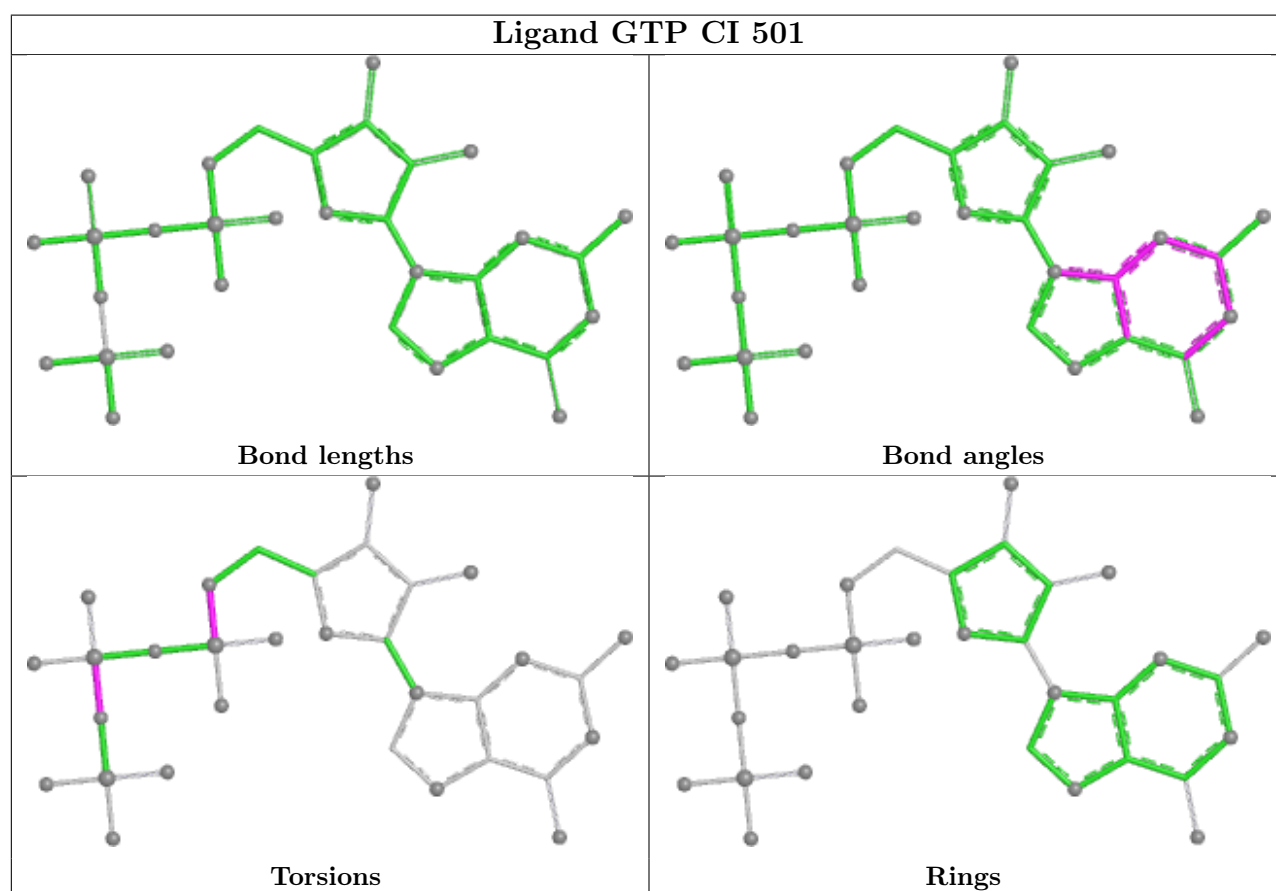
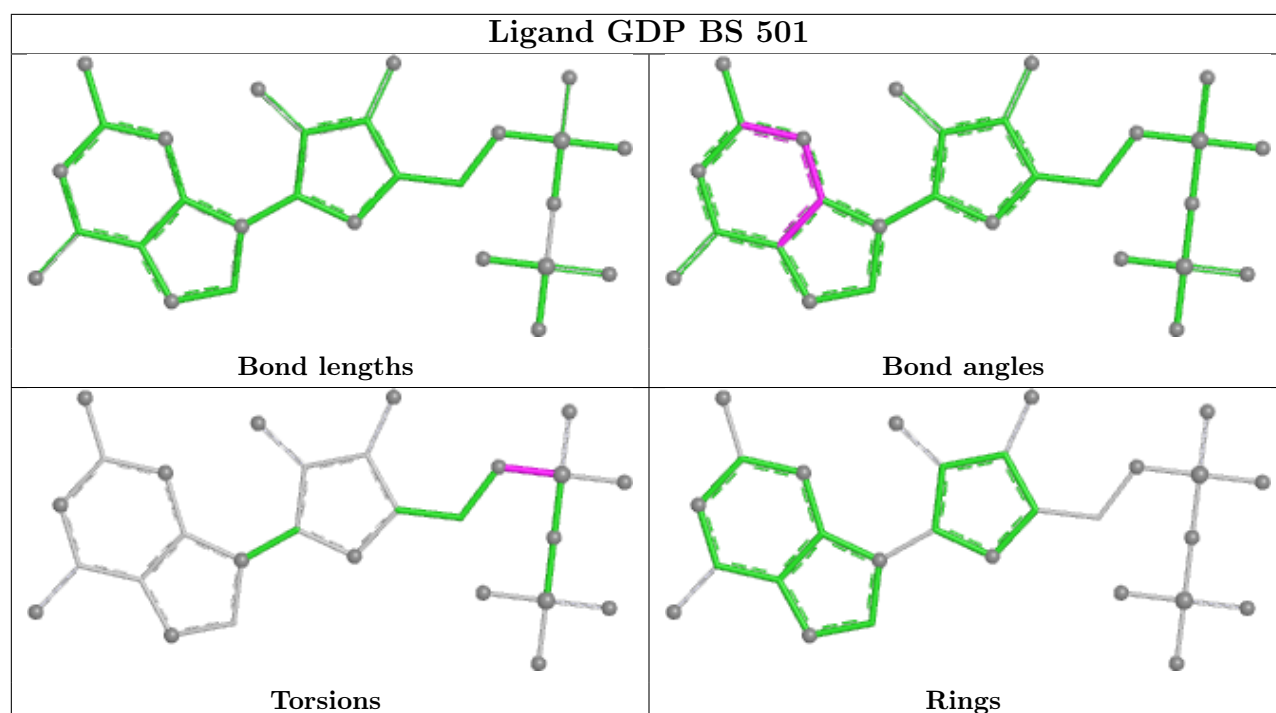


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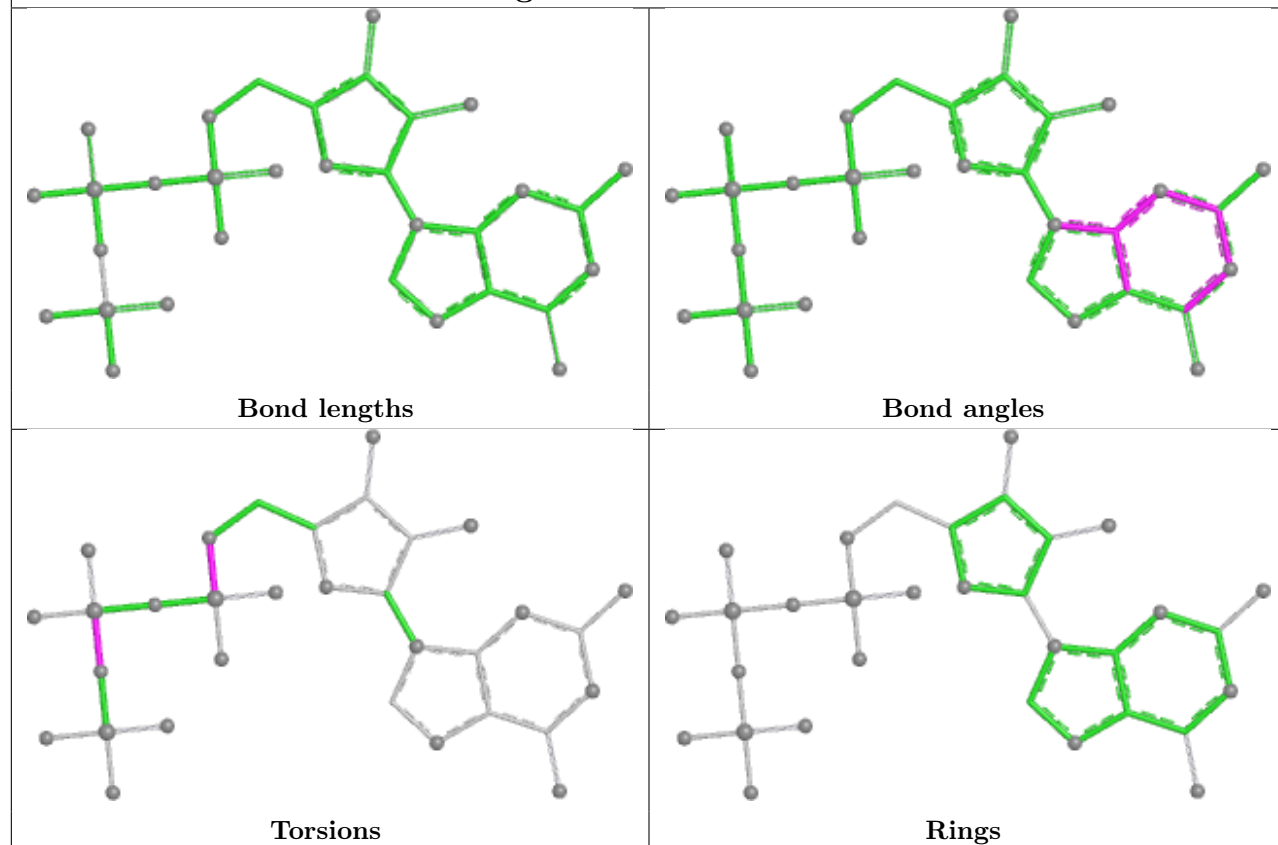
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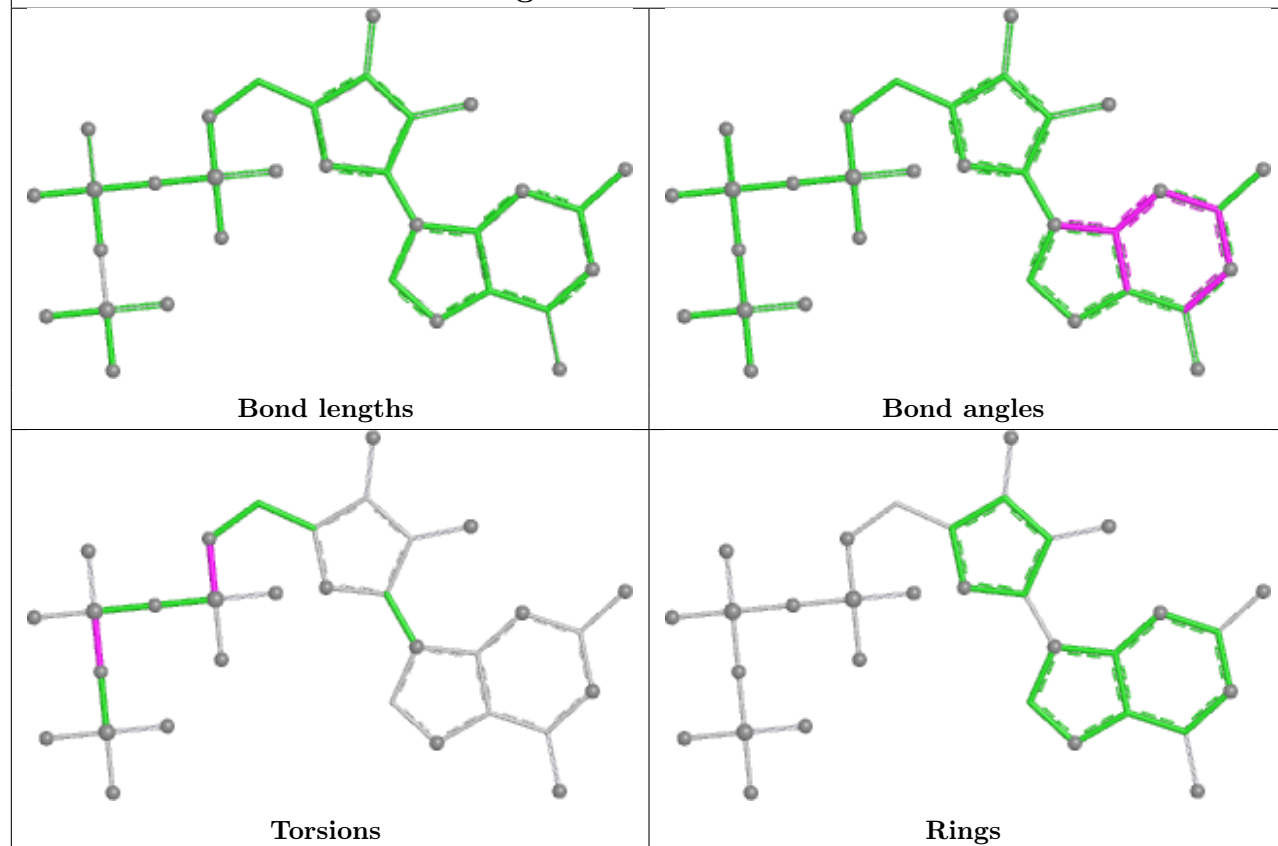




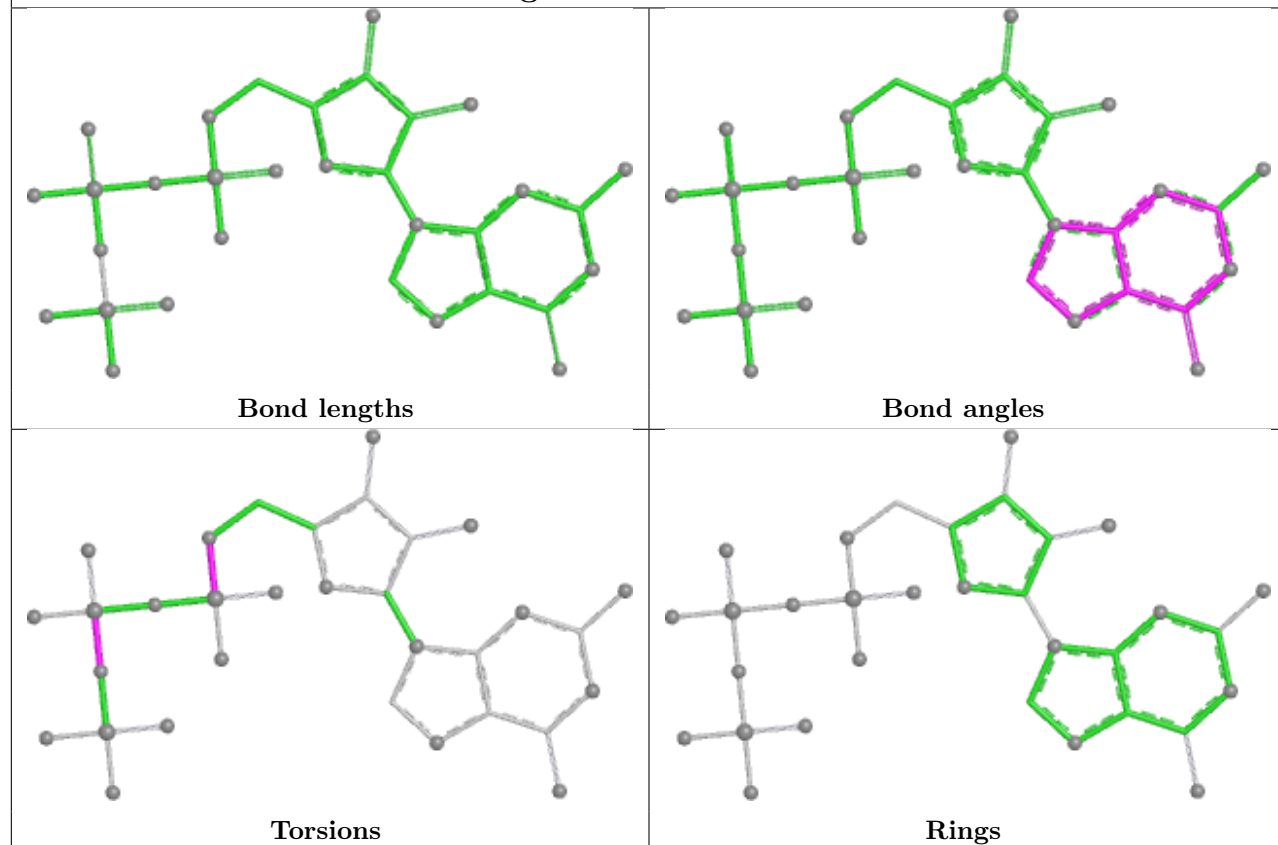
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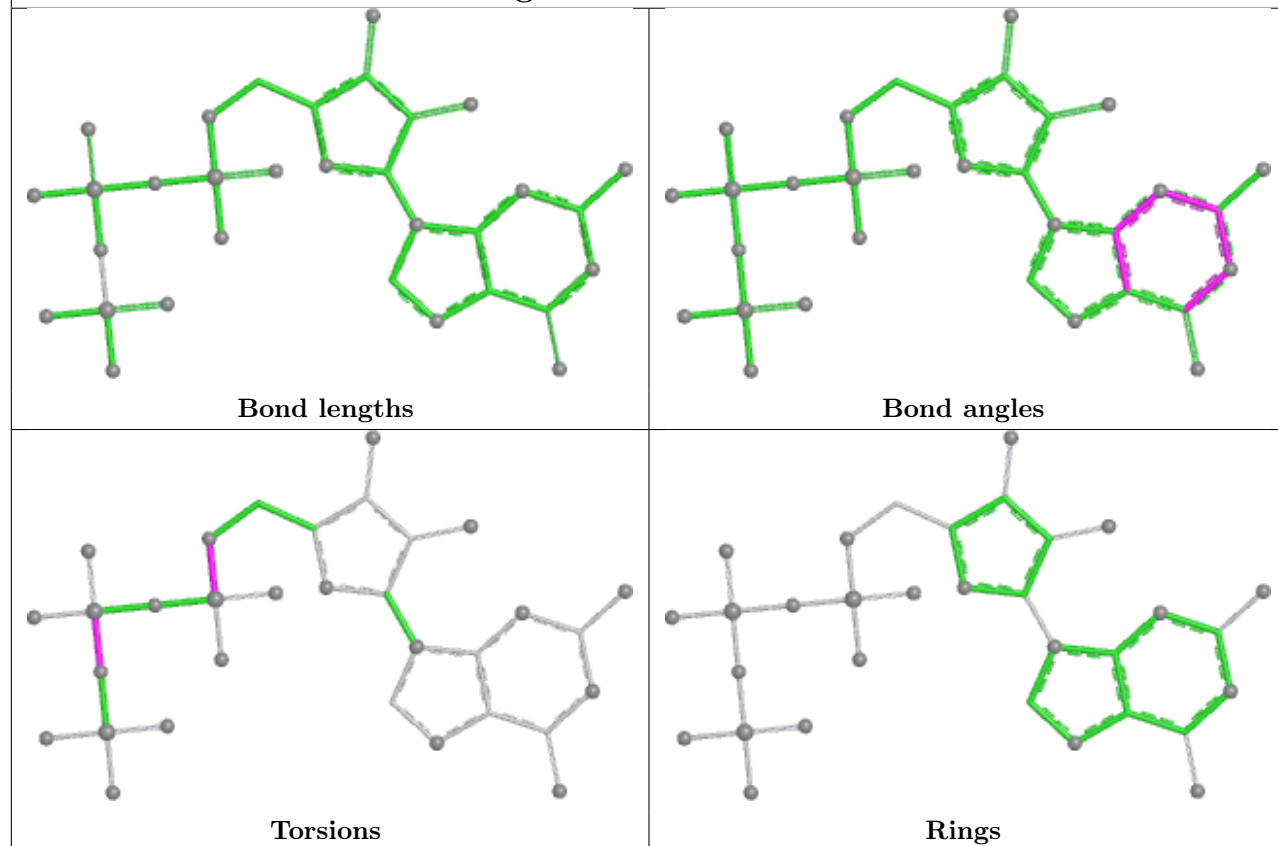
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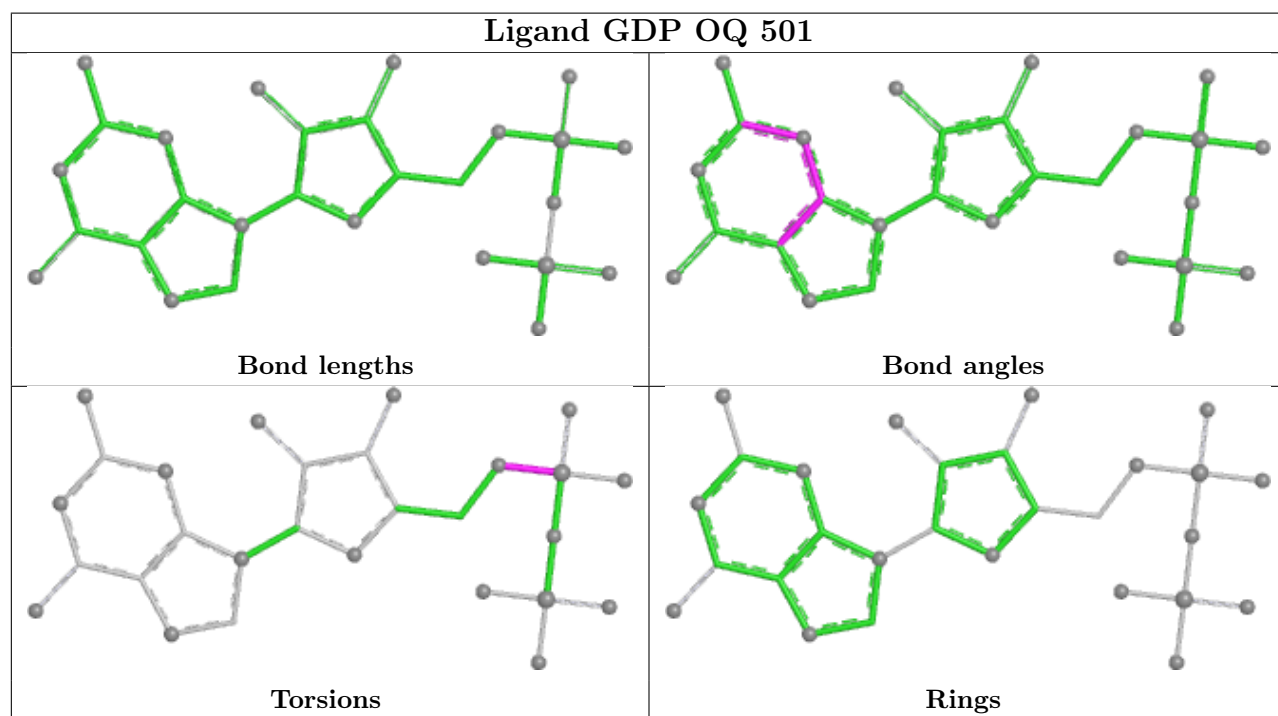
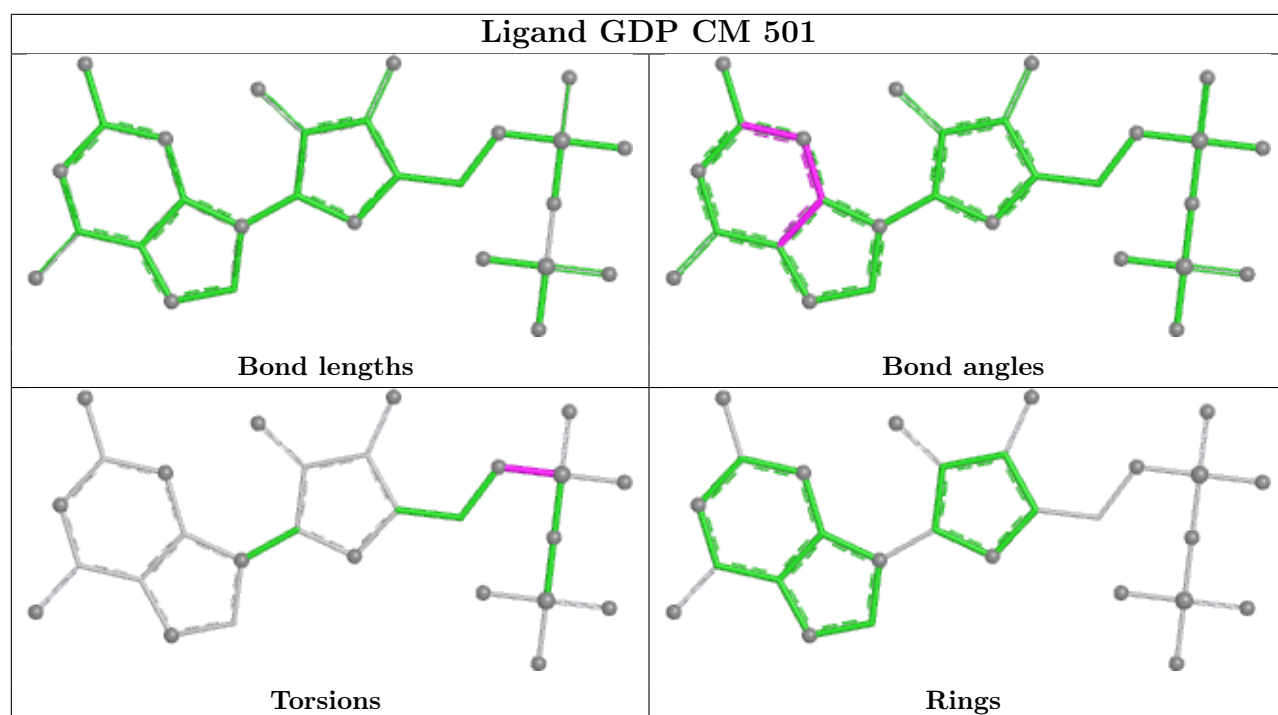


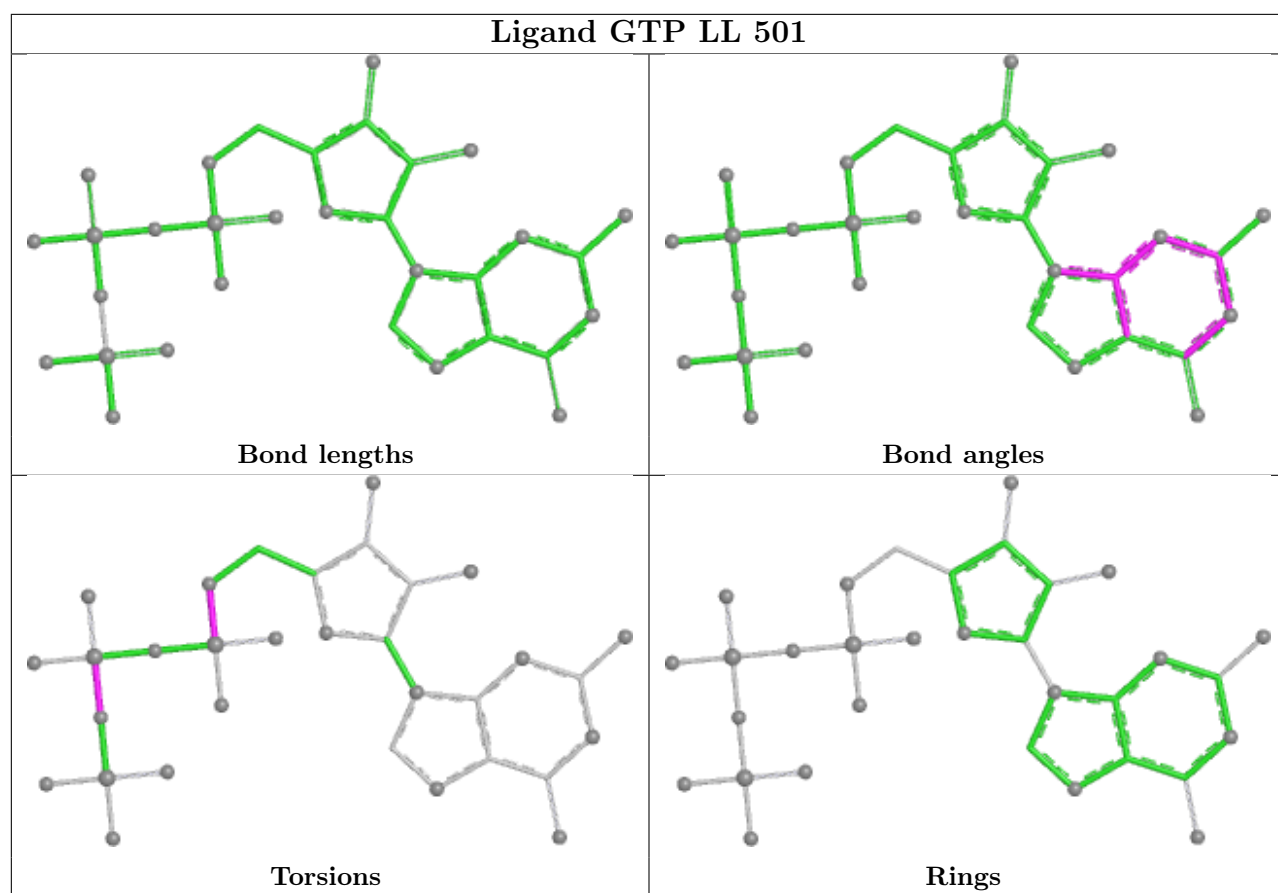
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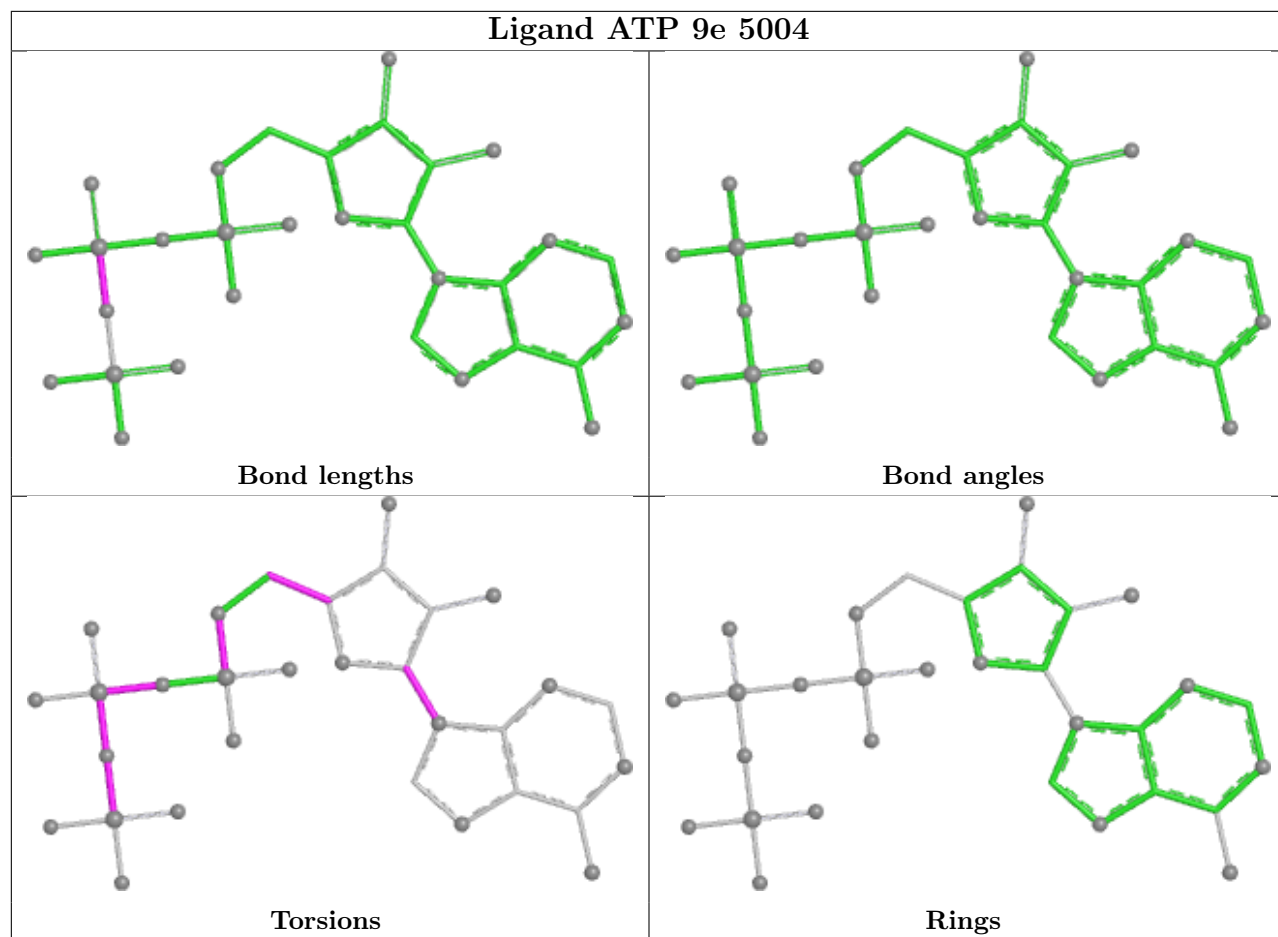


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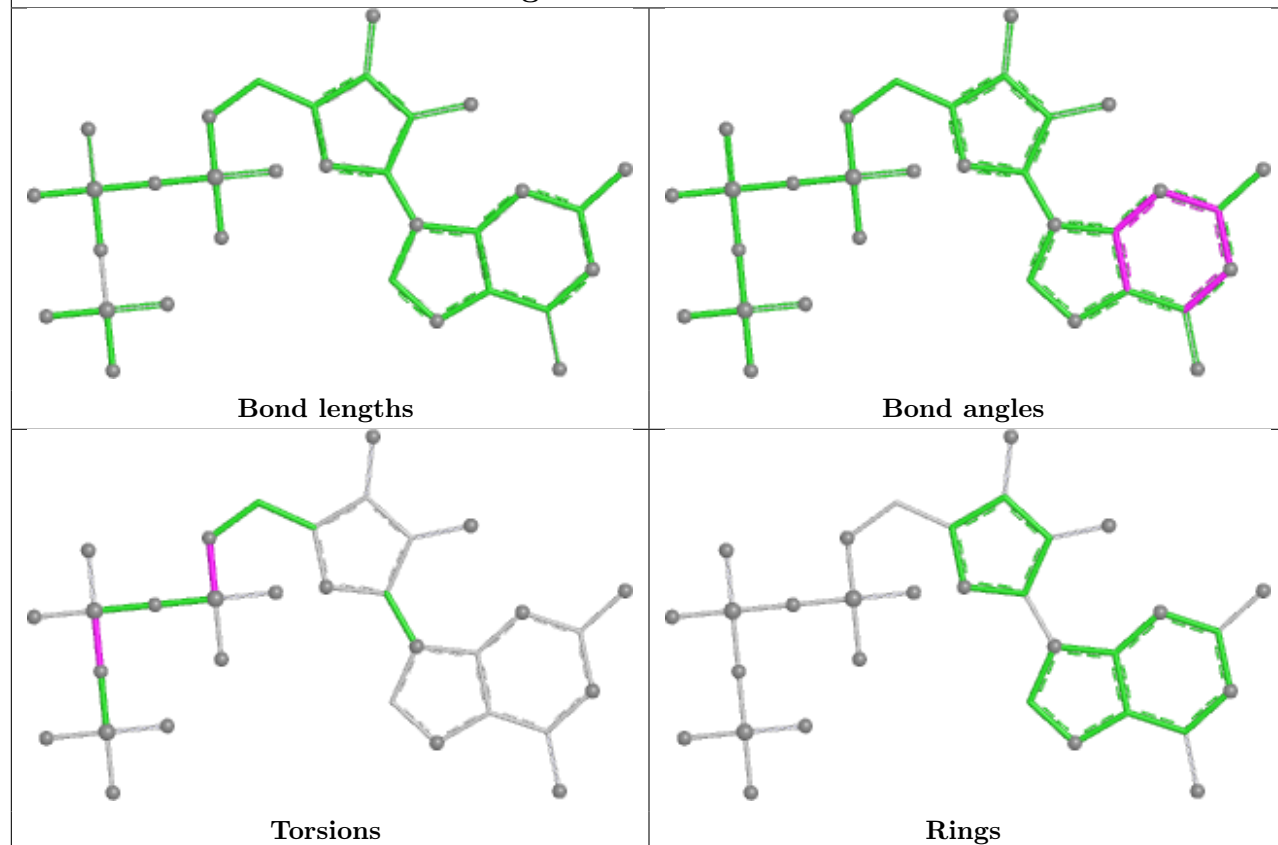




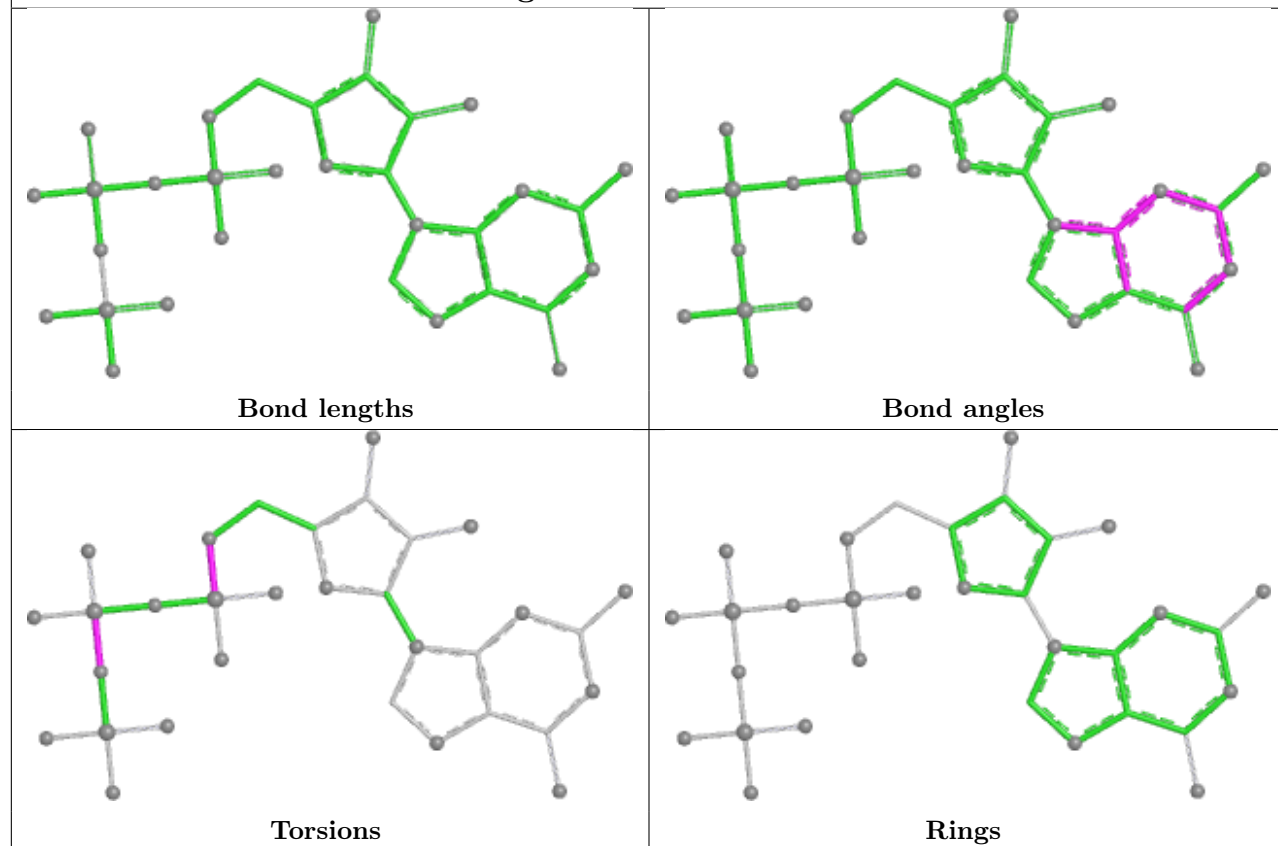




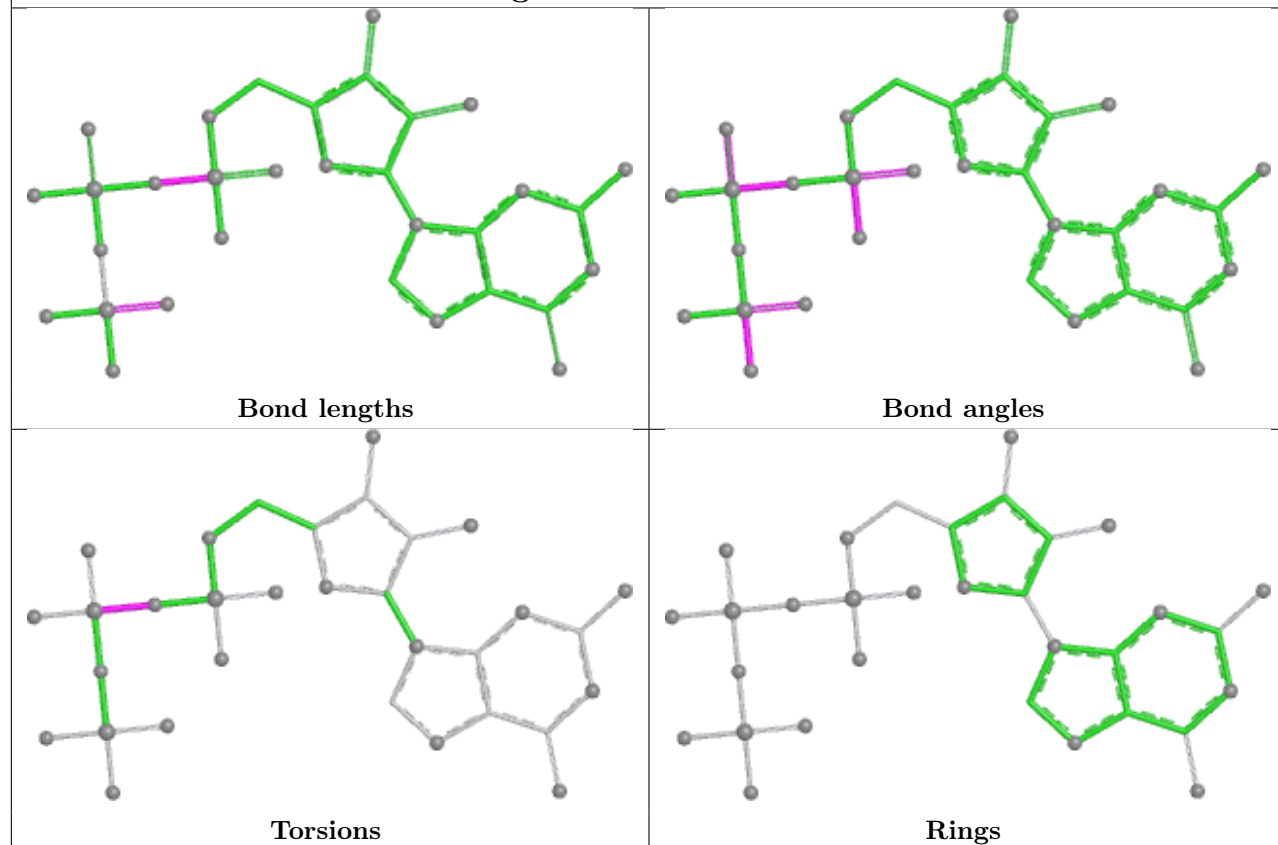
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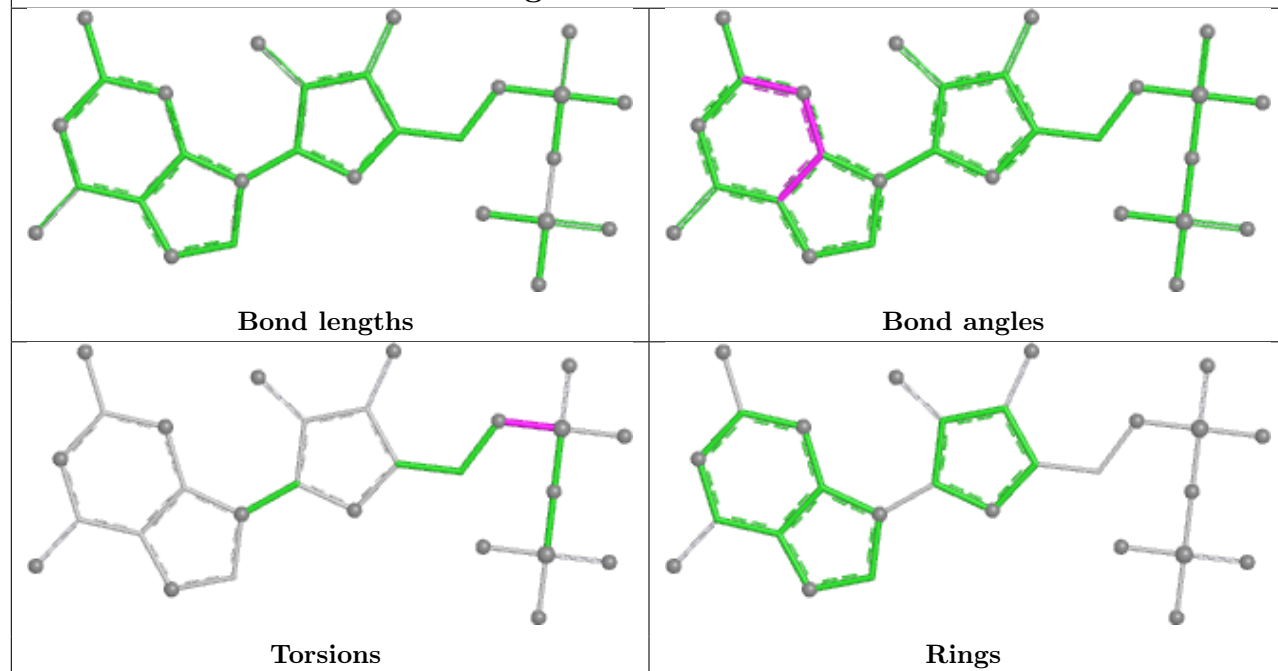
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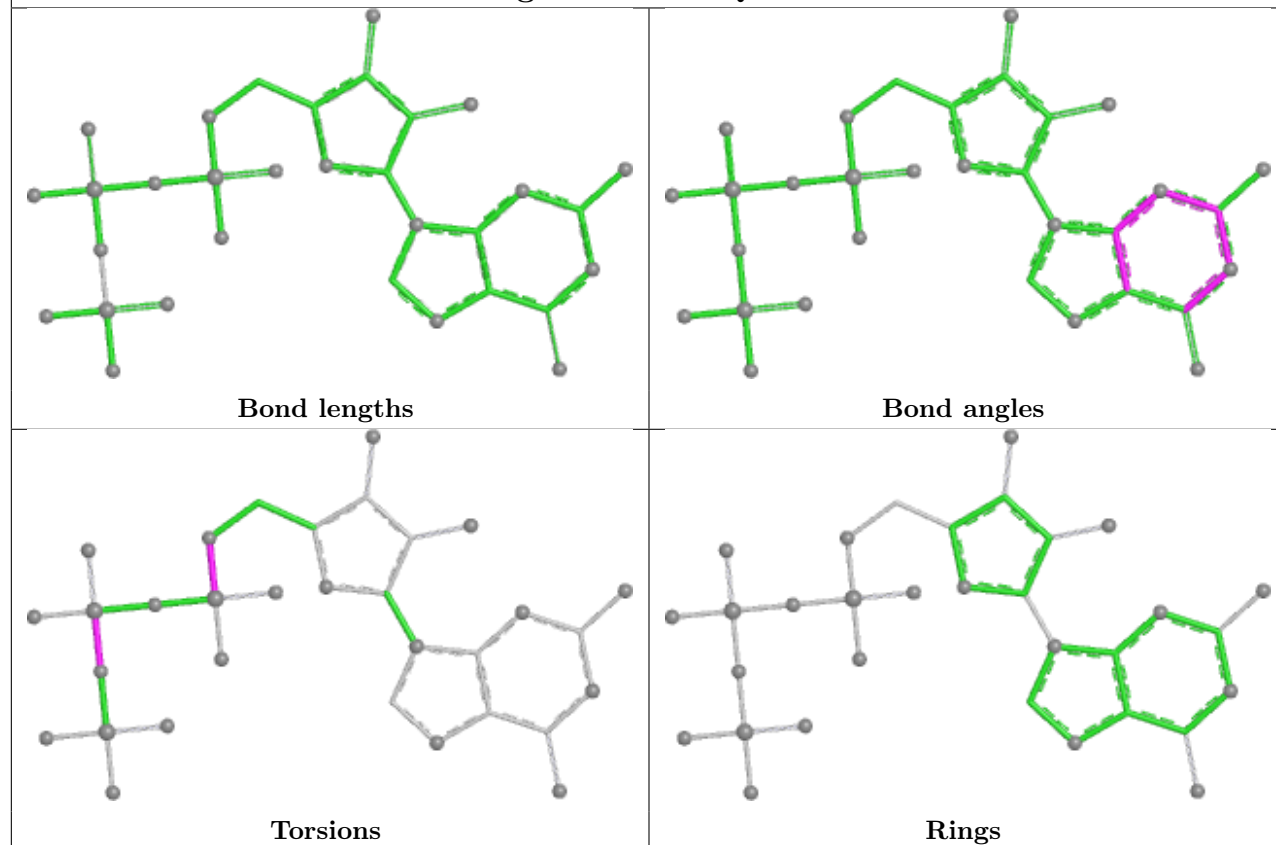
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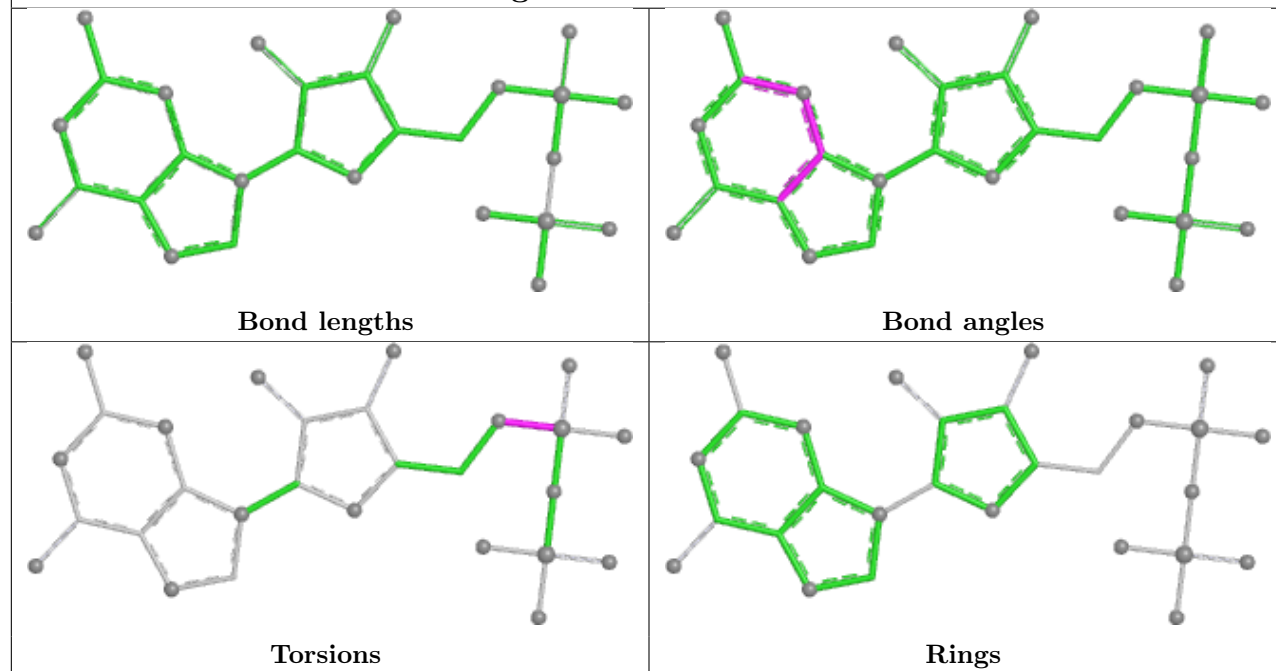
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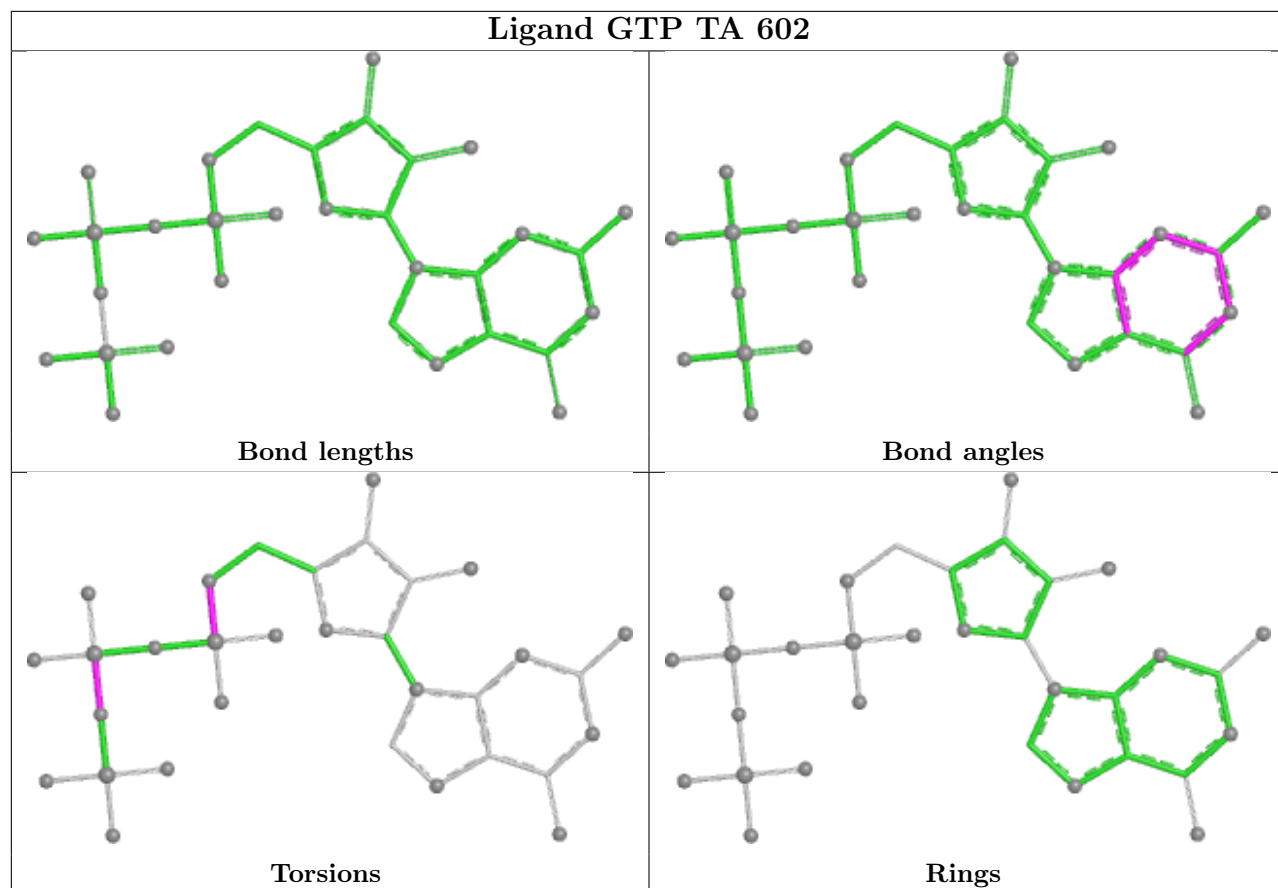


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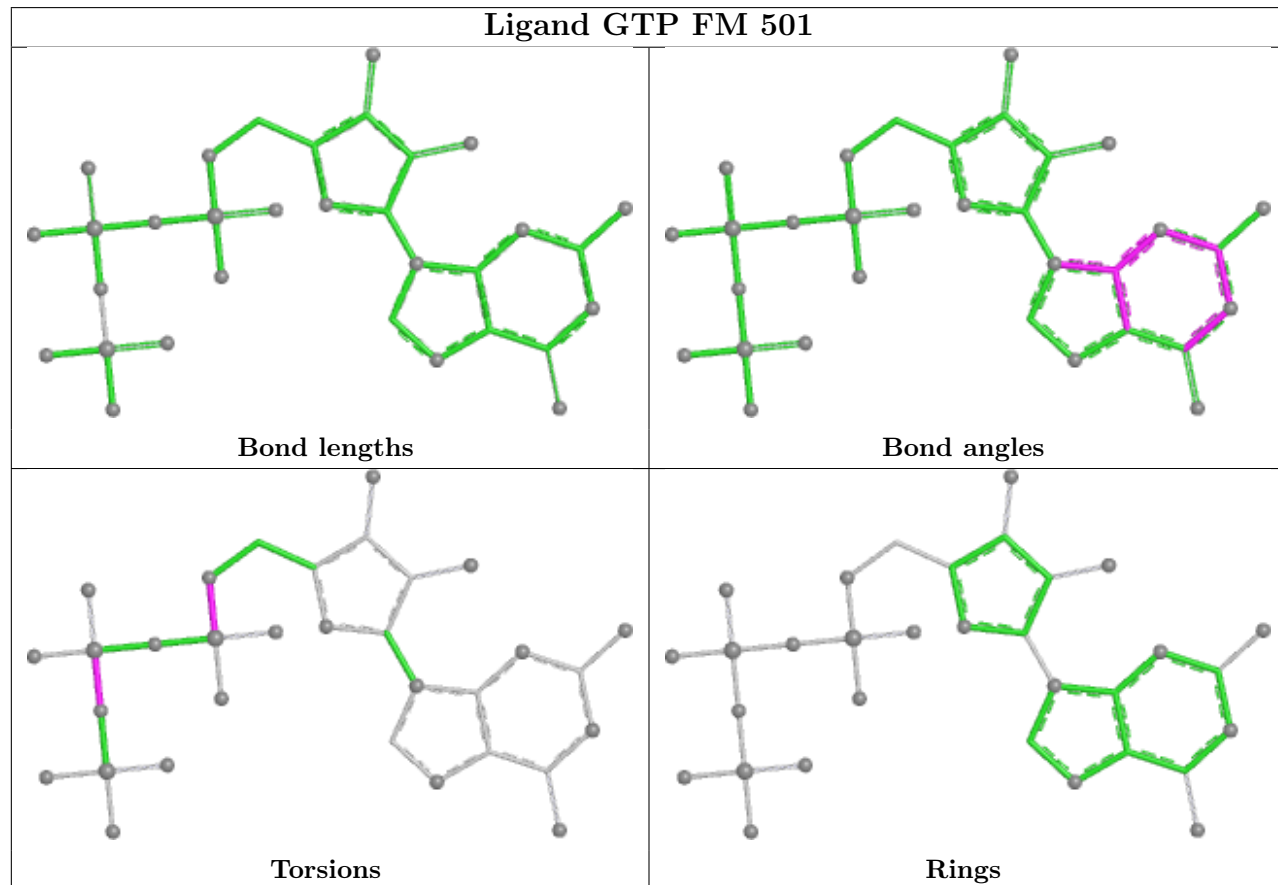


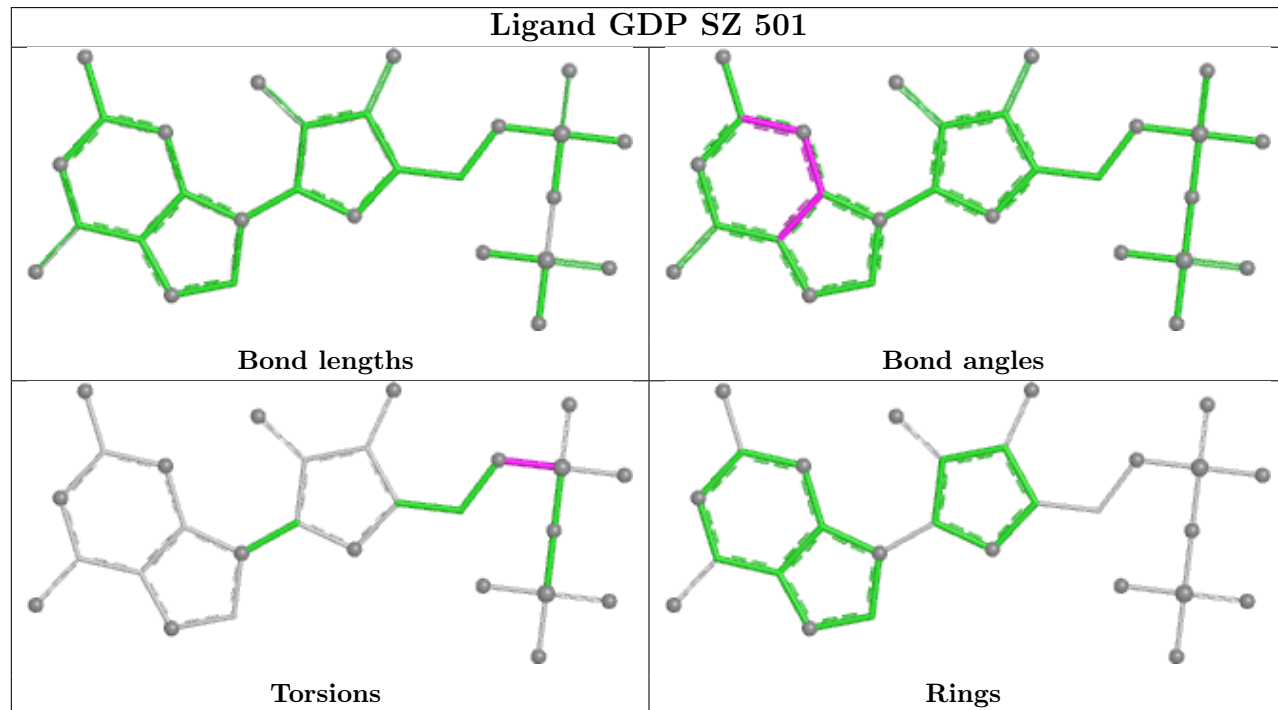
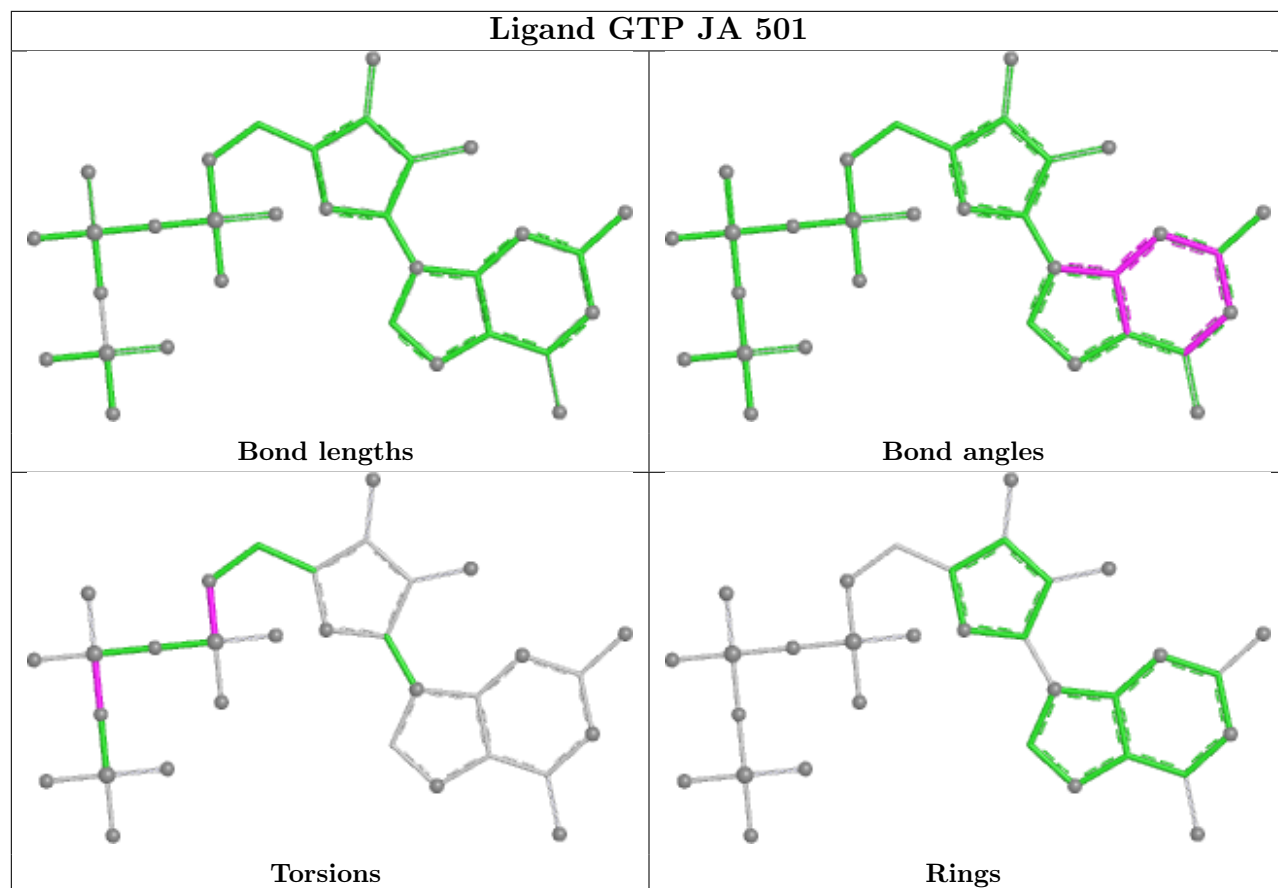


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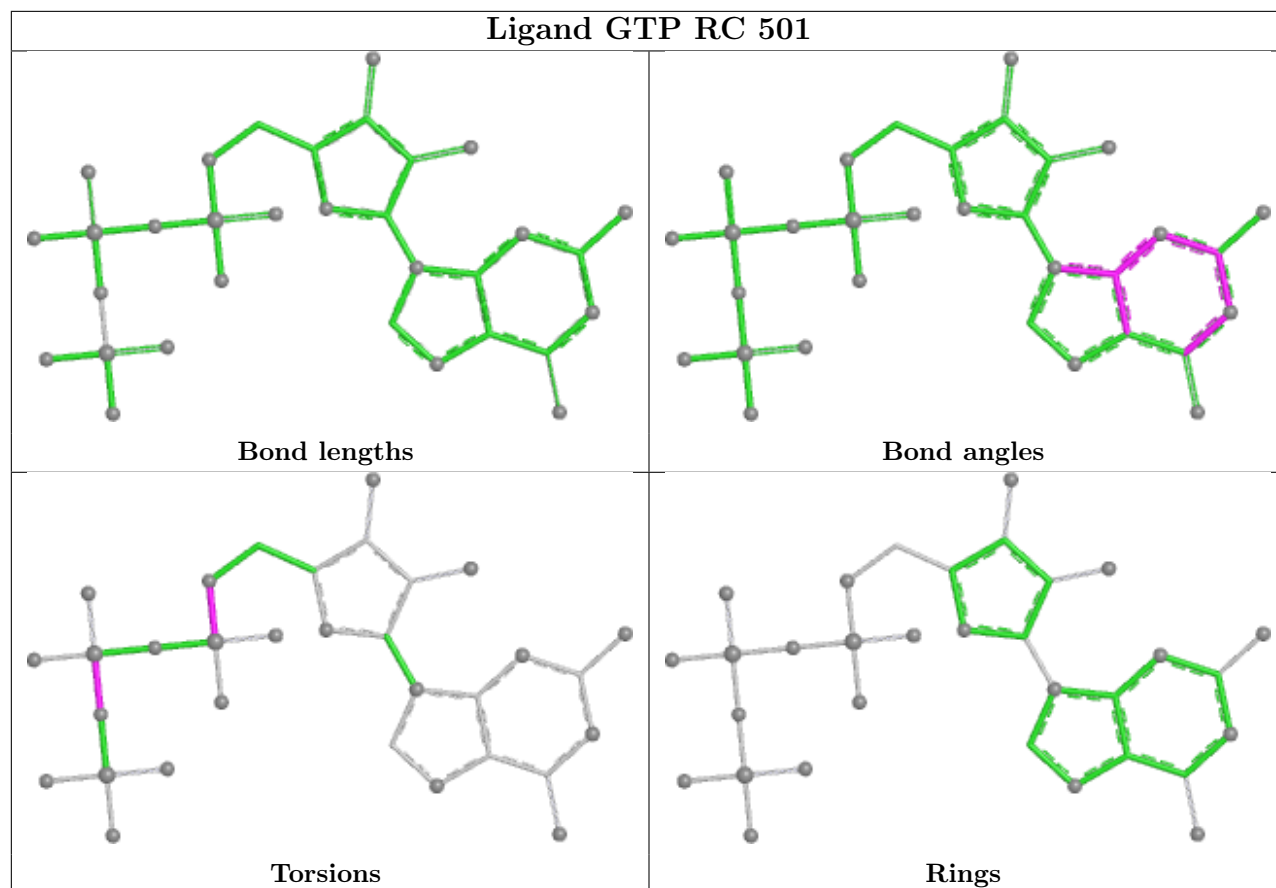


## Ligand GTP FM 501

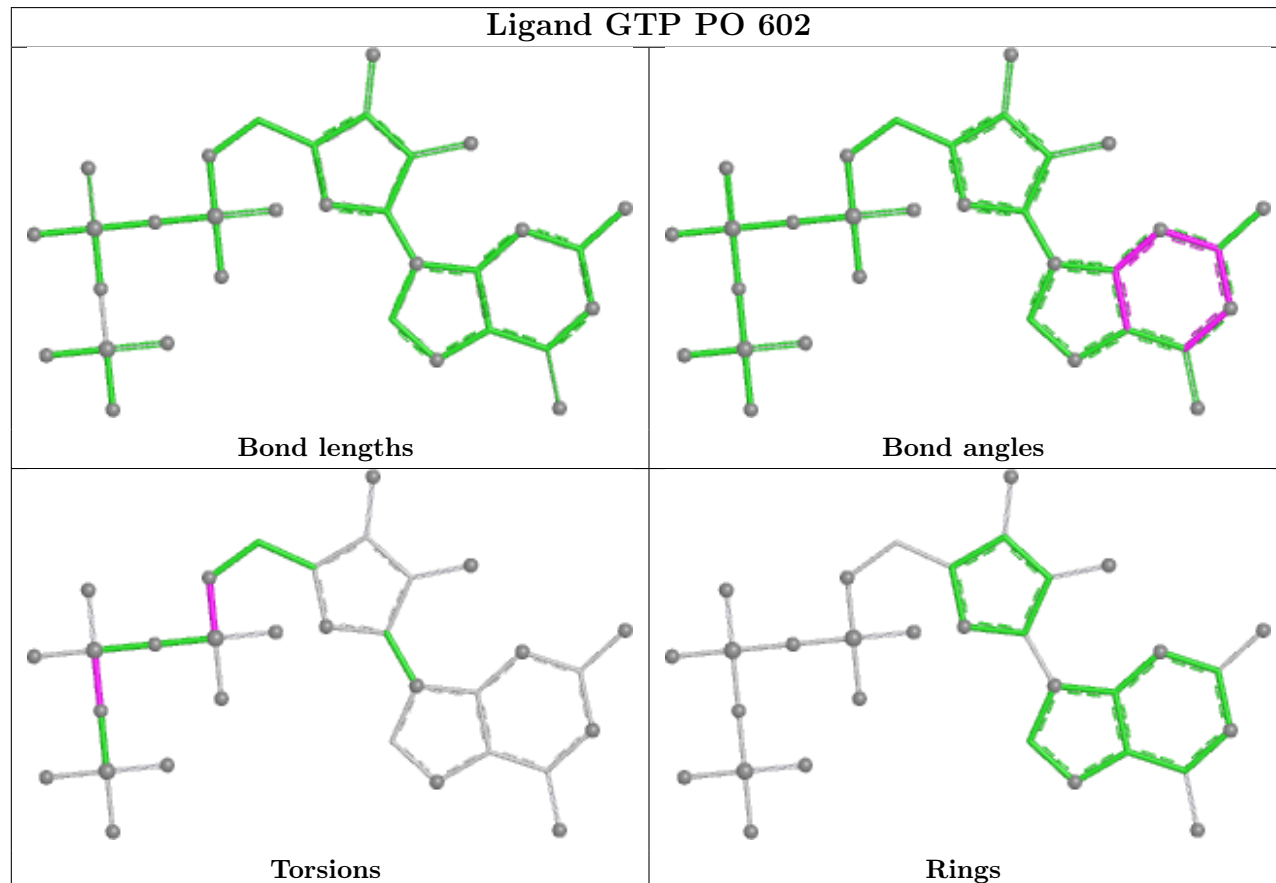


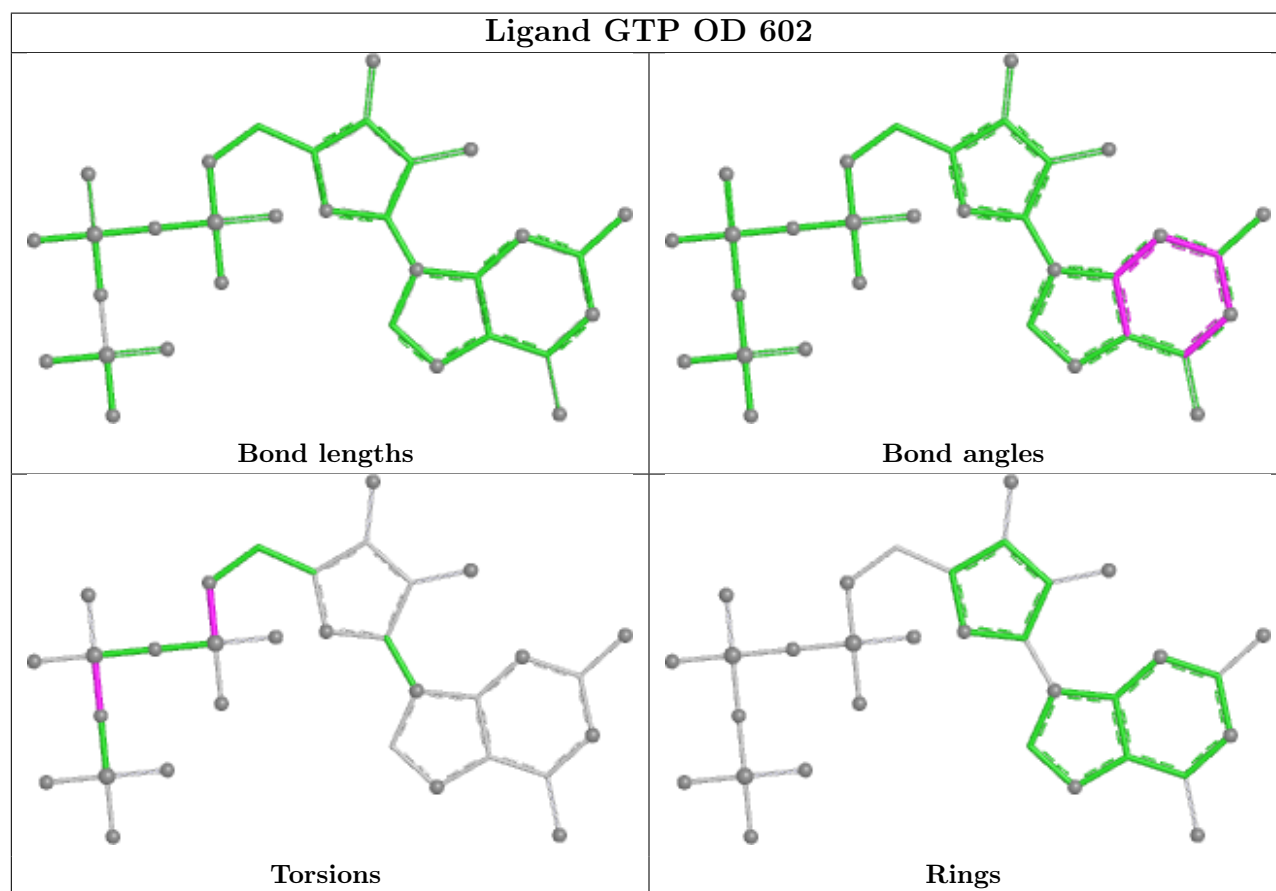
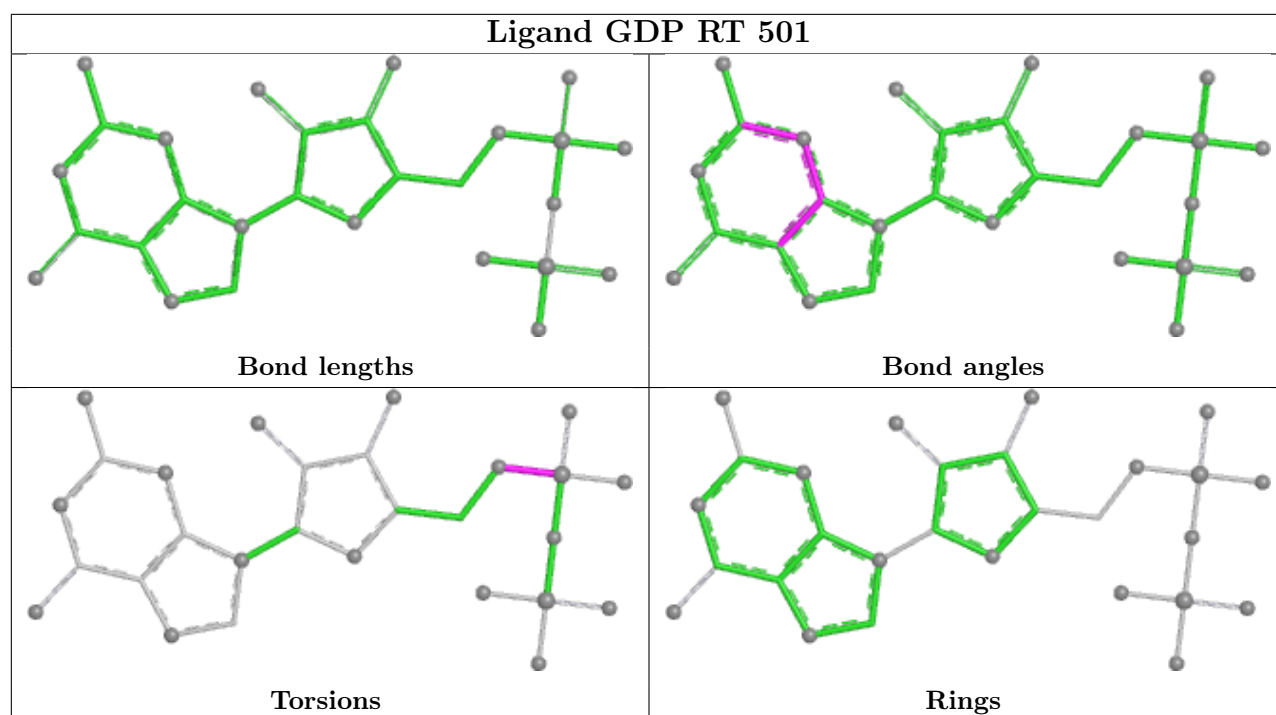


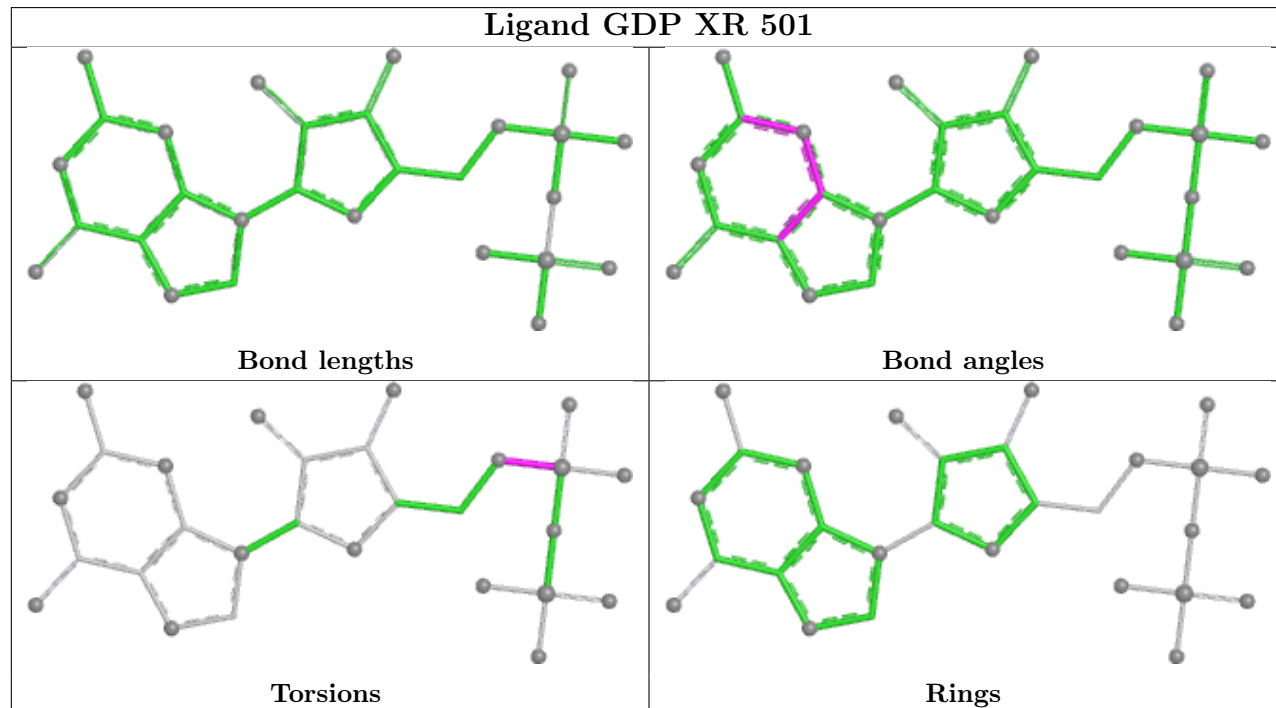
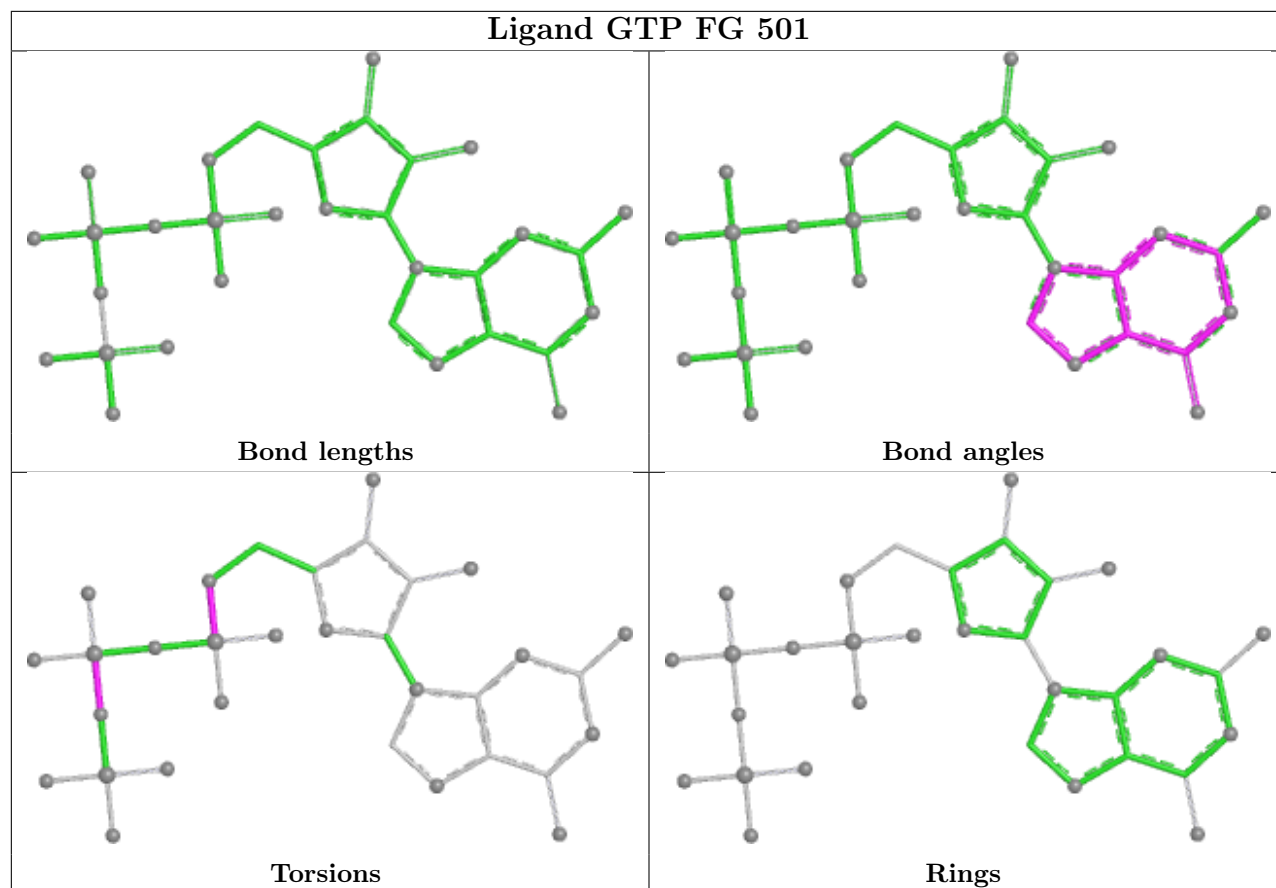
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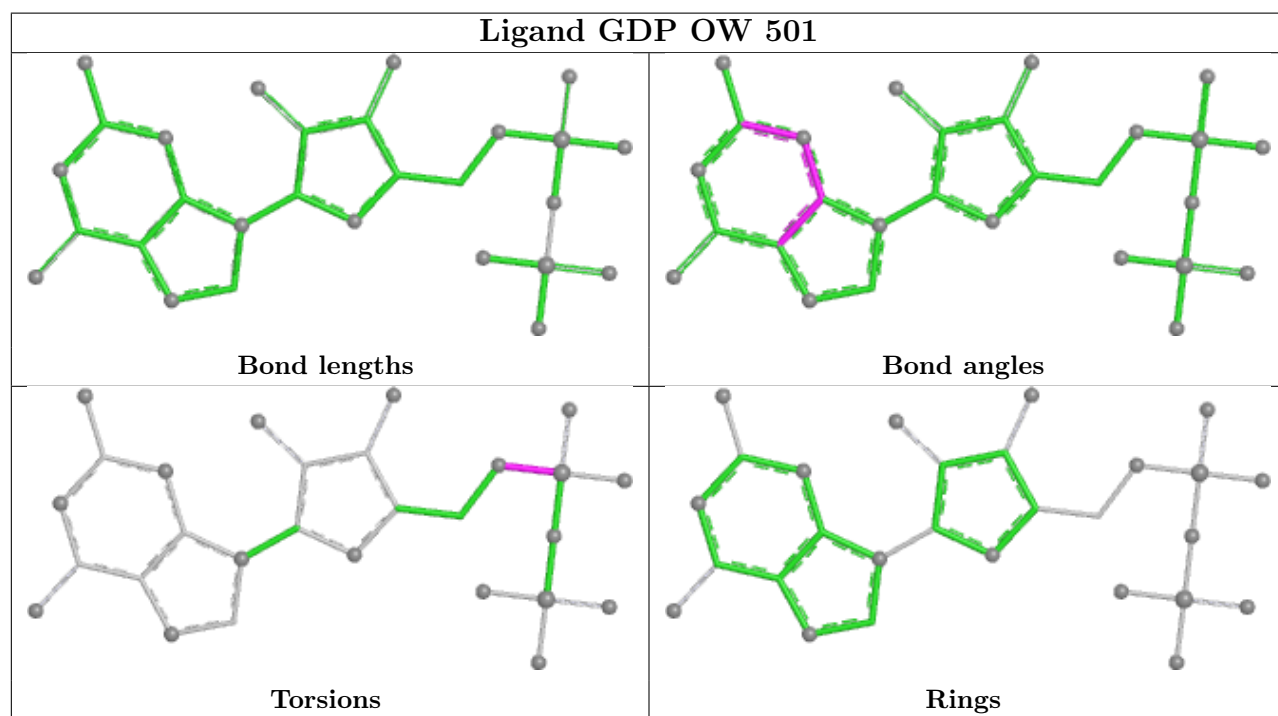
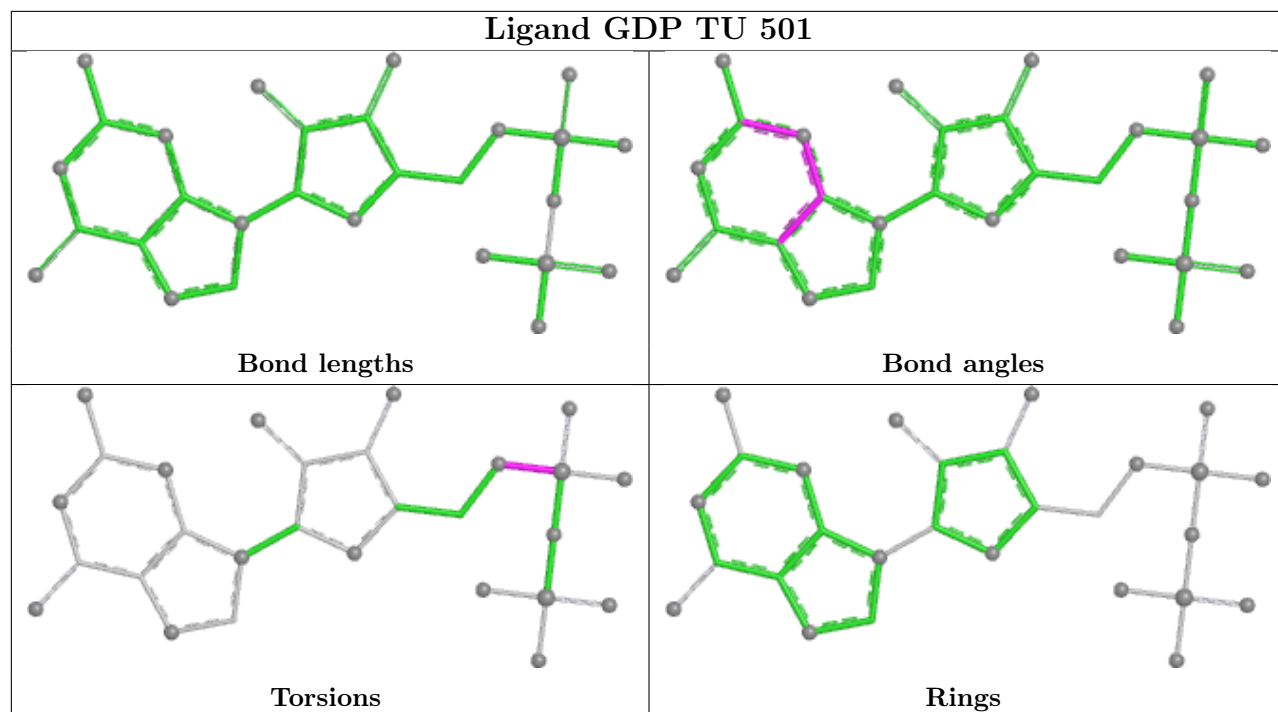


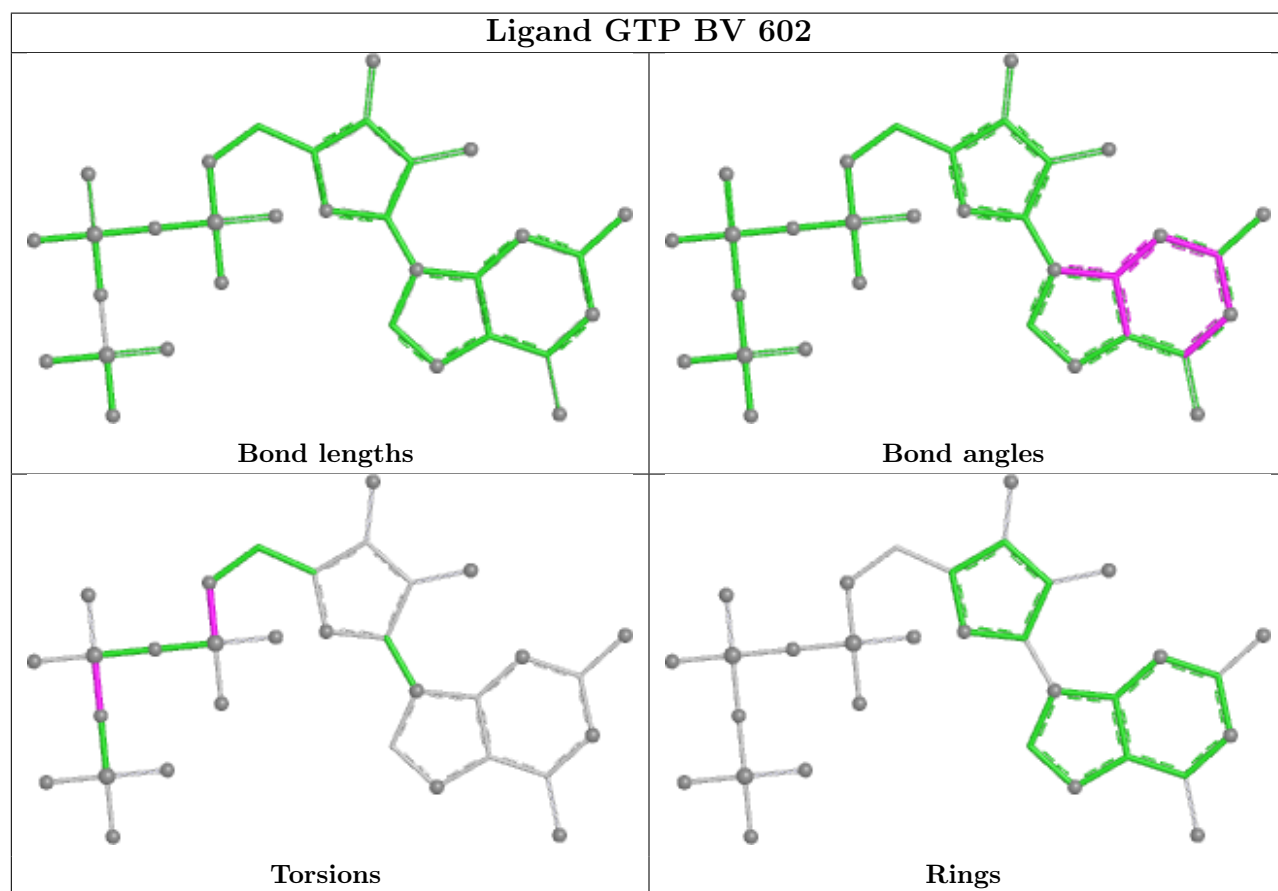
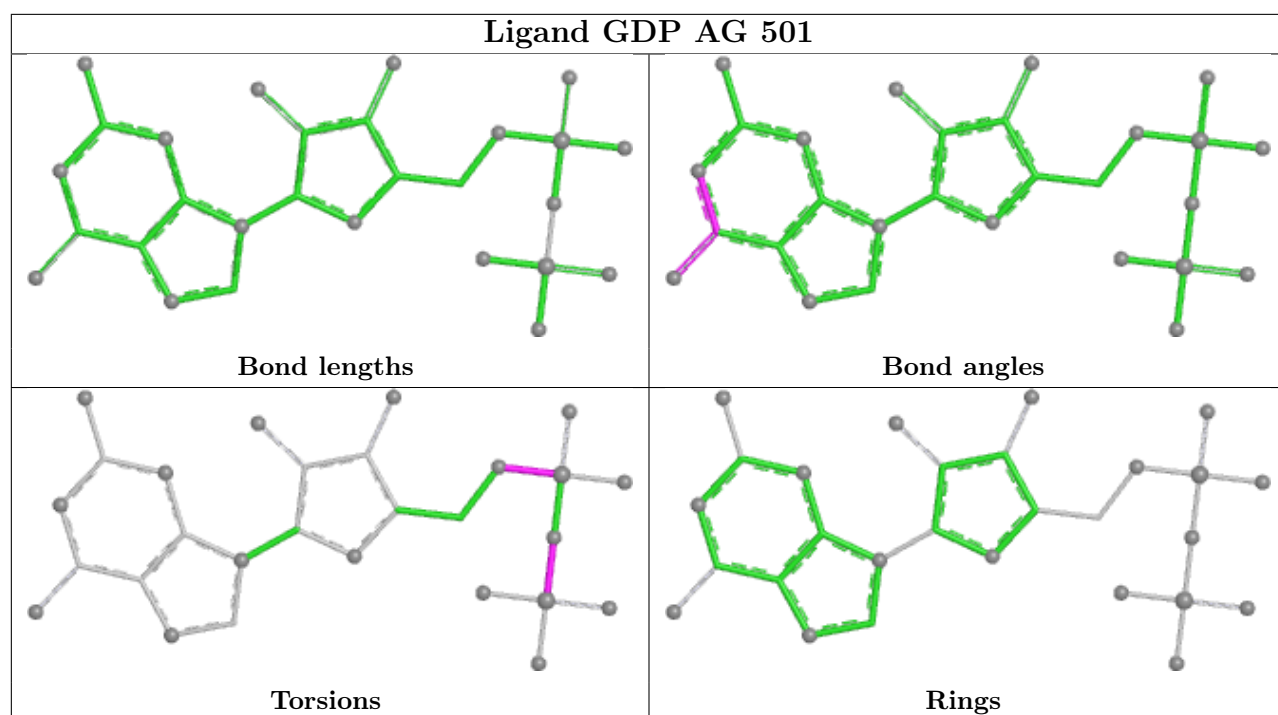
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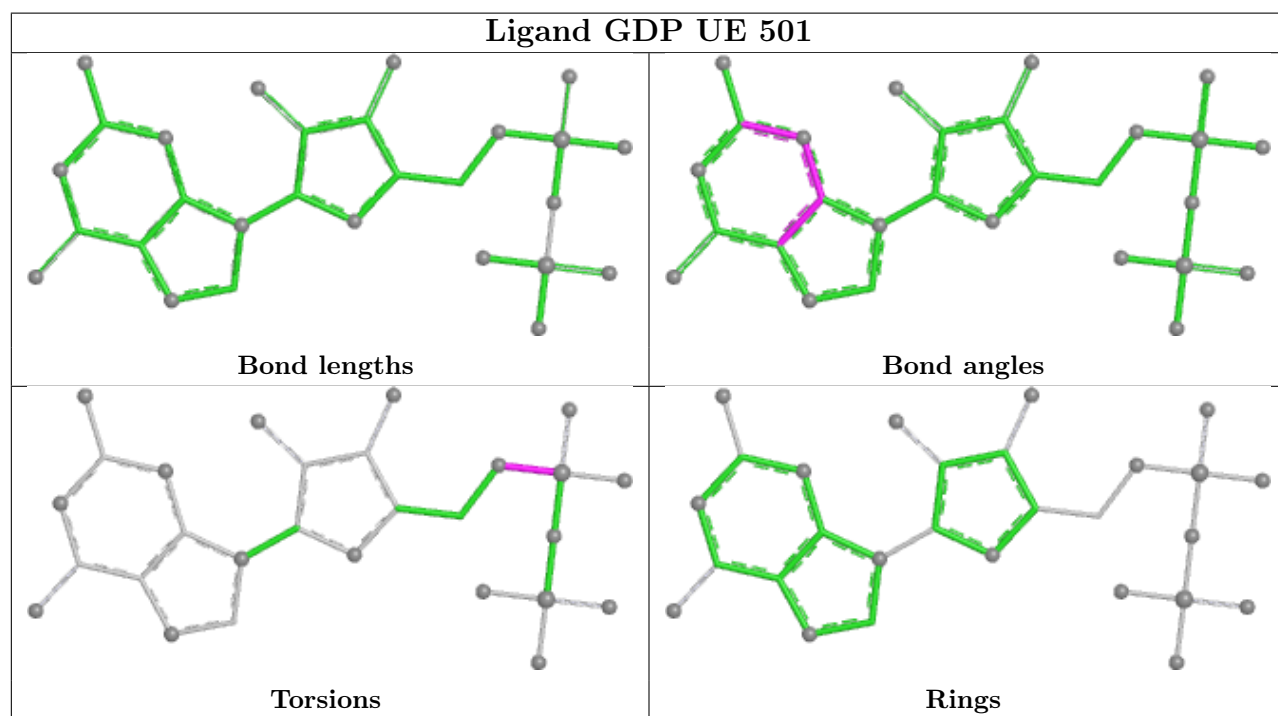
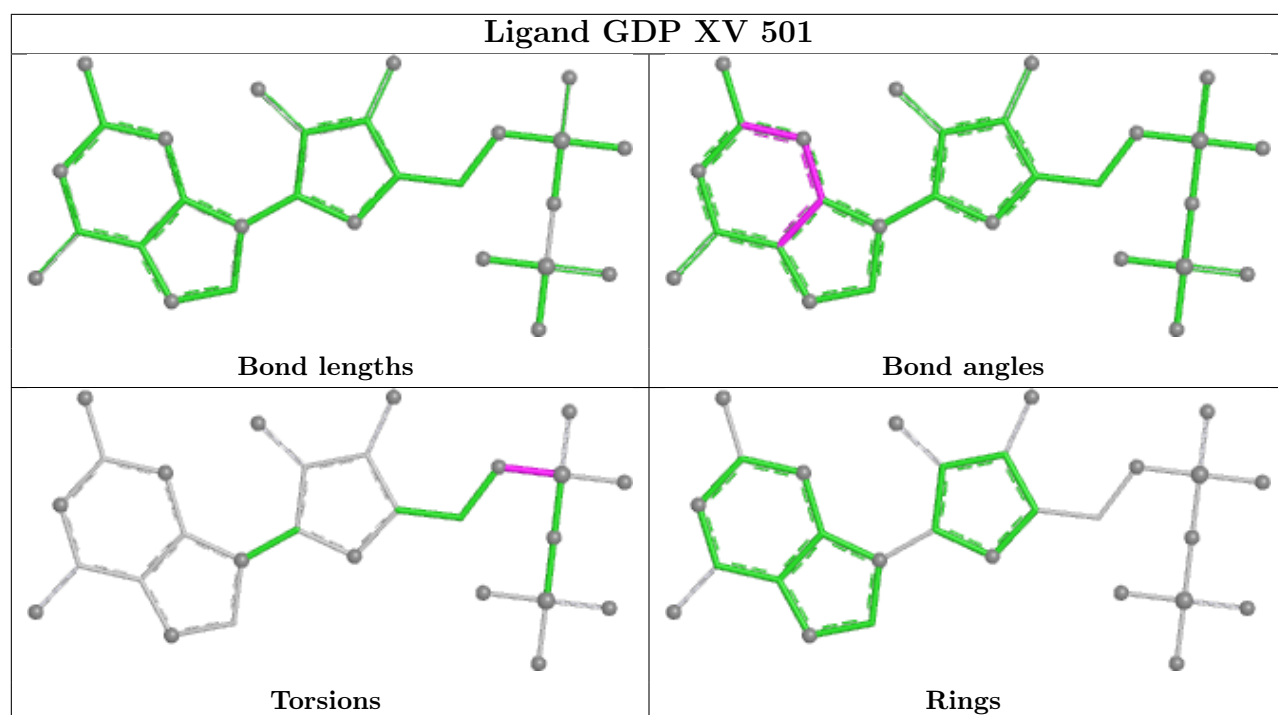






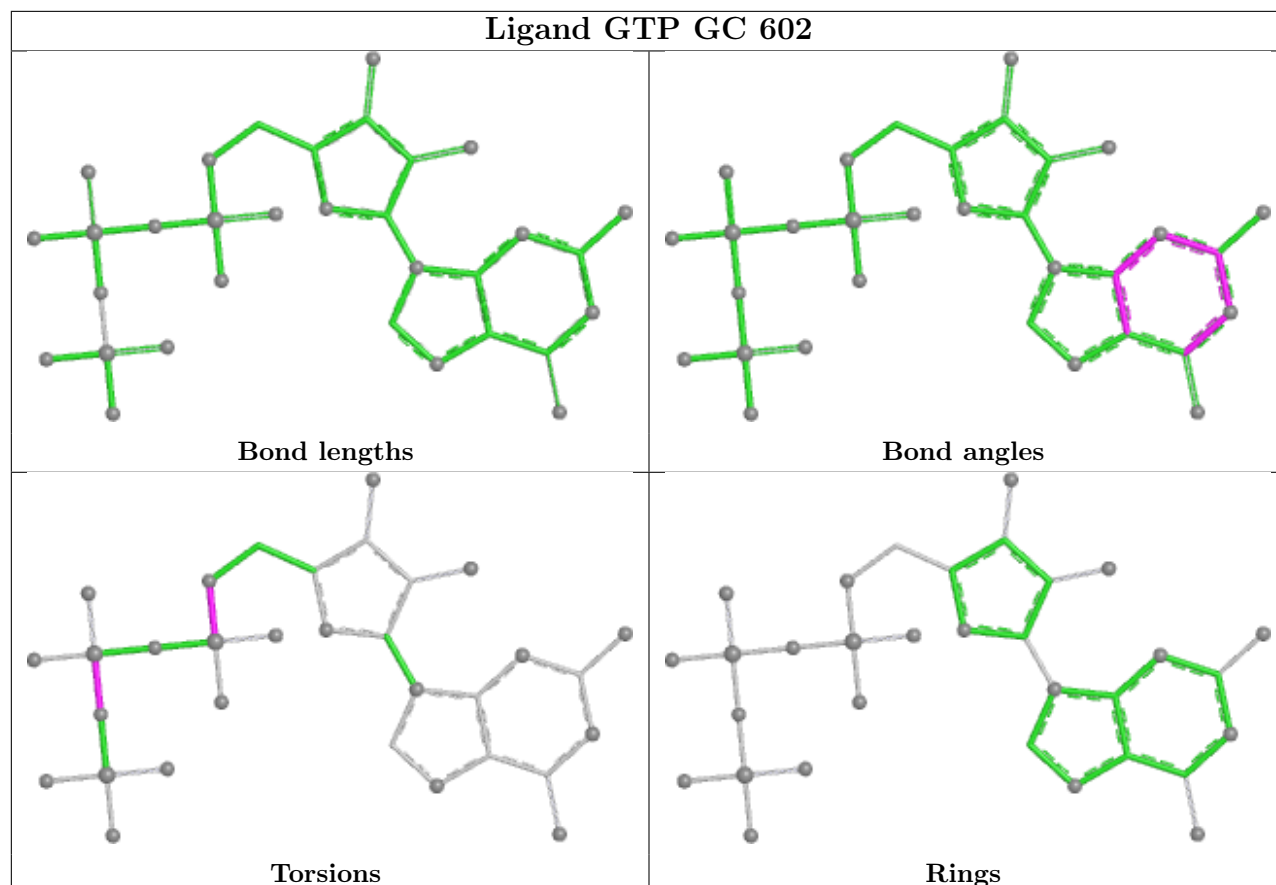




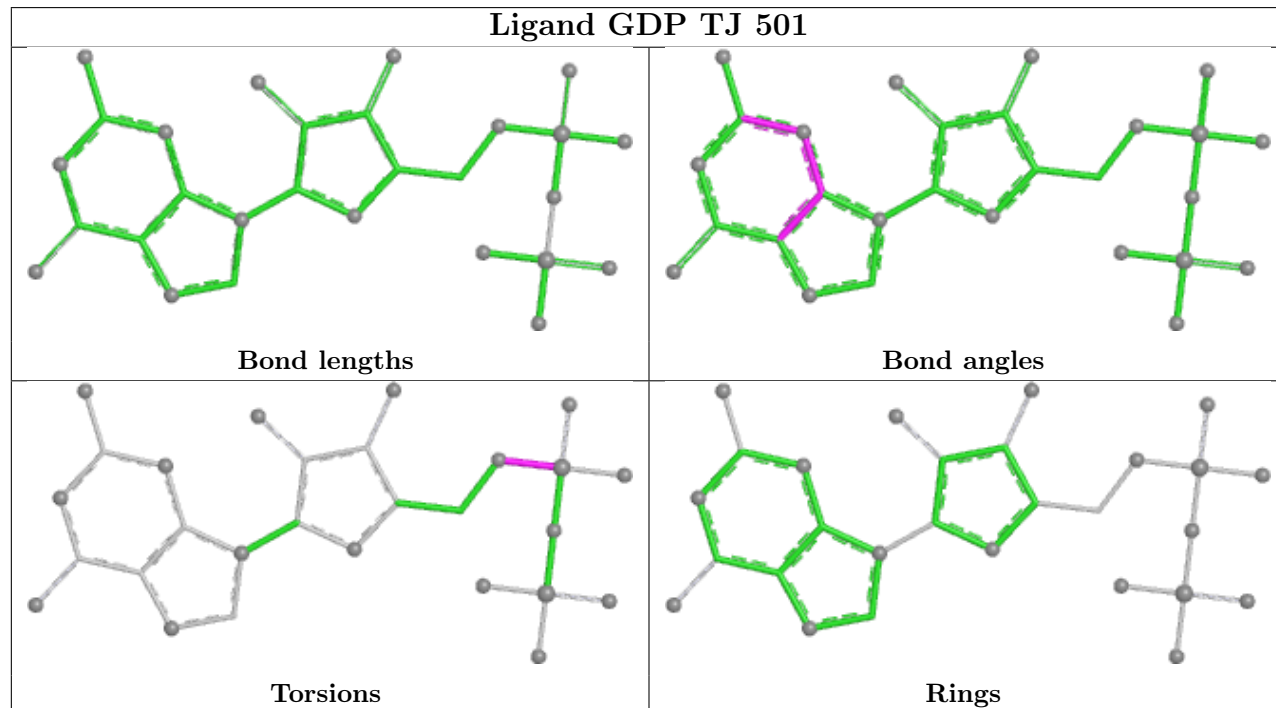


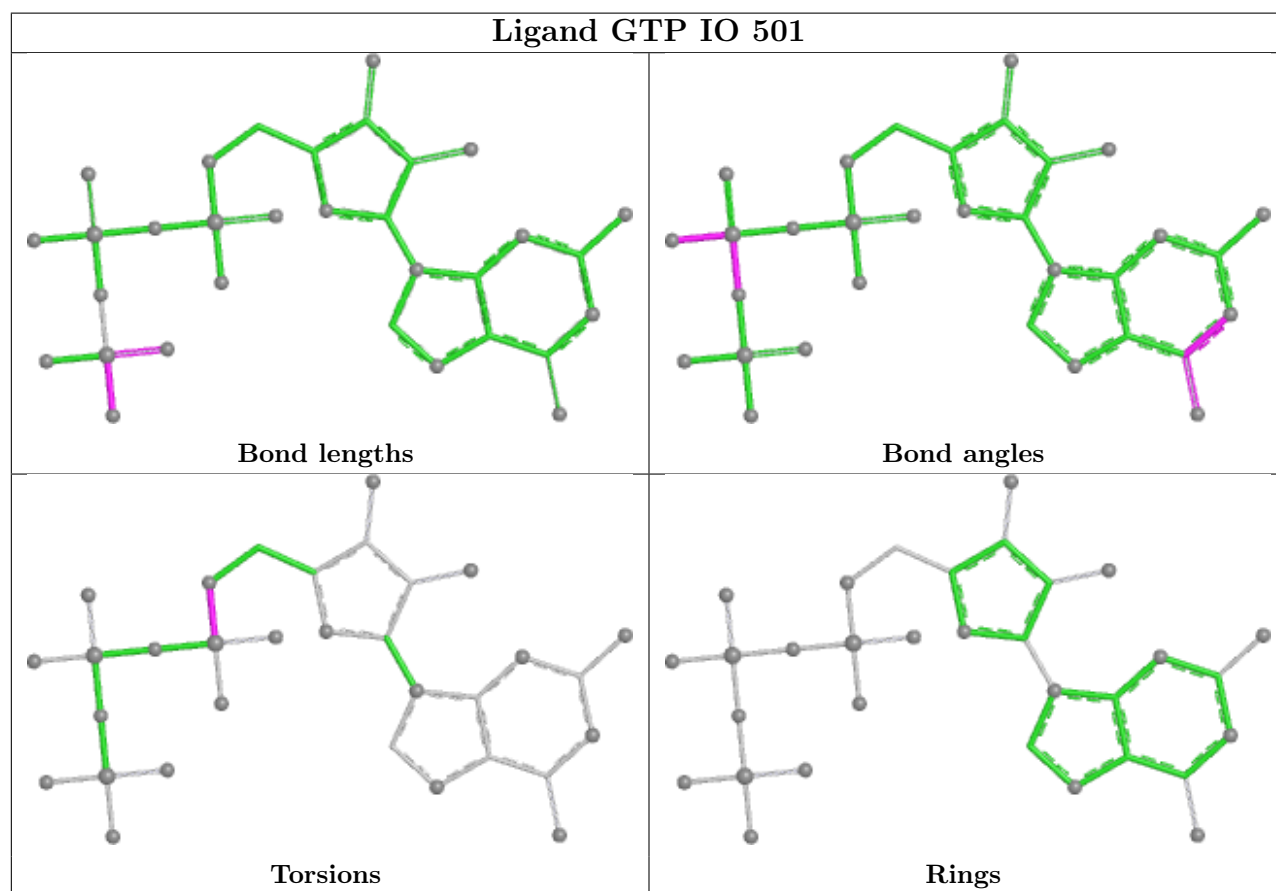
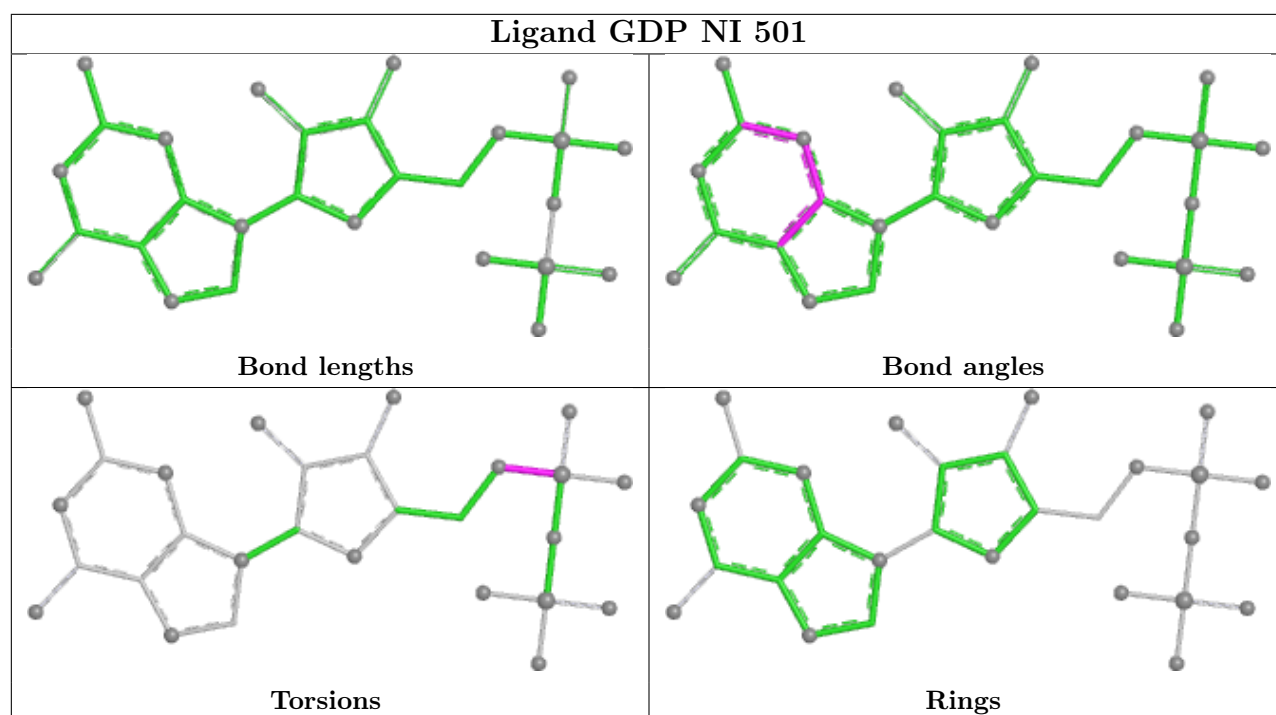


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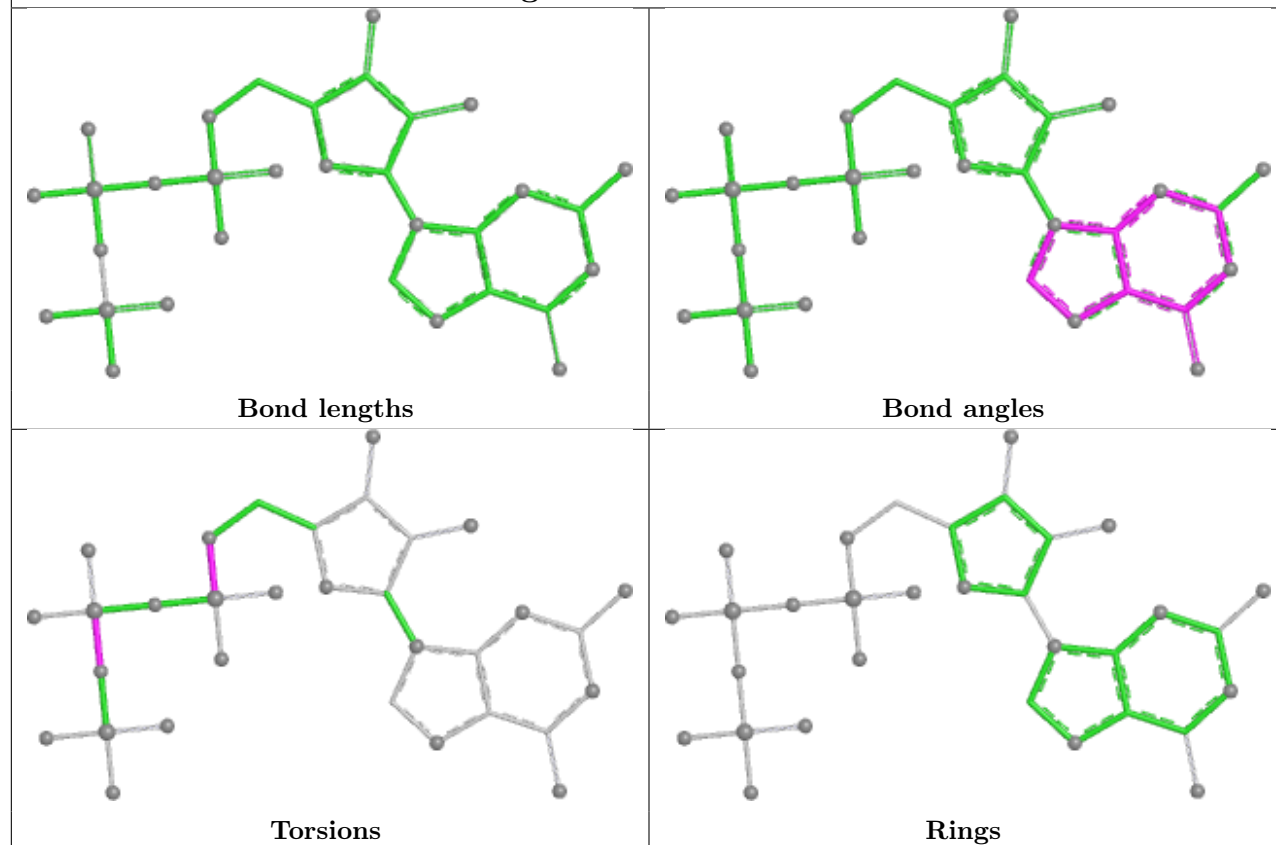


## Ligand GDP TJ 501

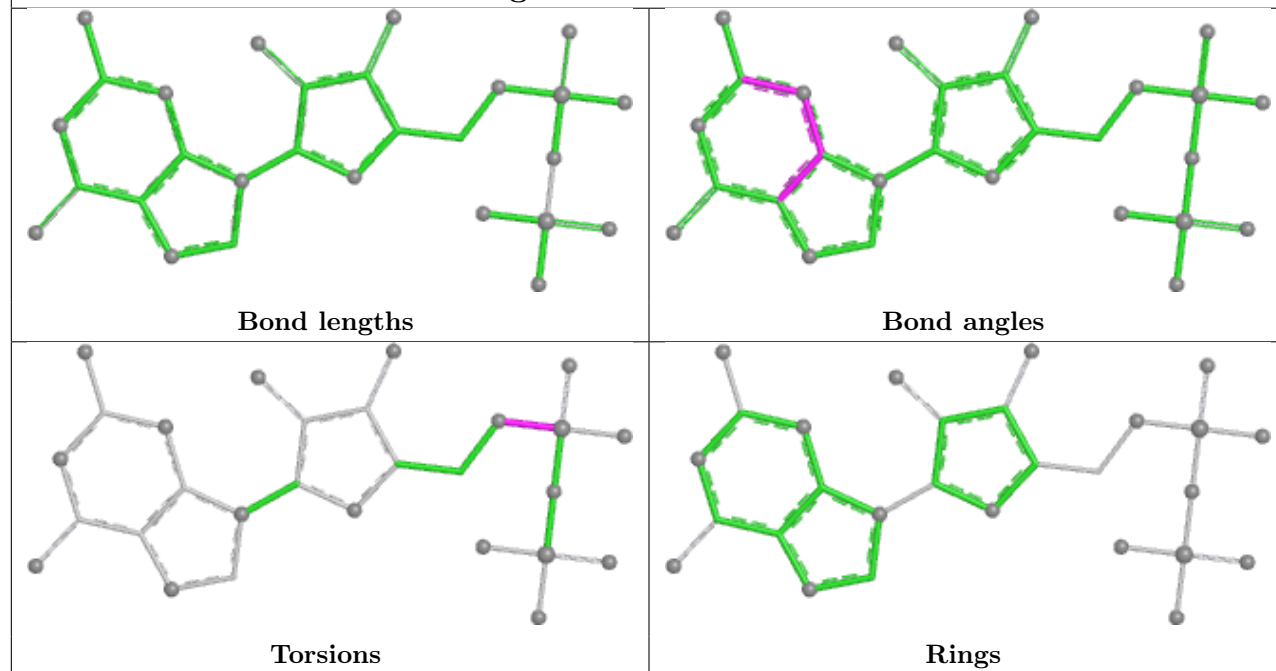




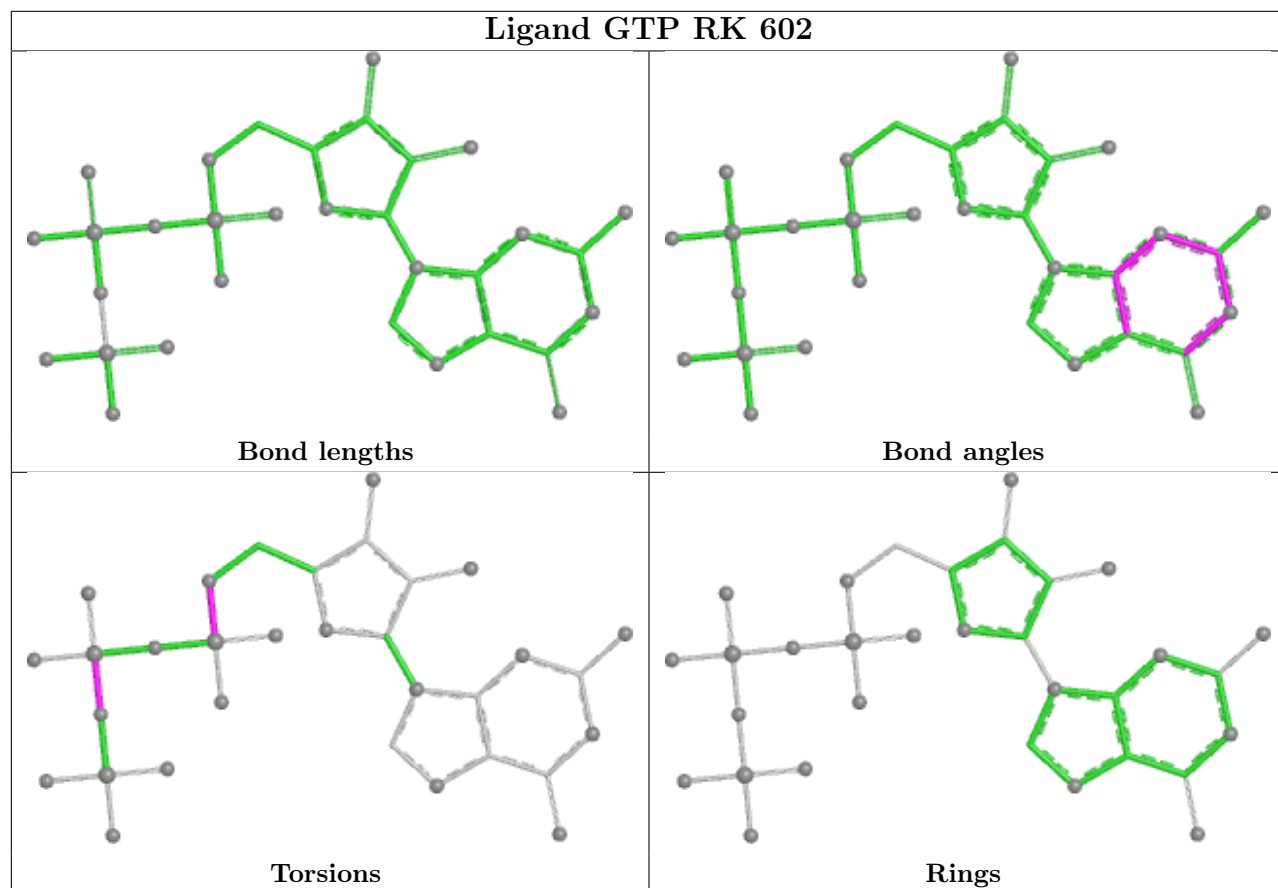
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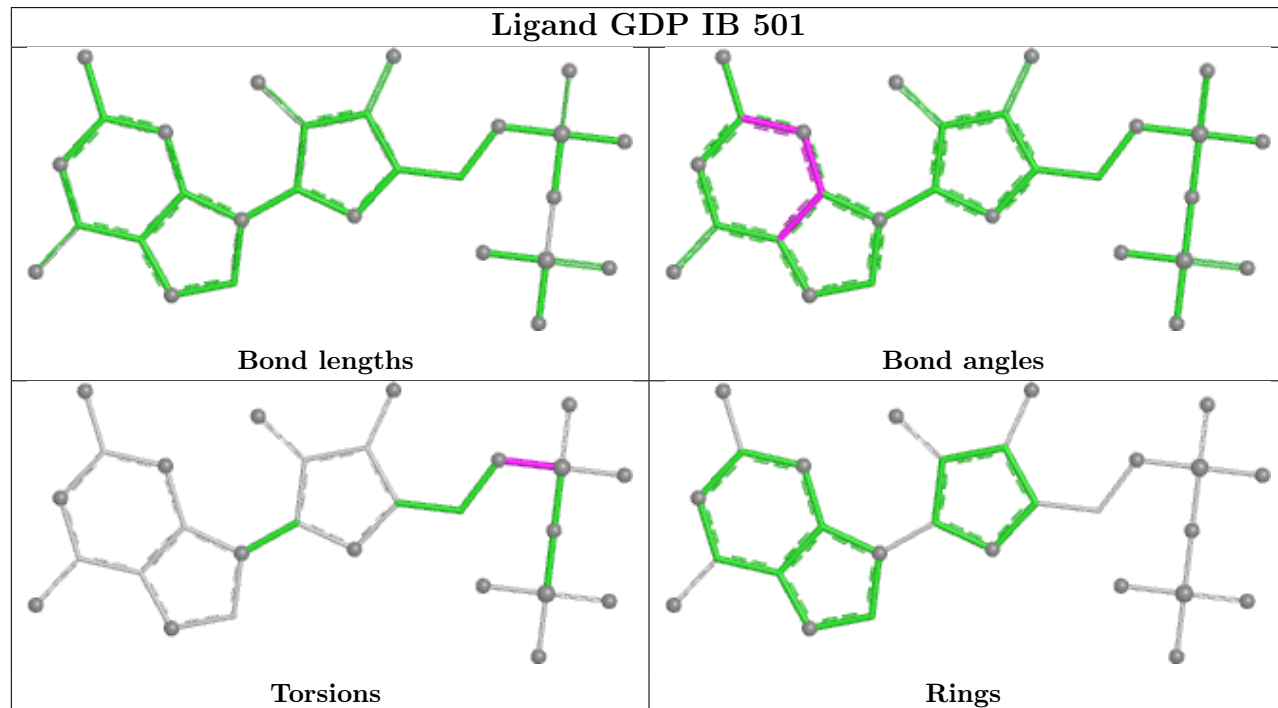
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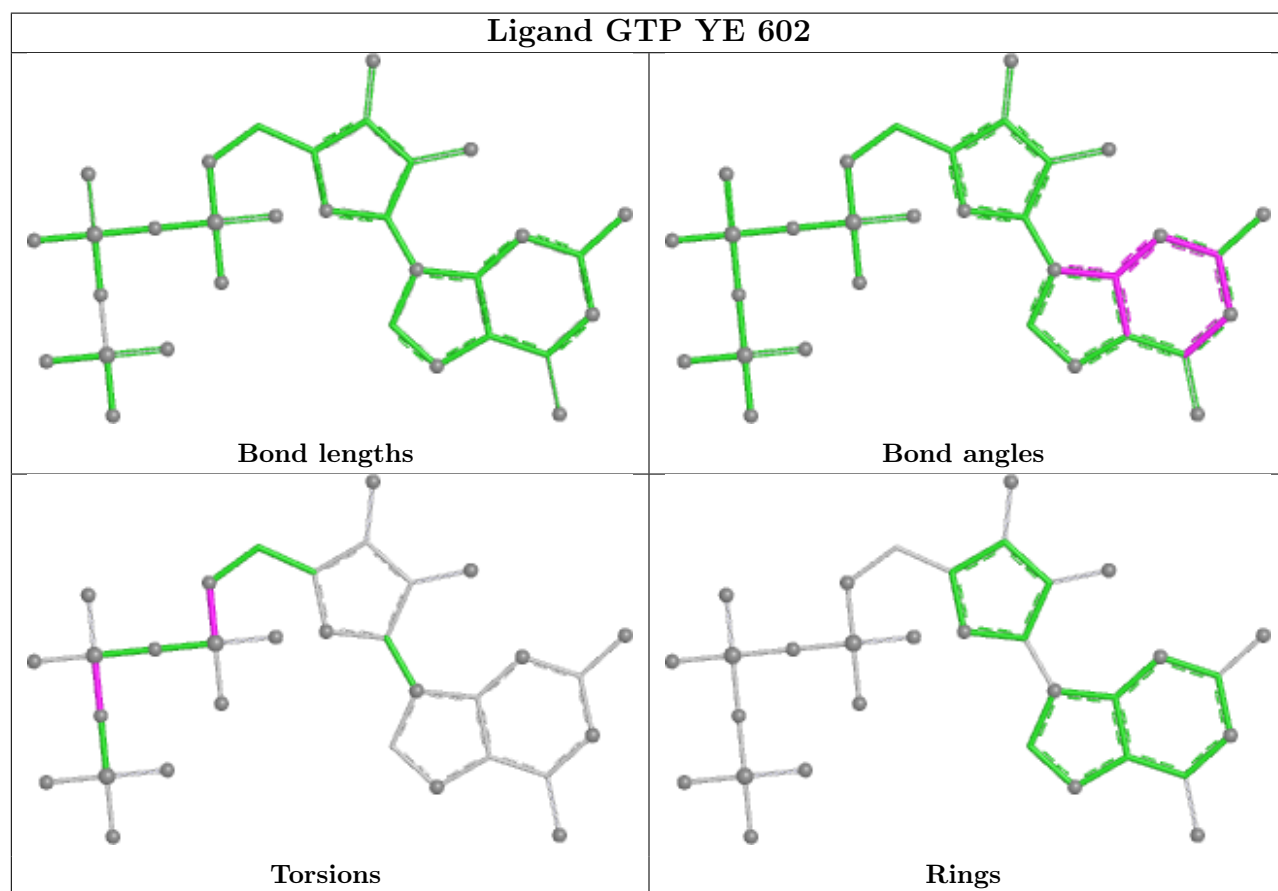
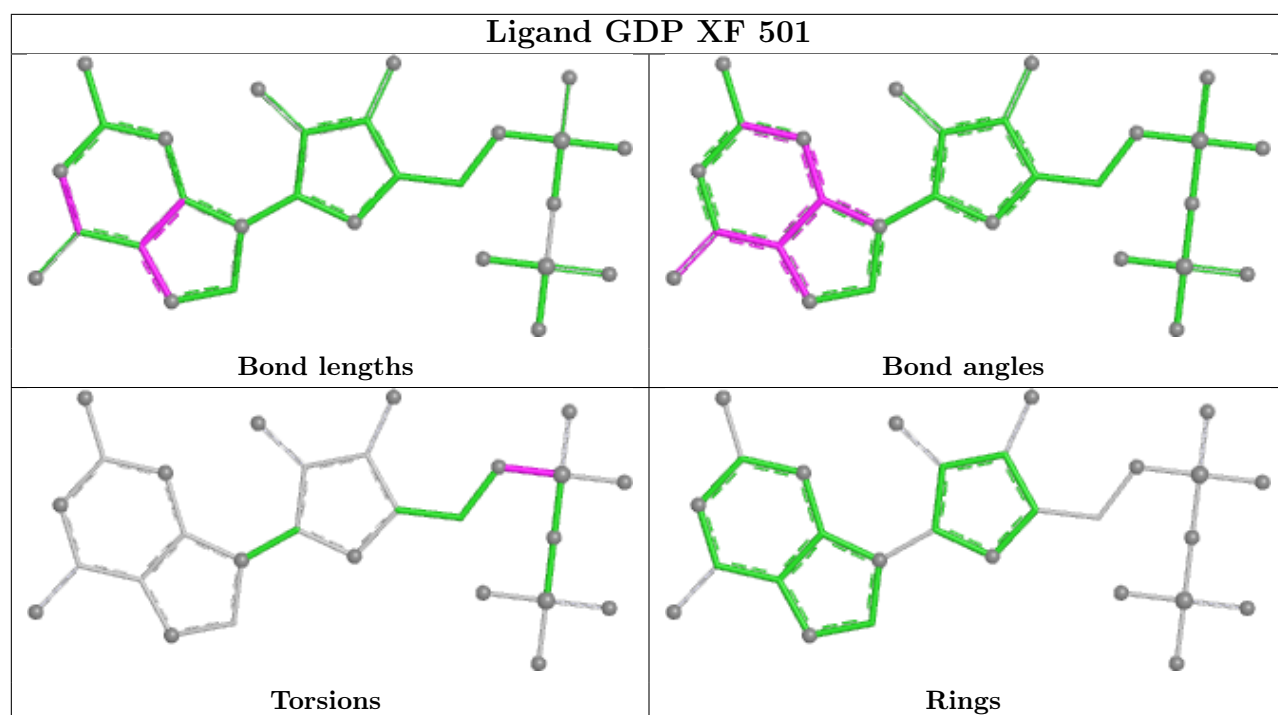


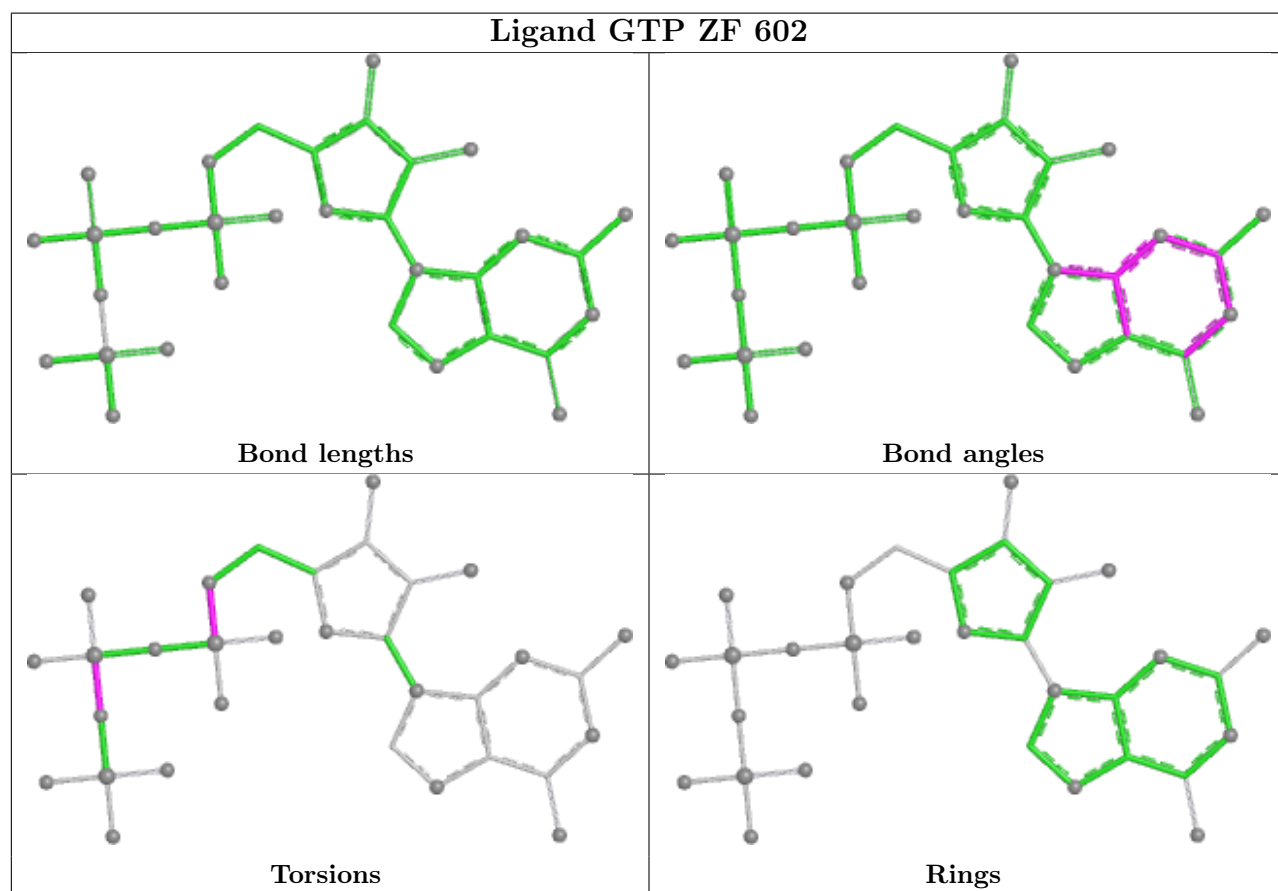
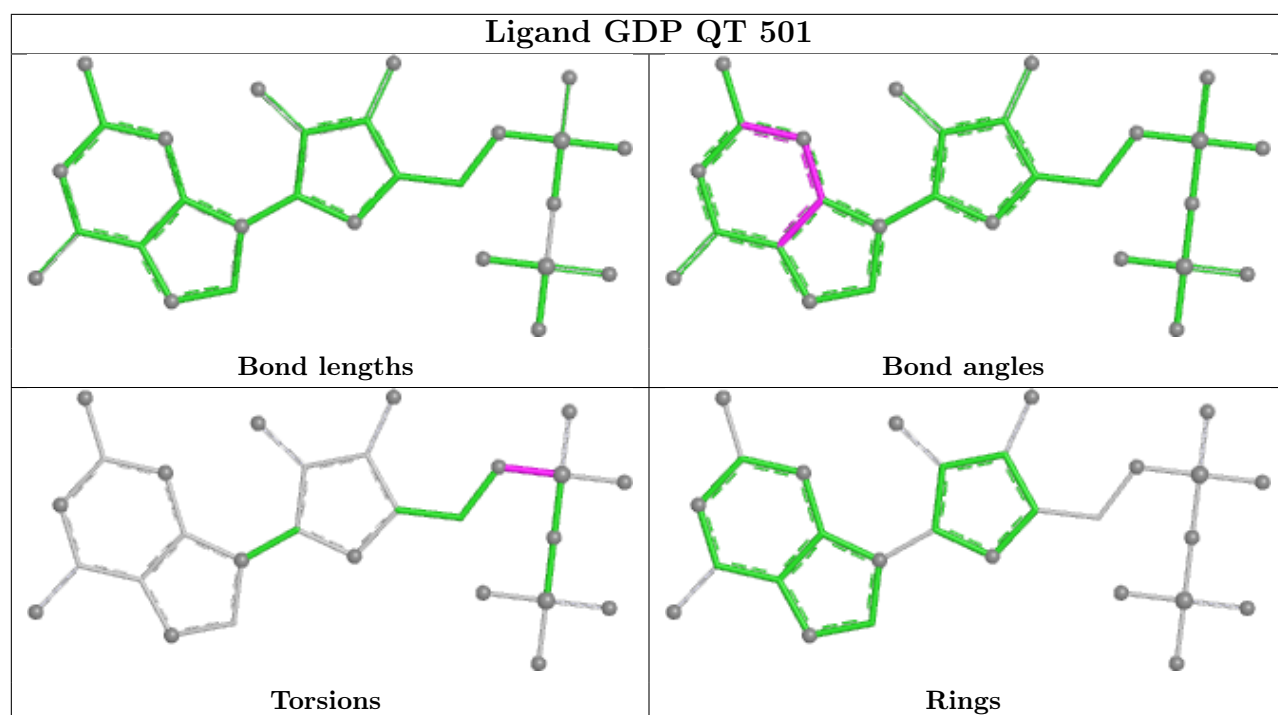
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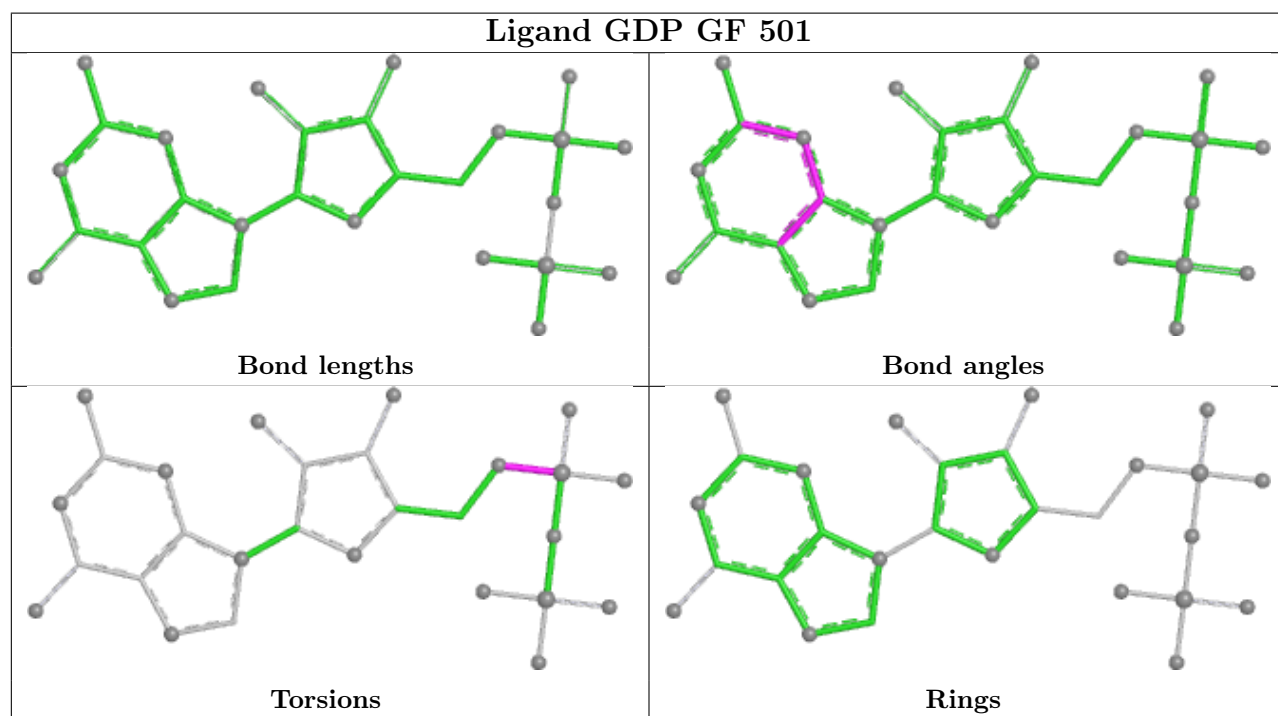
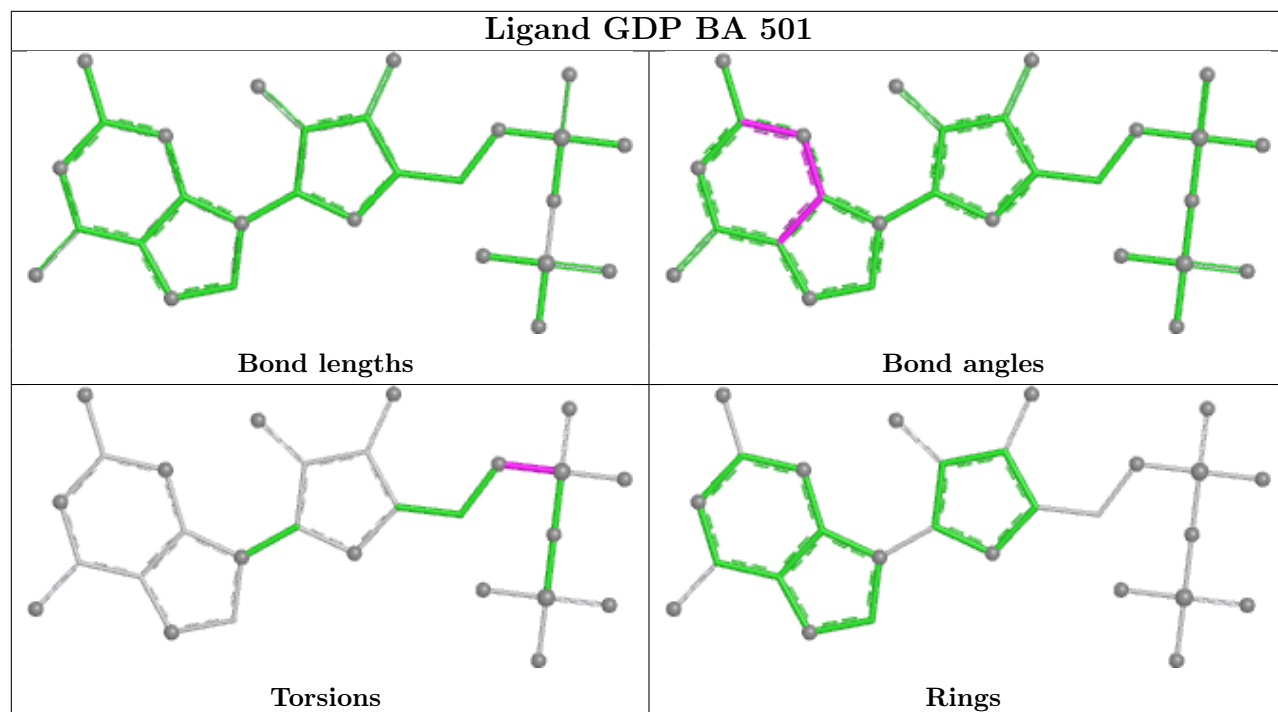


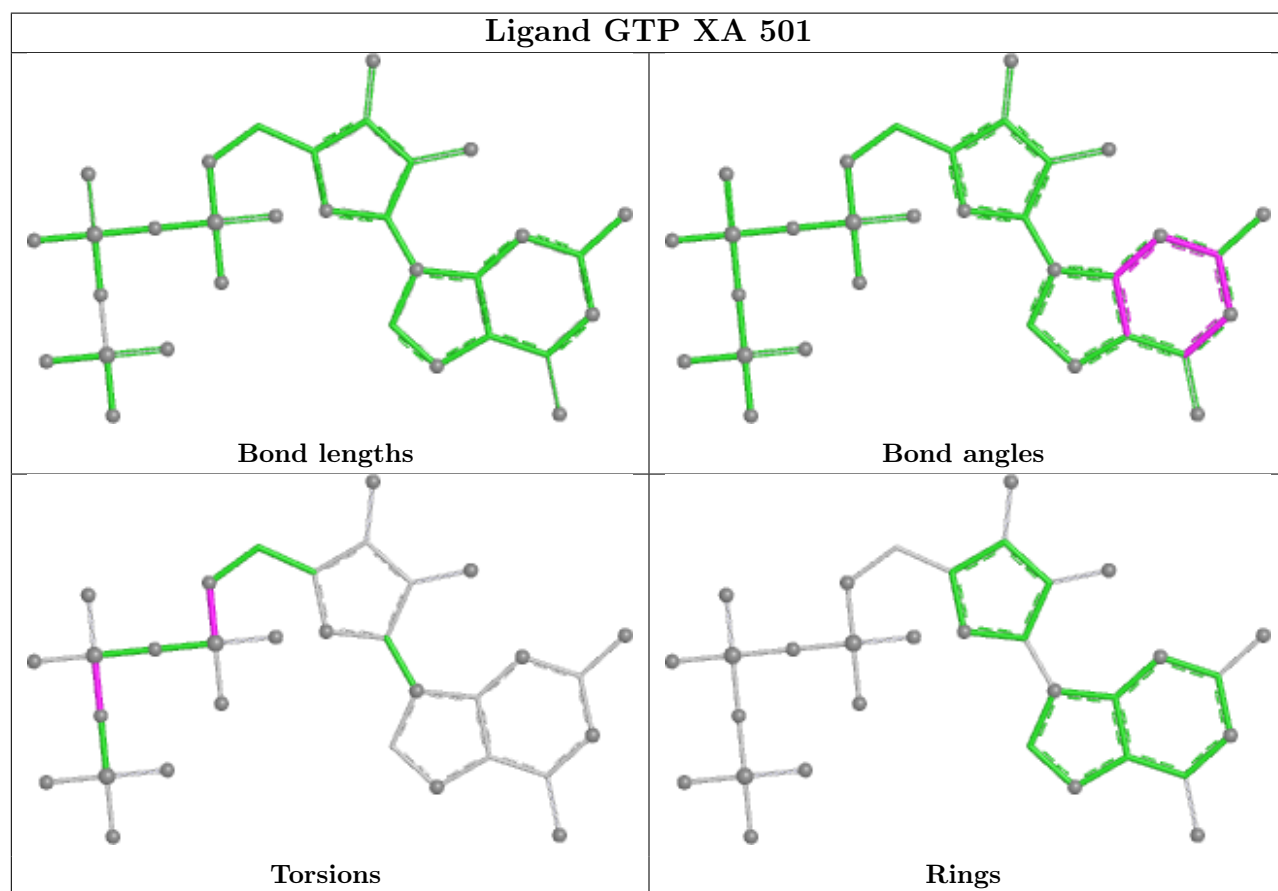
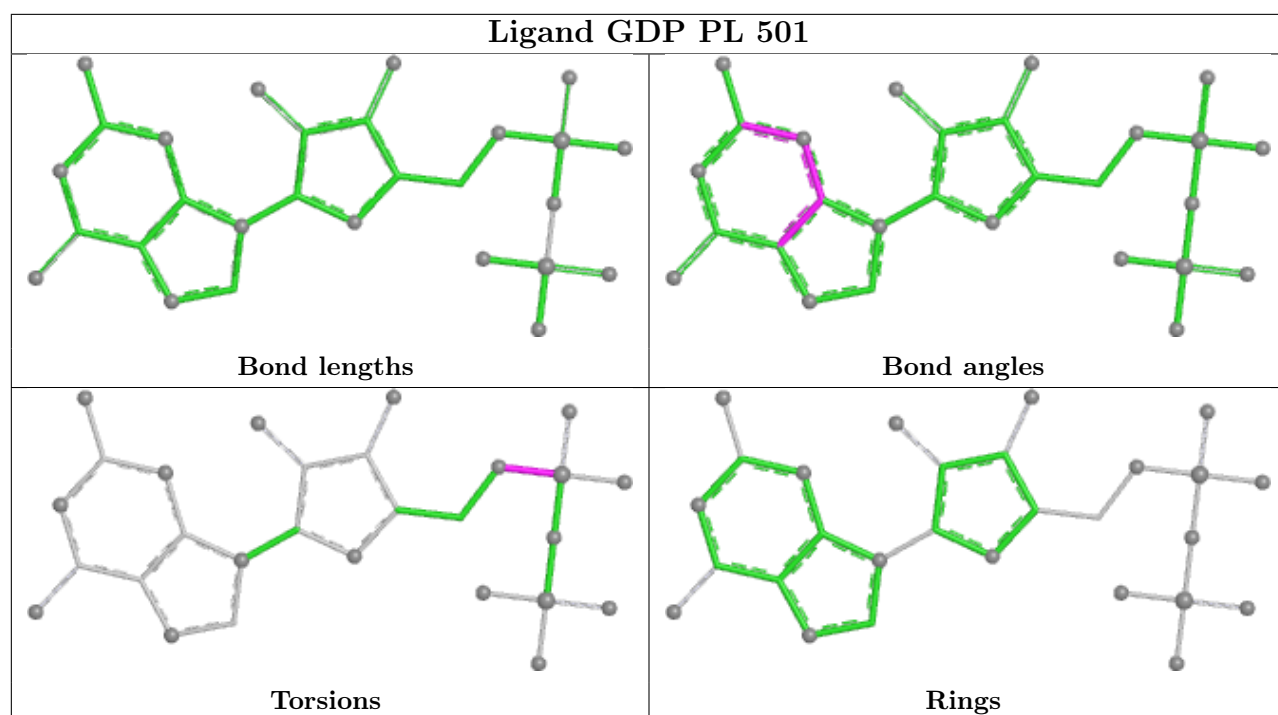
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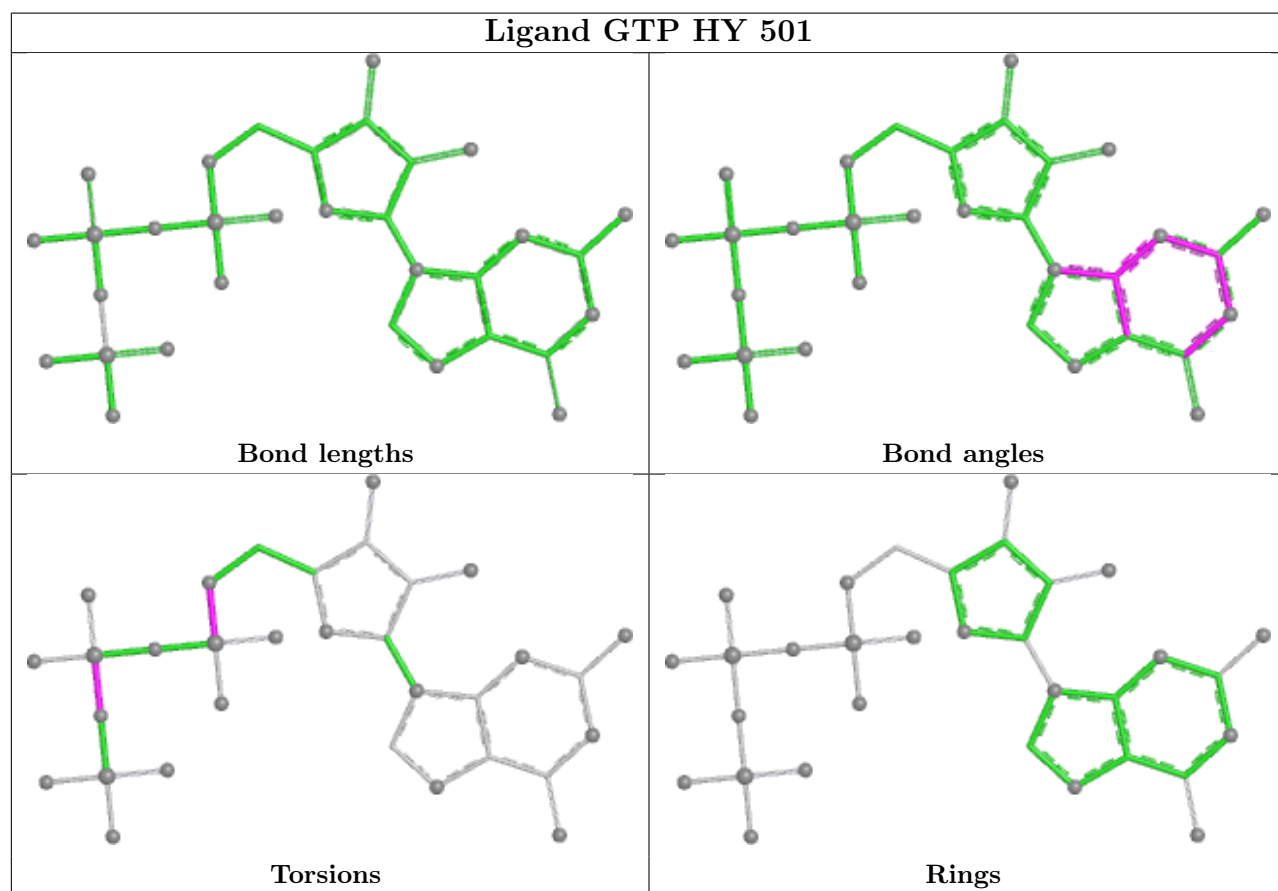
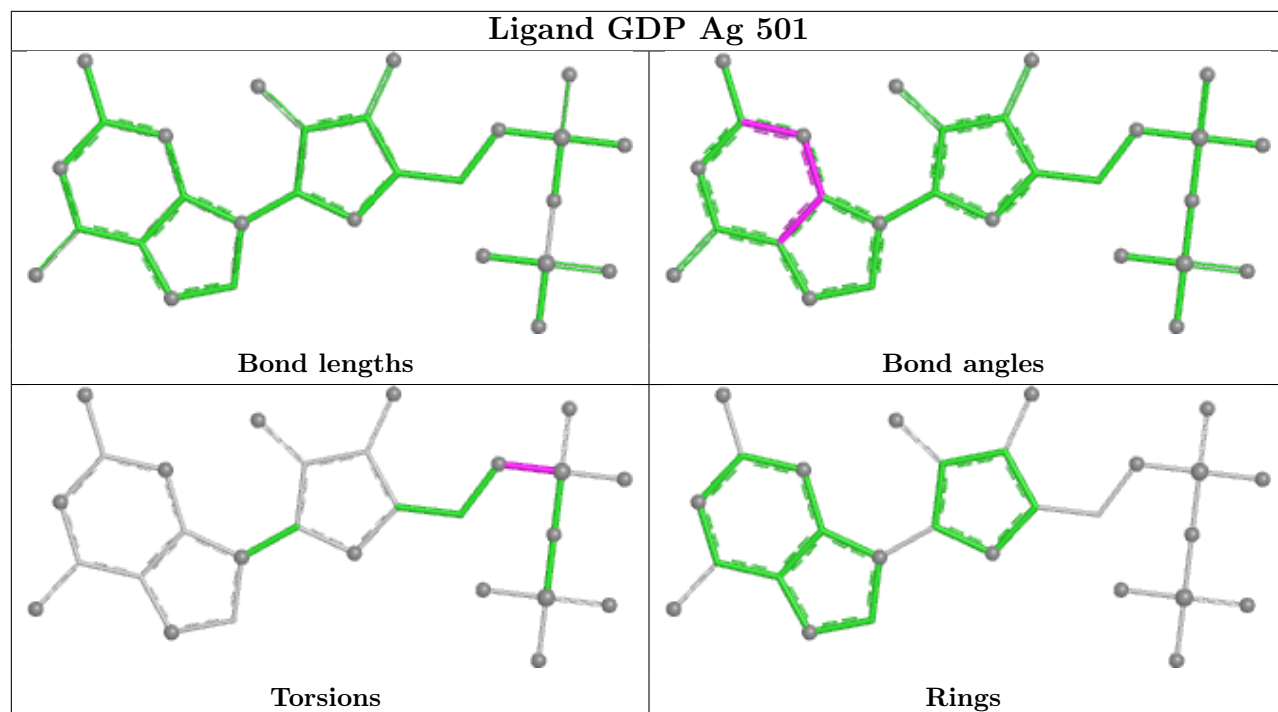


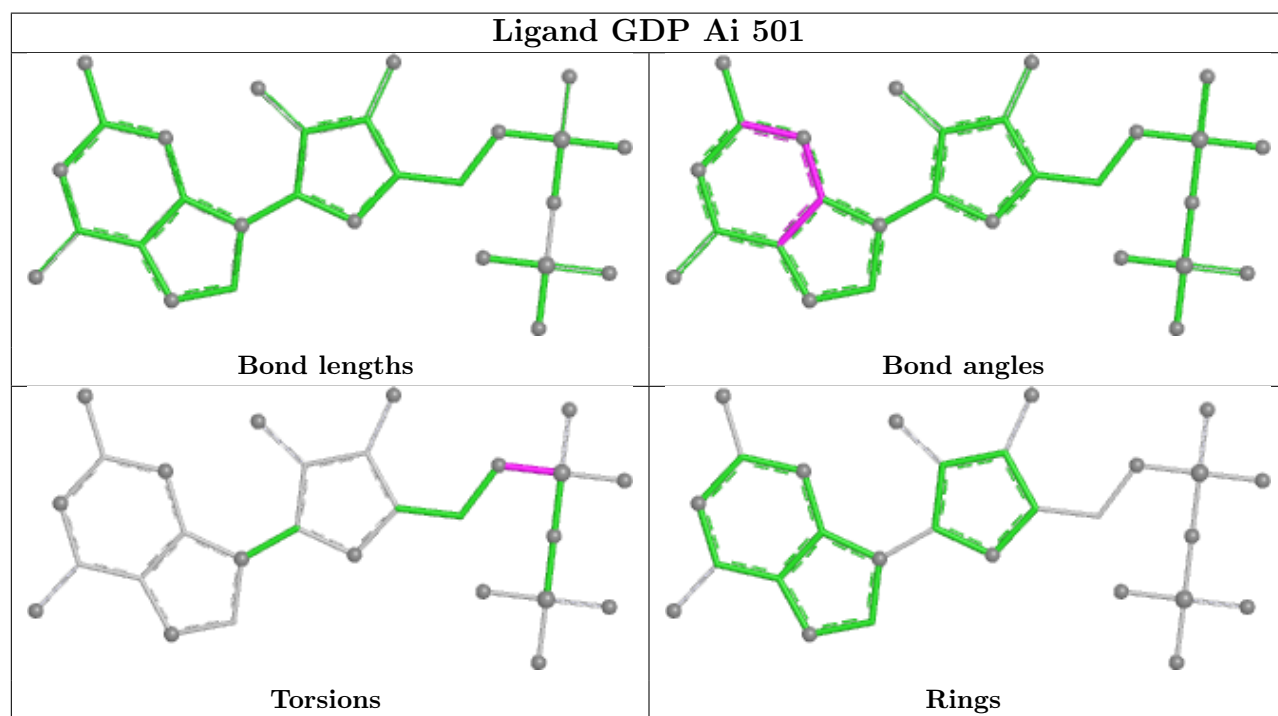
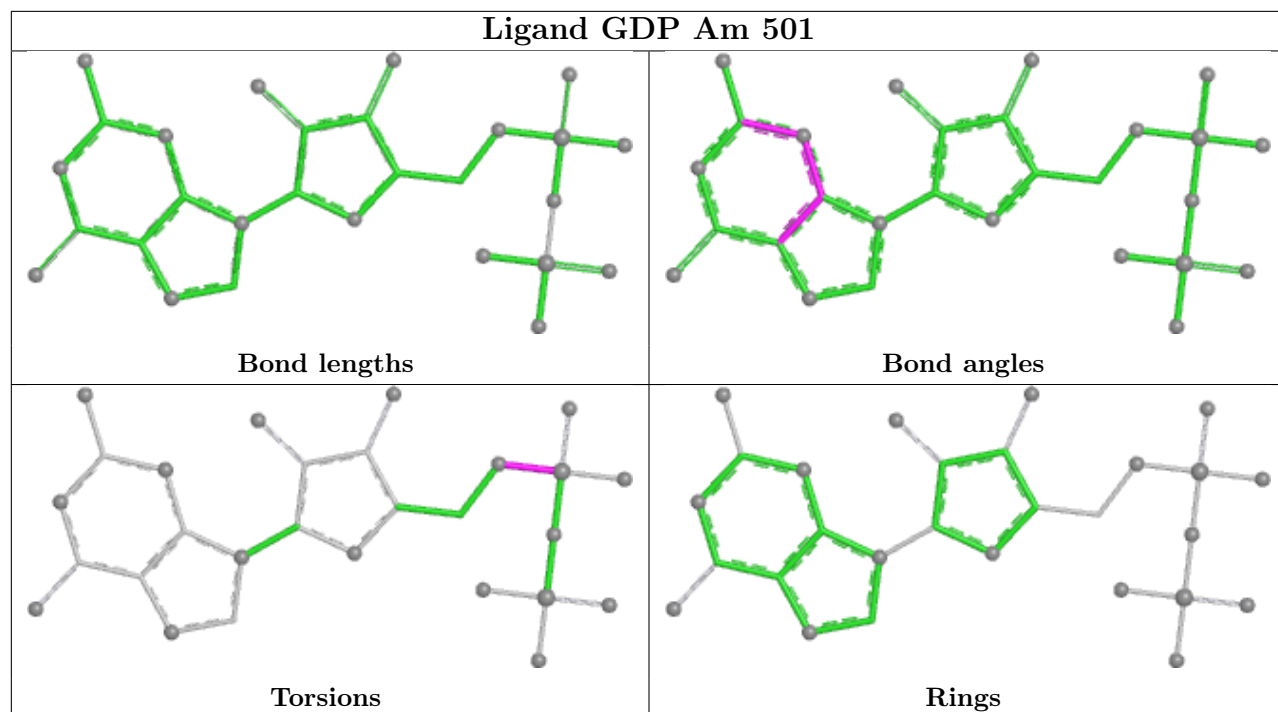


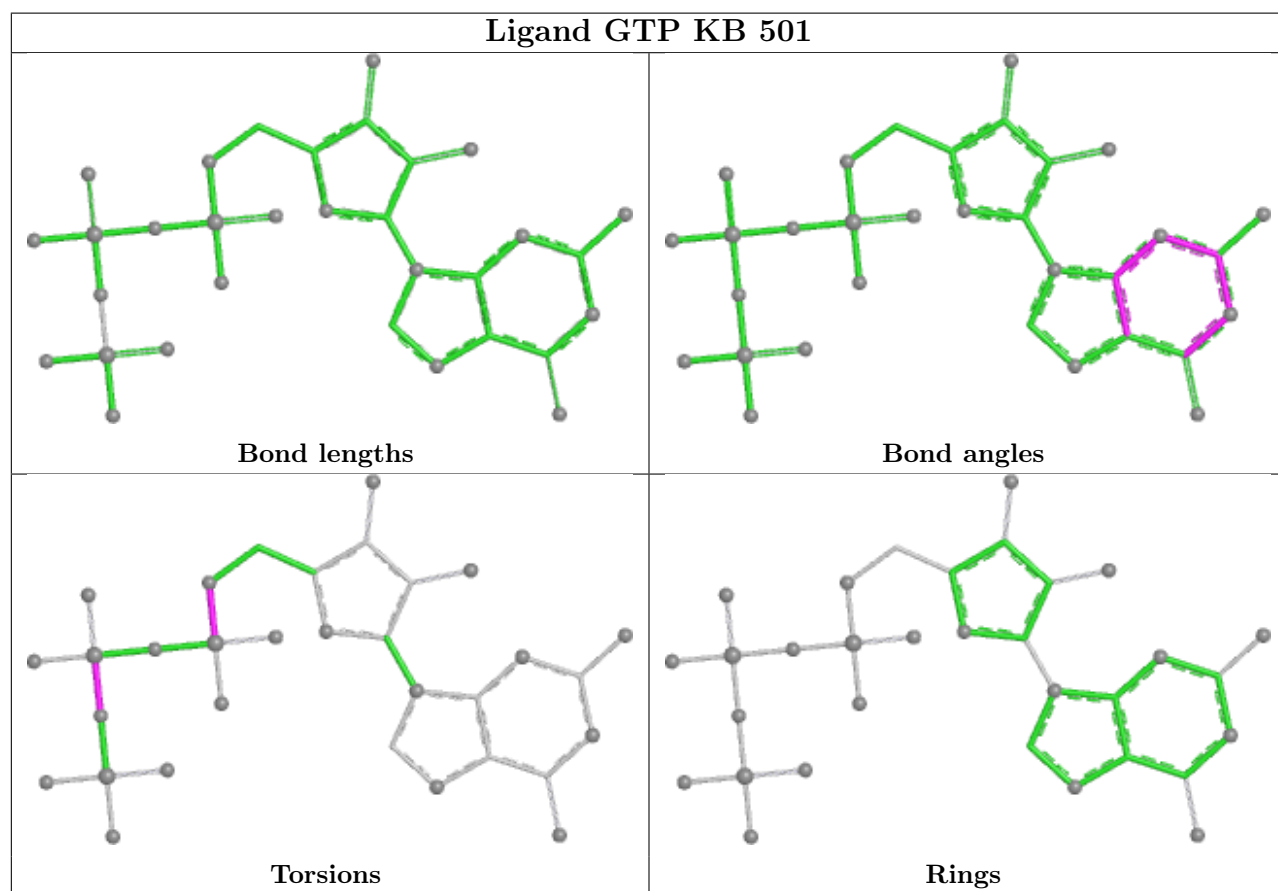
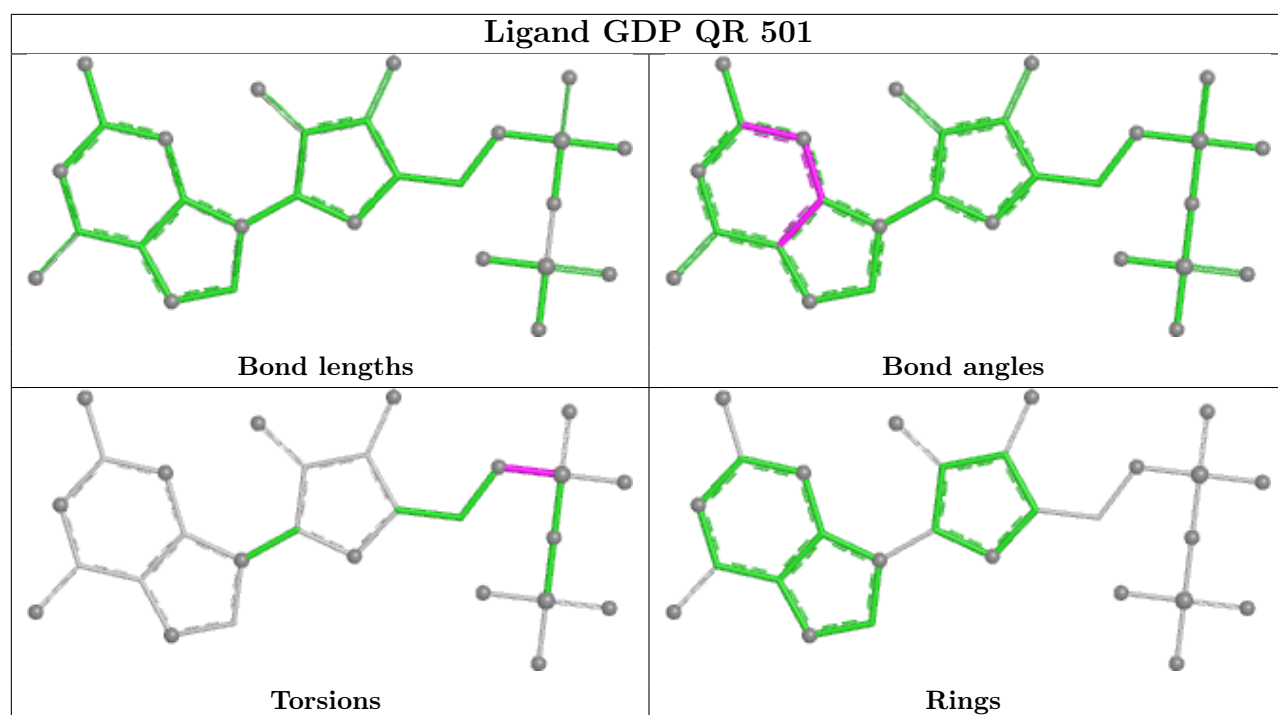


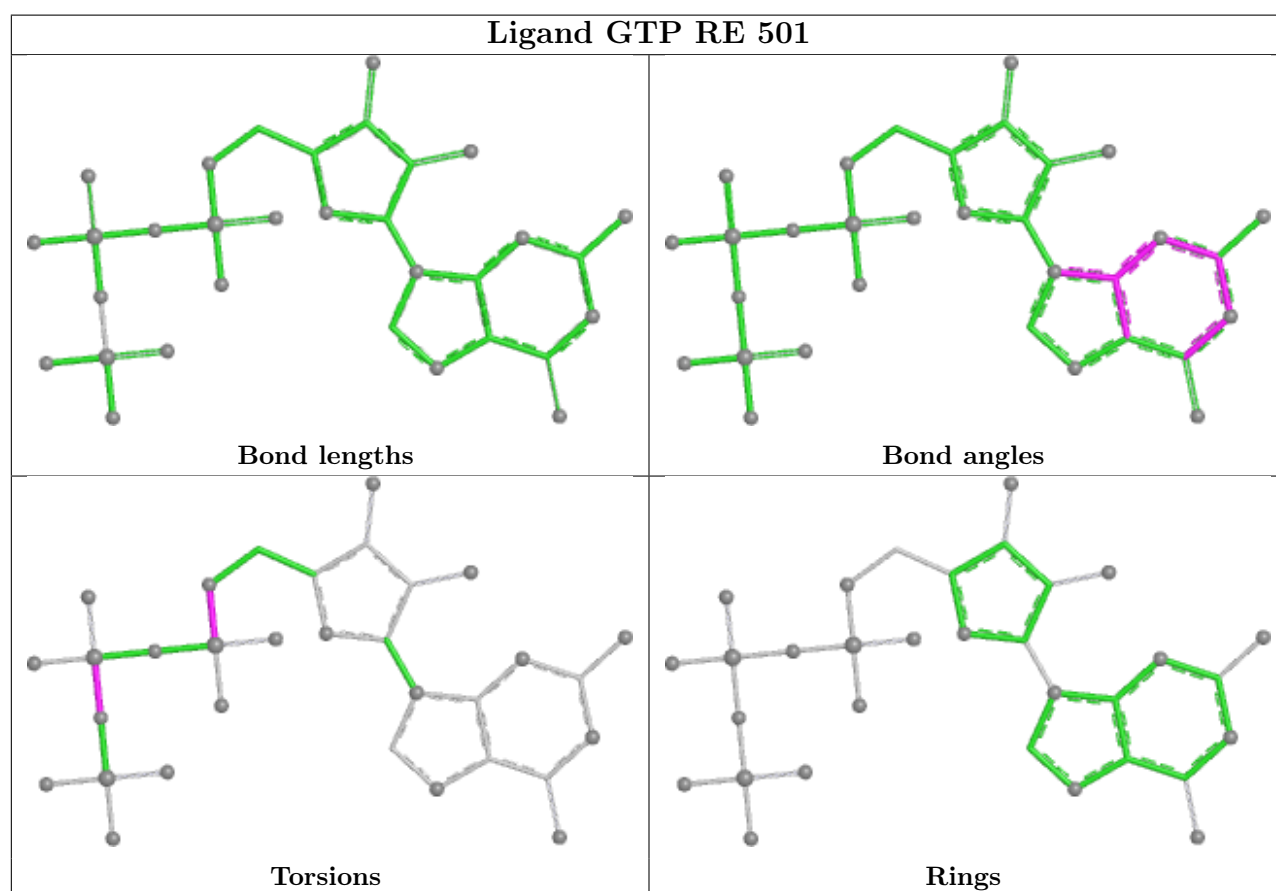
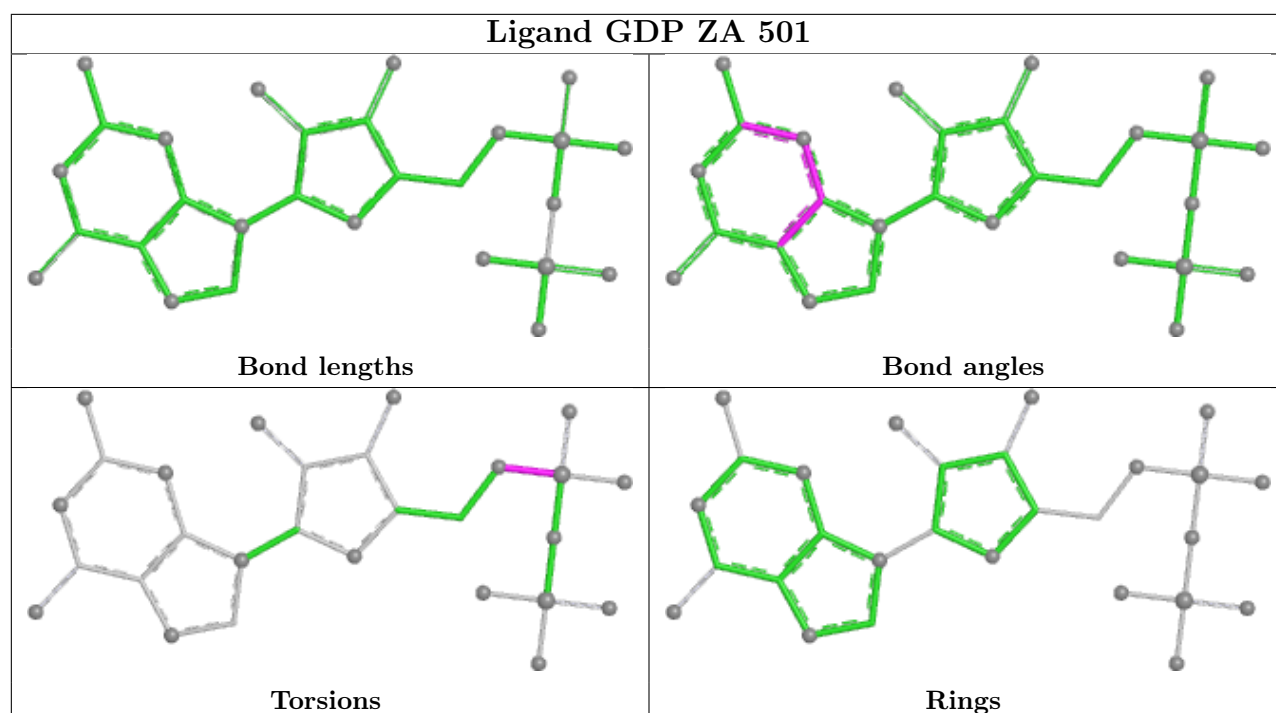




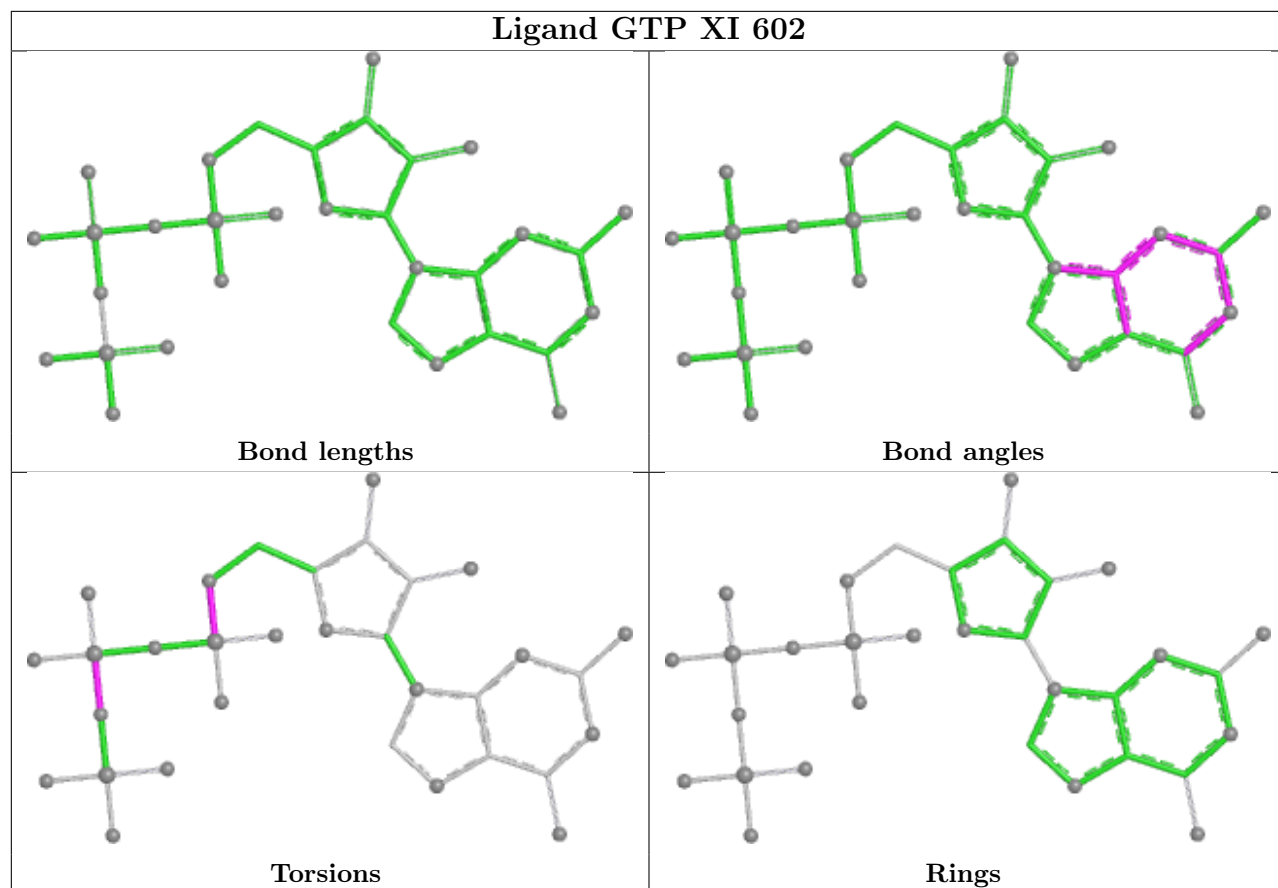




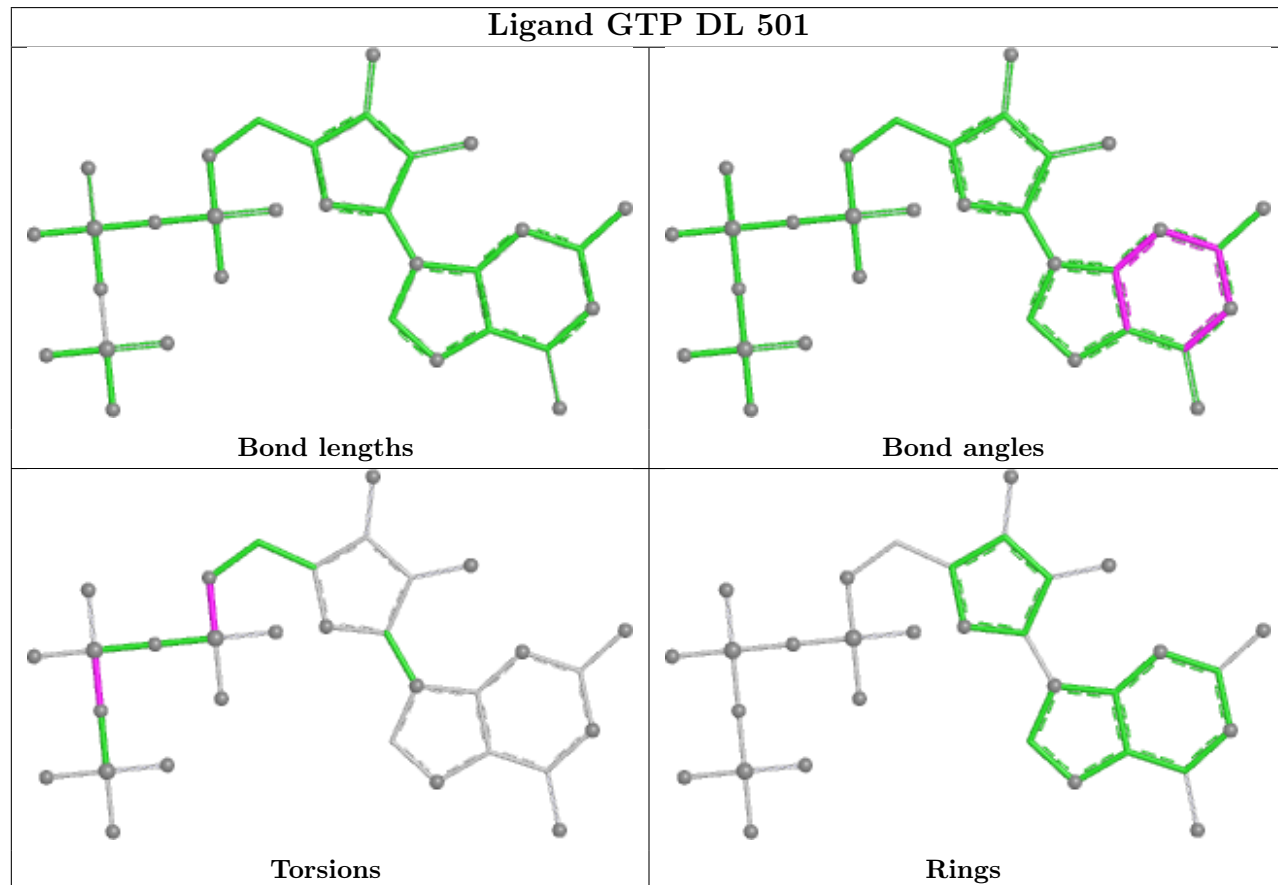


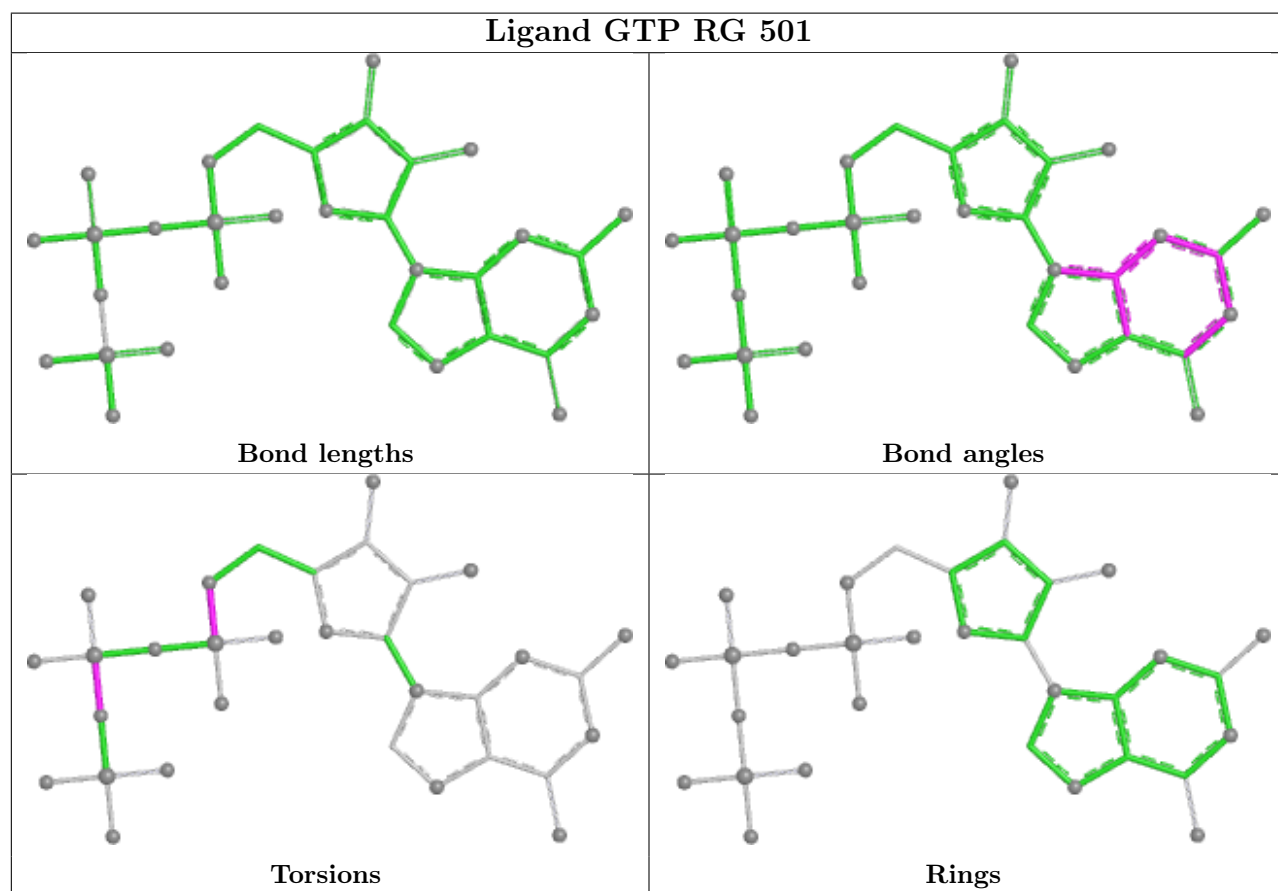
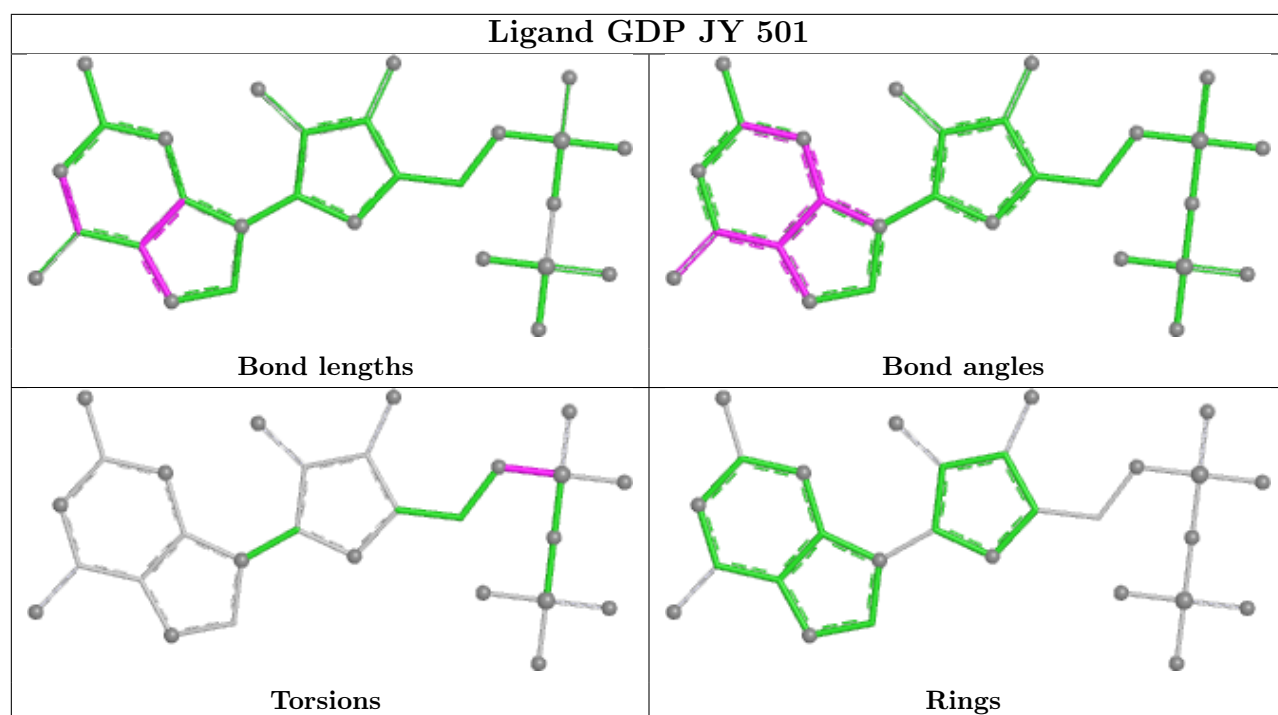


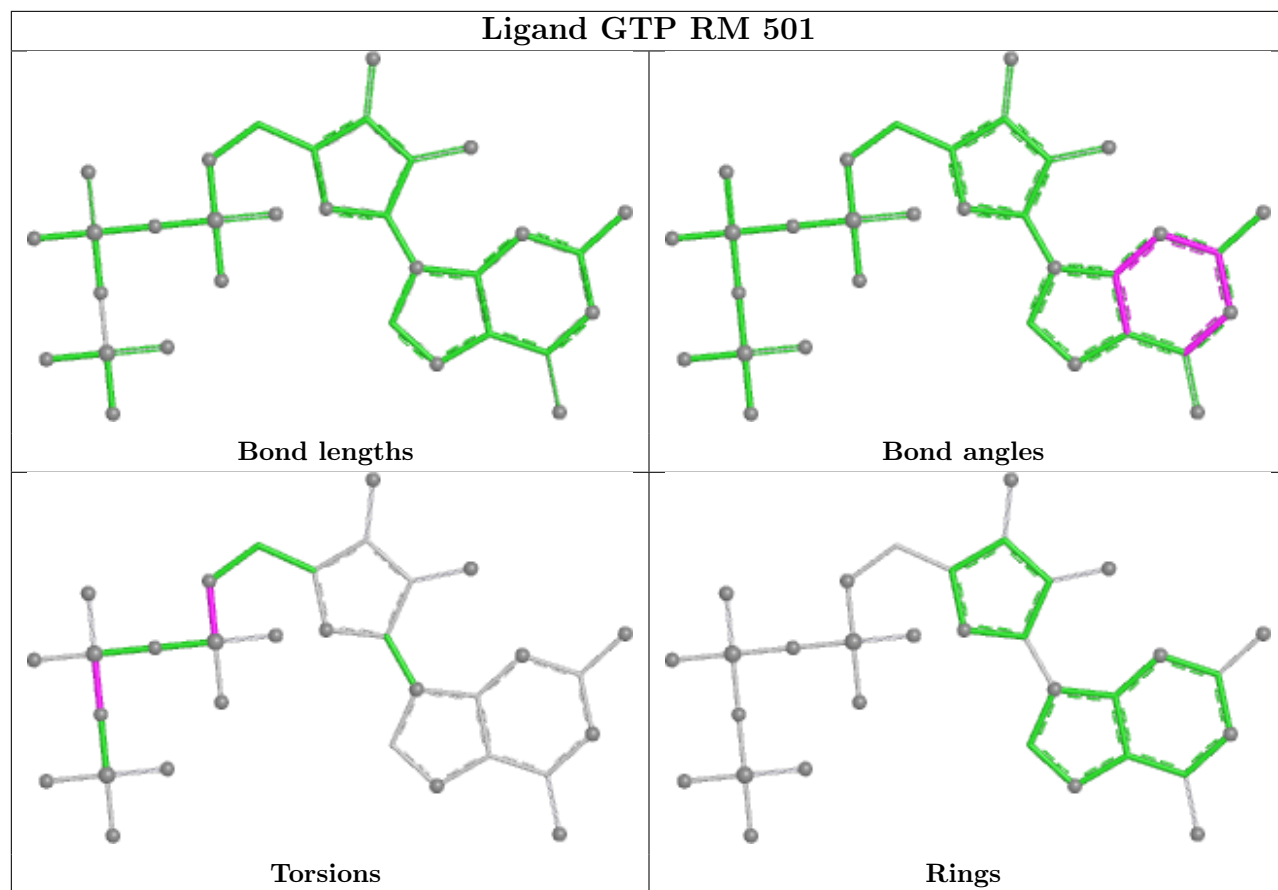
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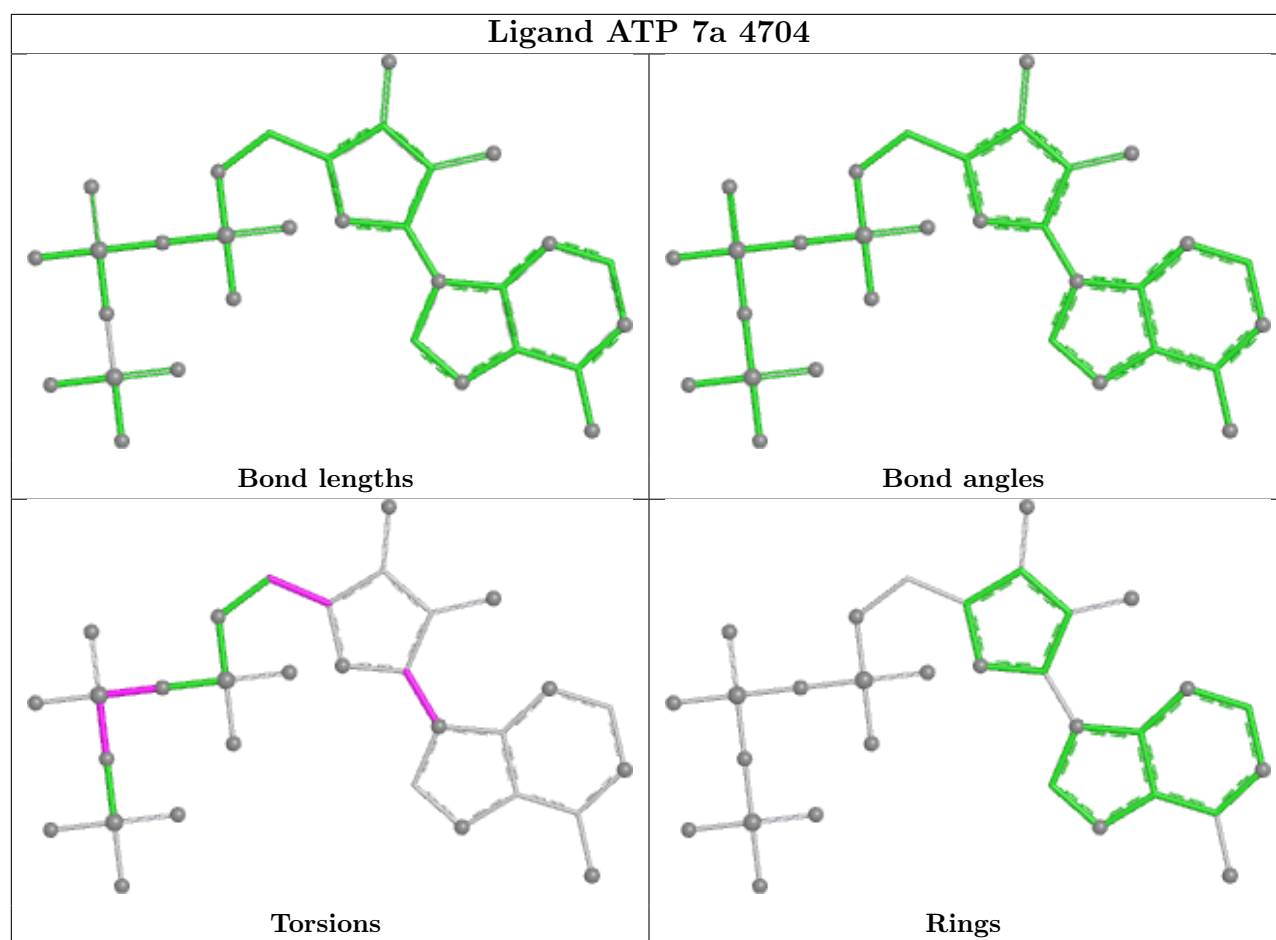


## Ligand GTP DL 501



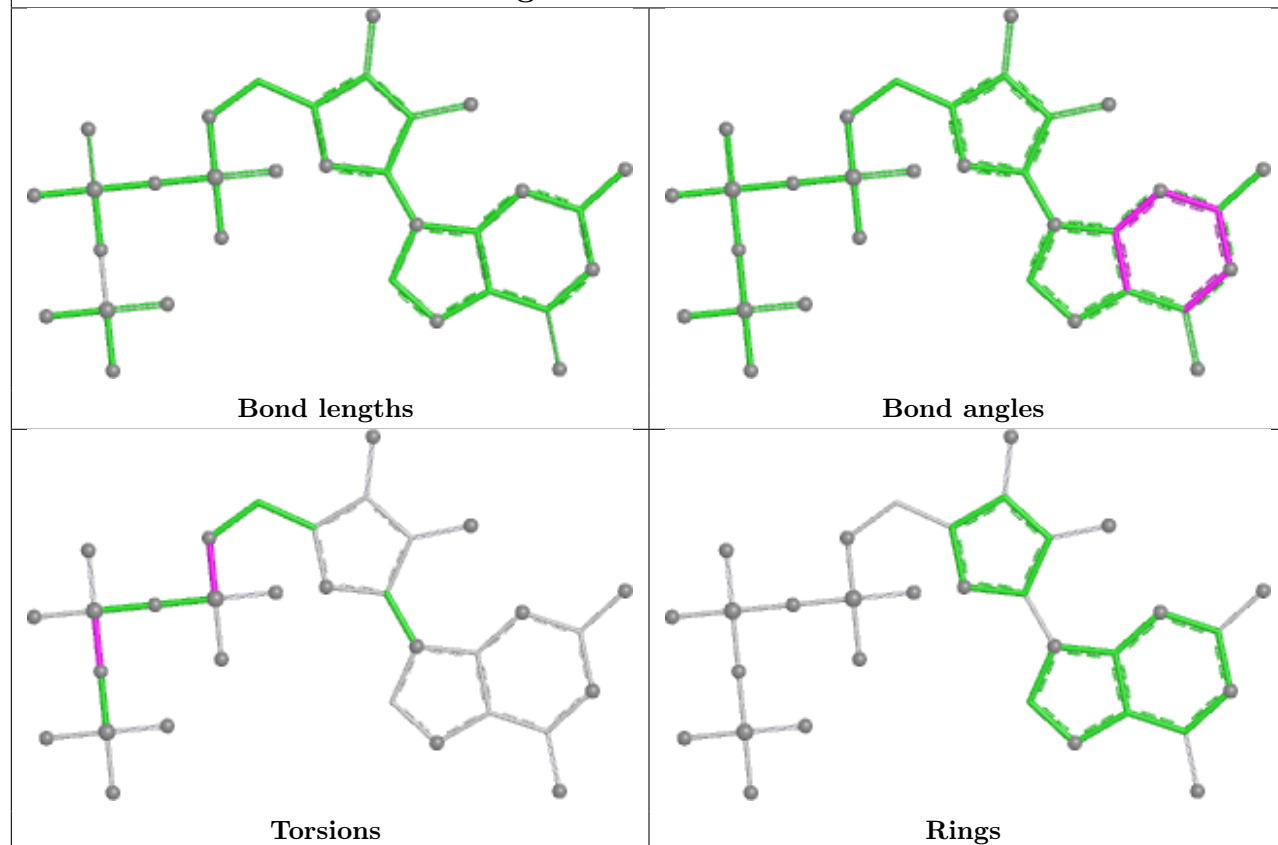




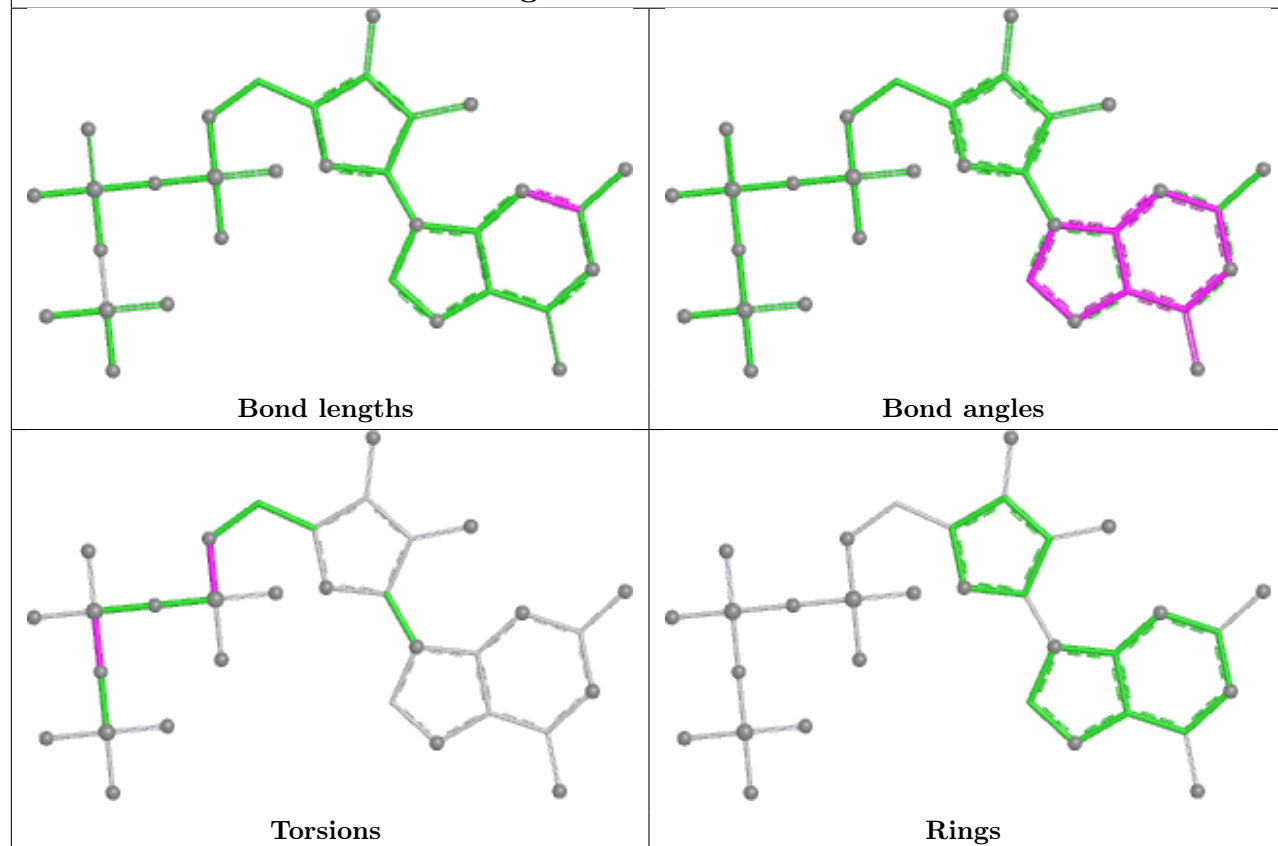


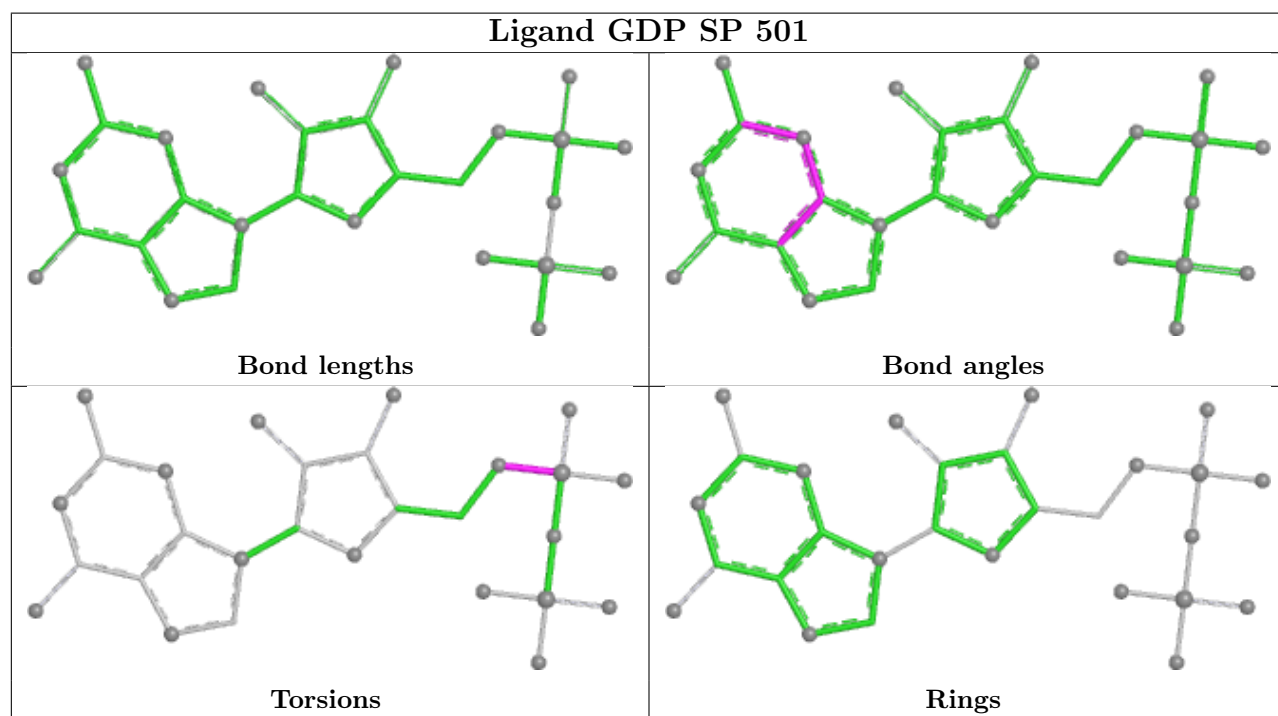
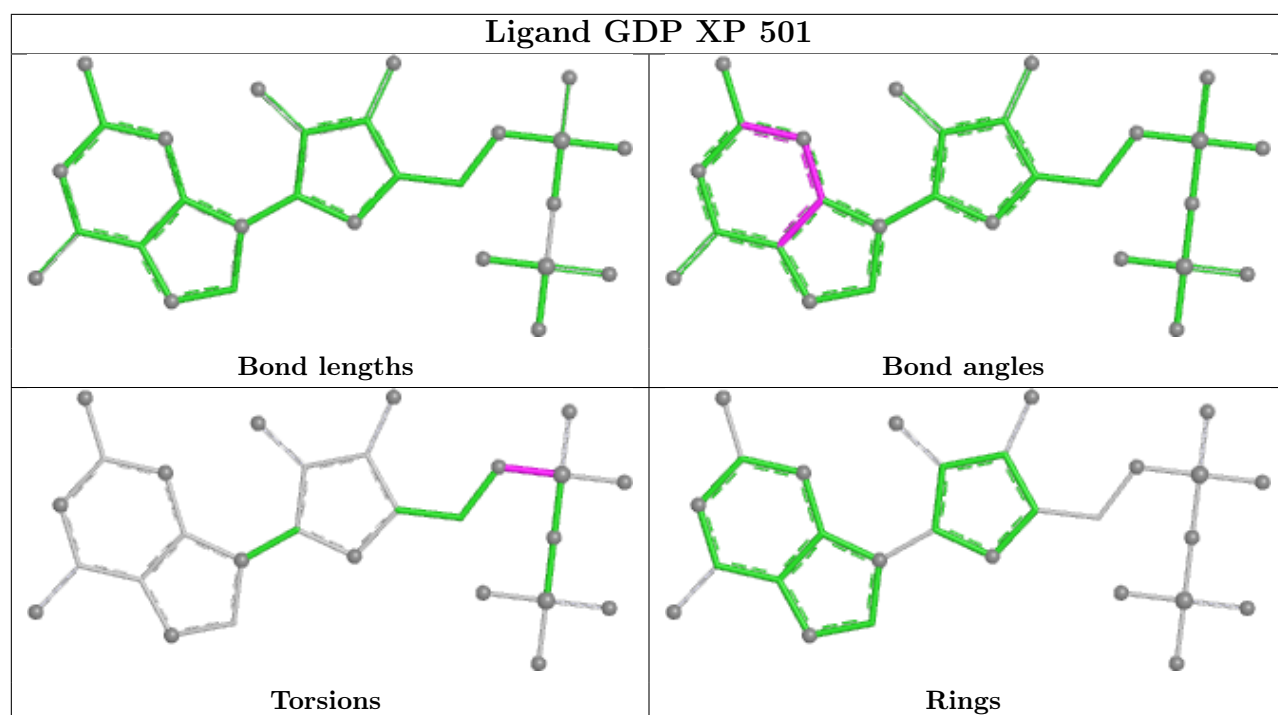


## Ligand GTP DB 501

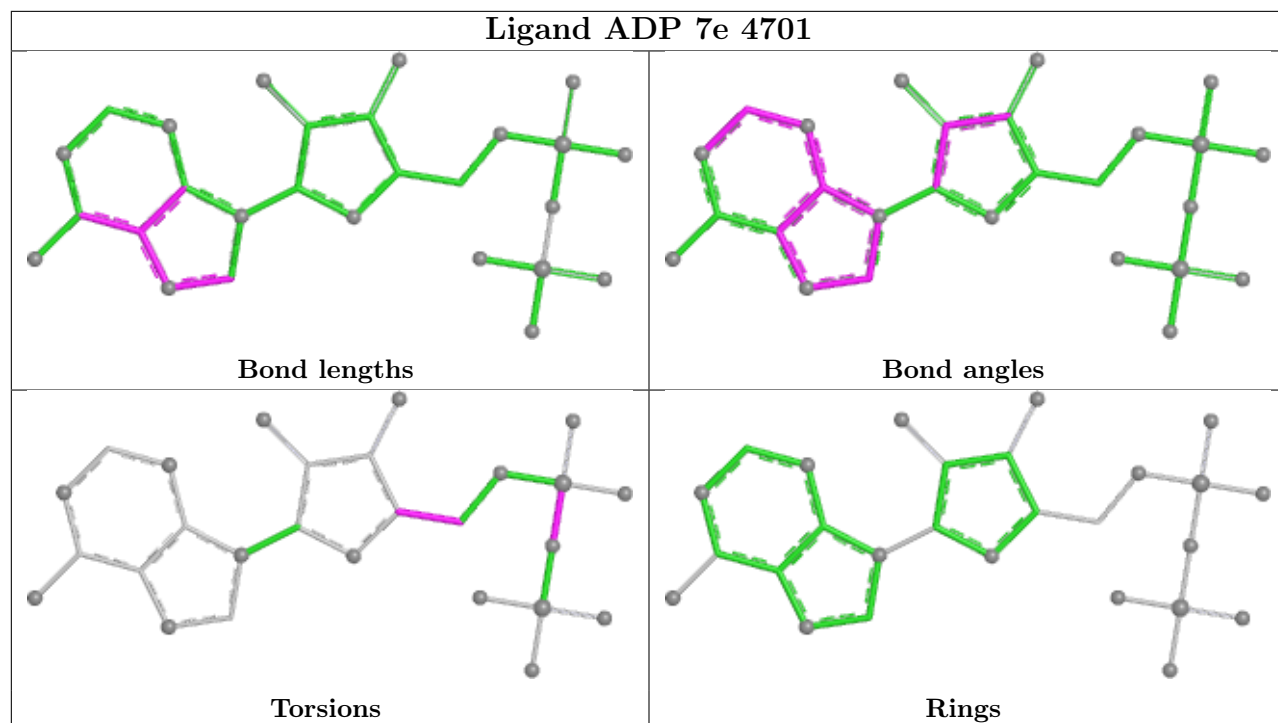


## Ligand GTP CL 501

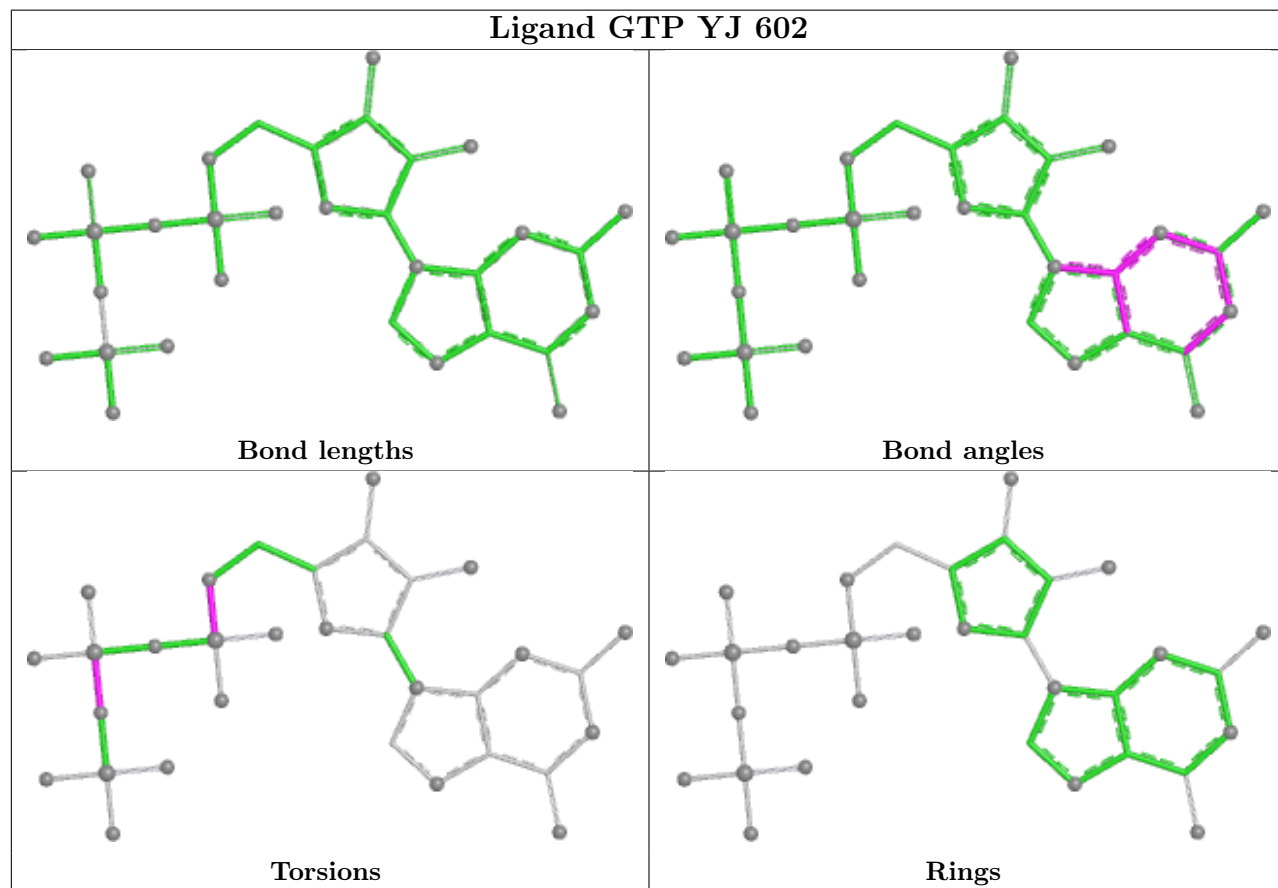


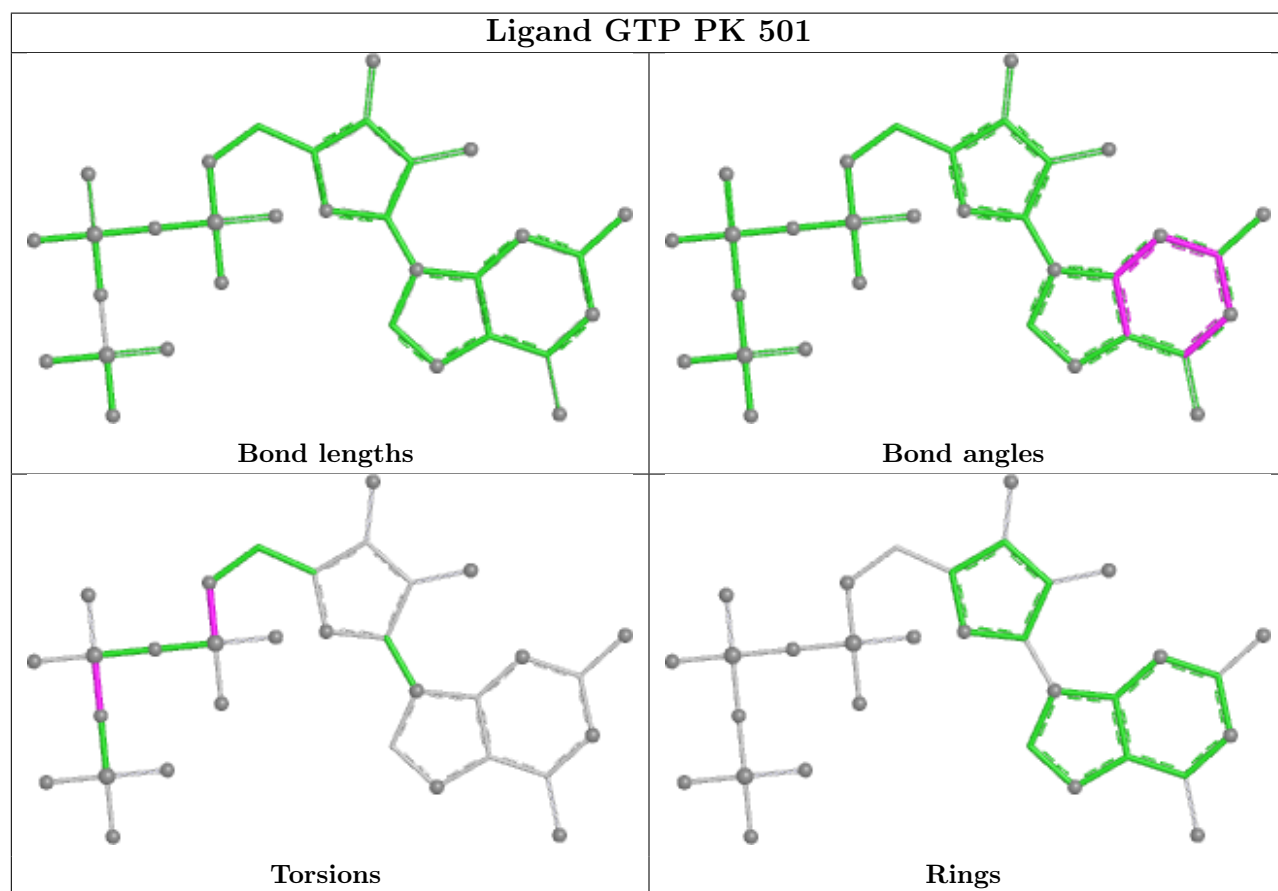
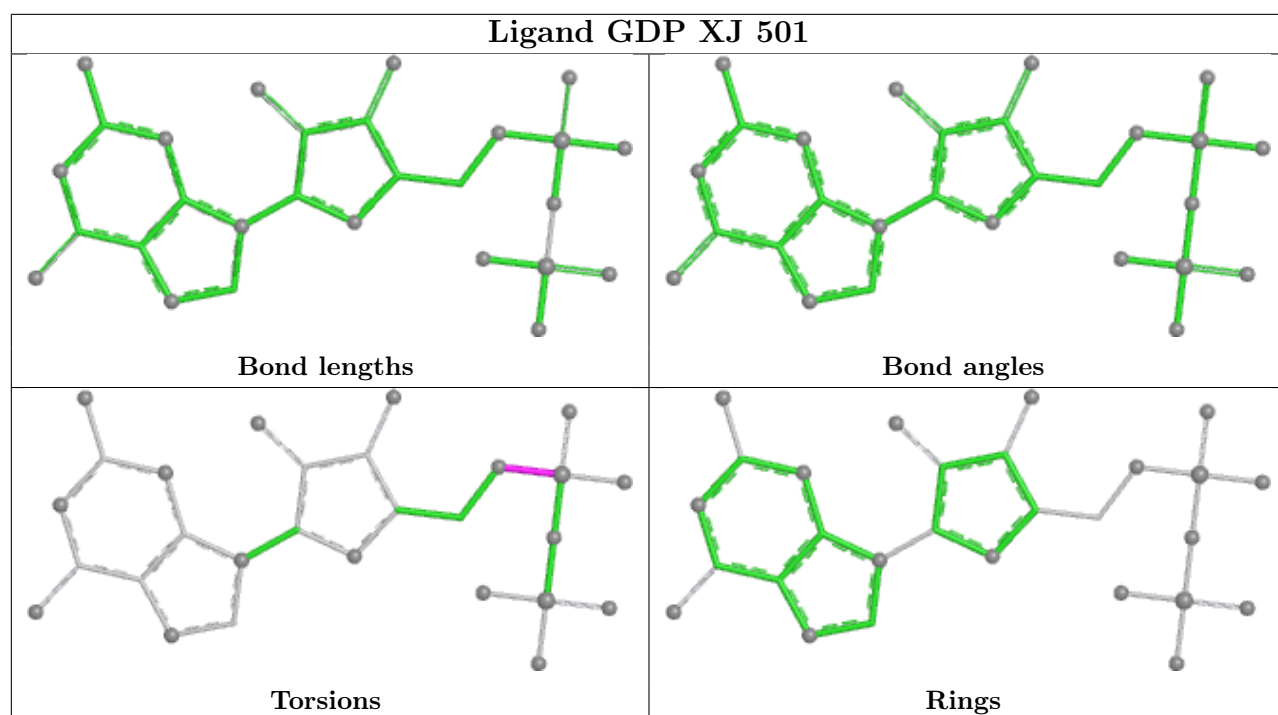


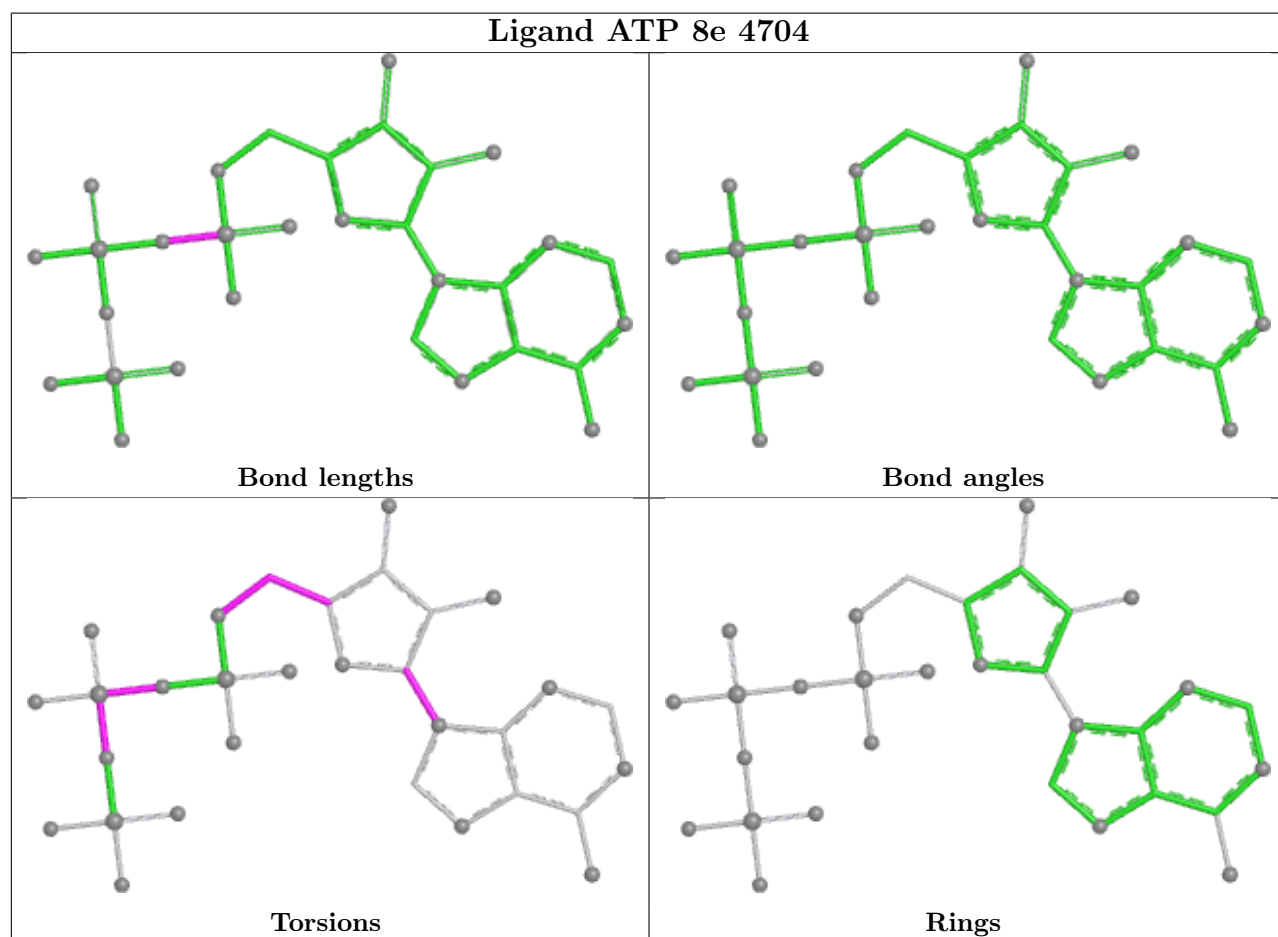
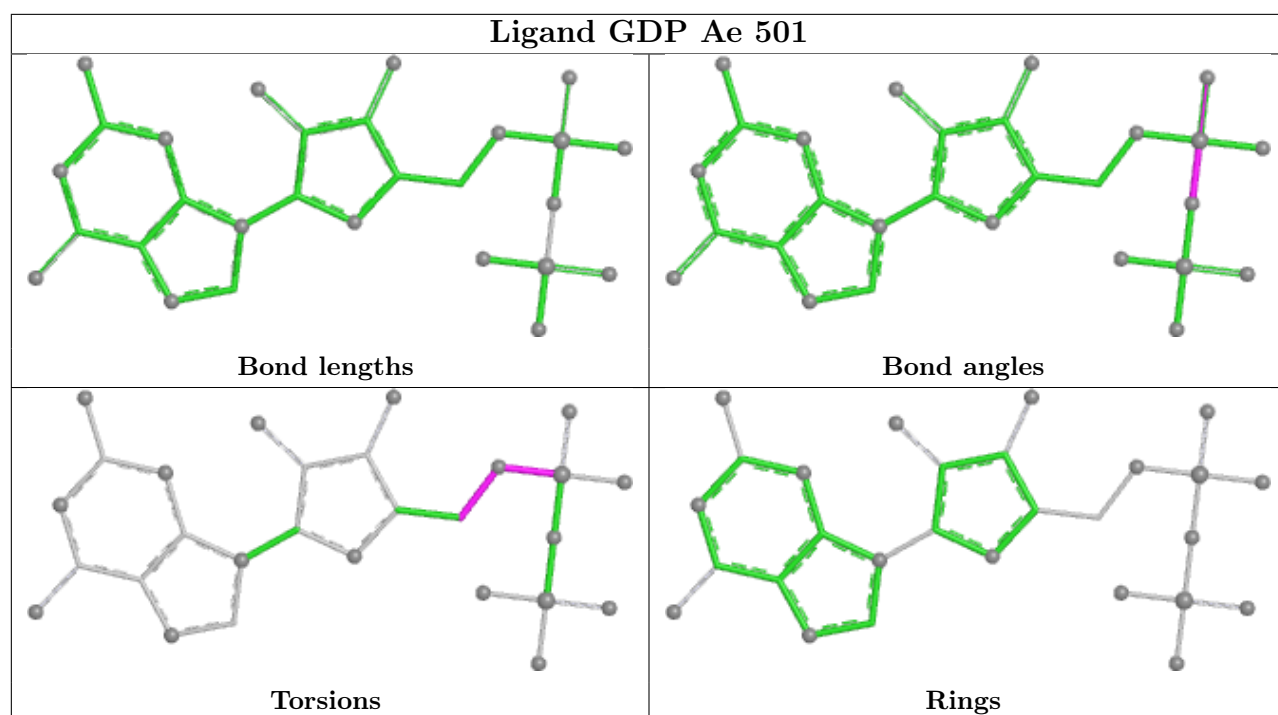
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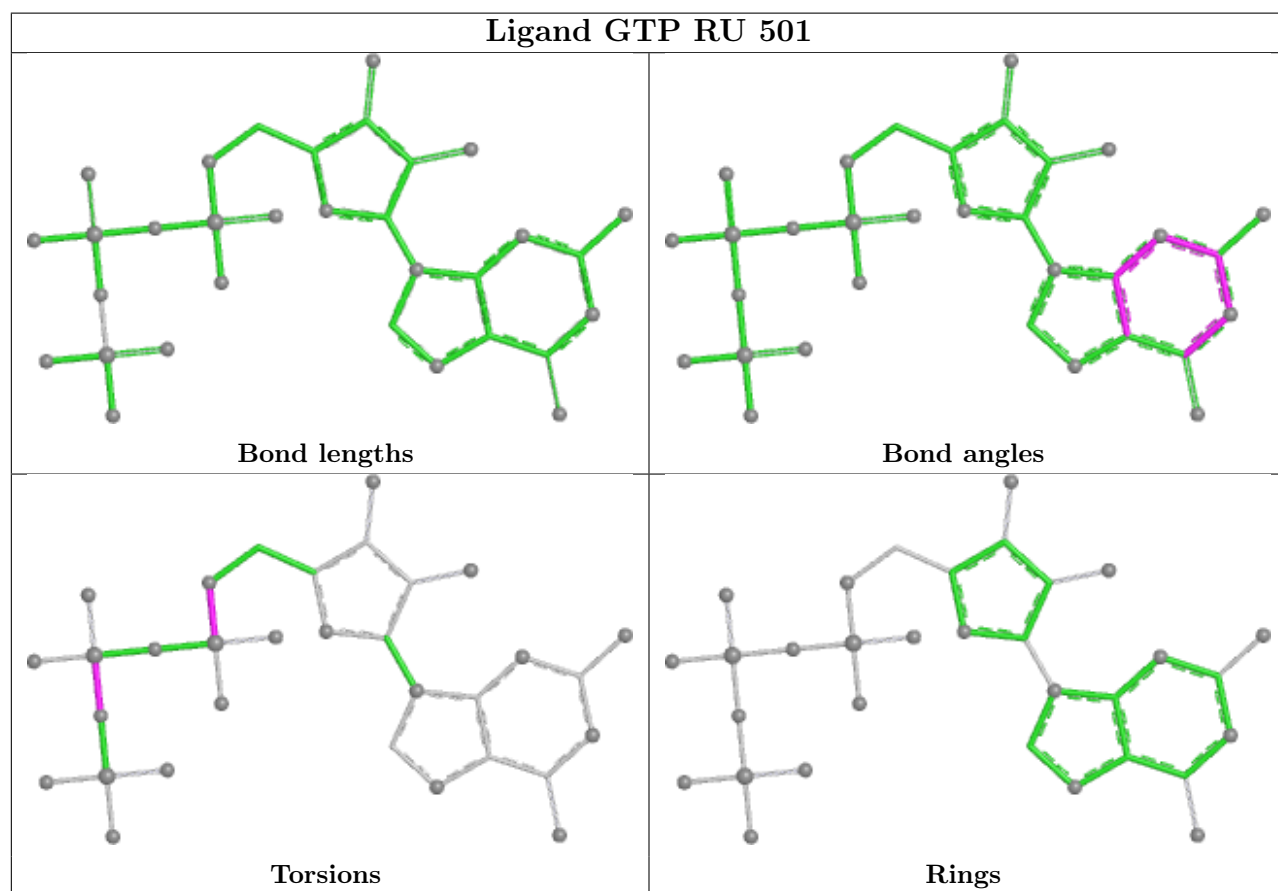
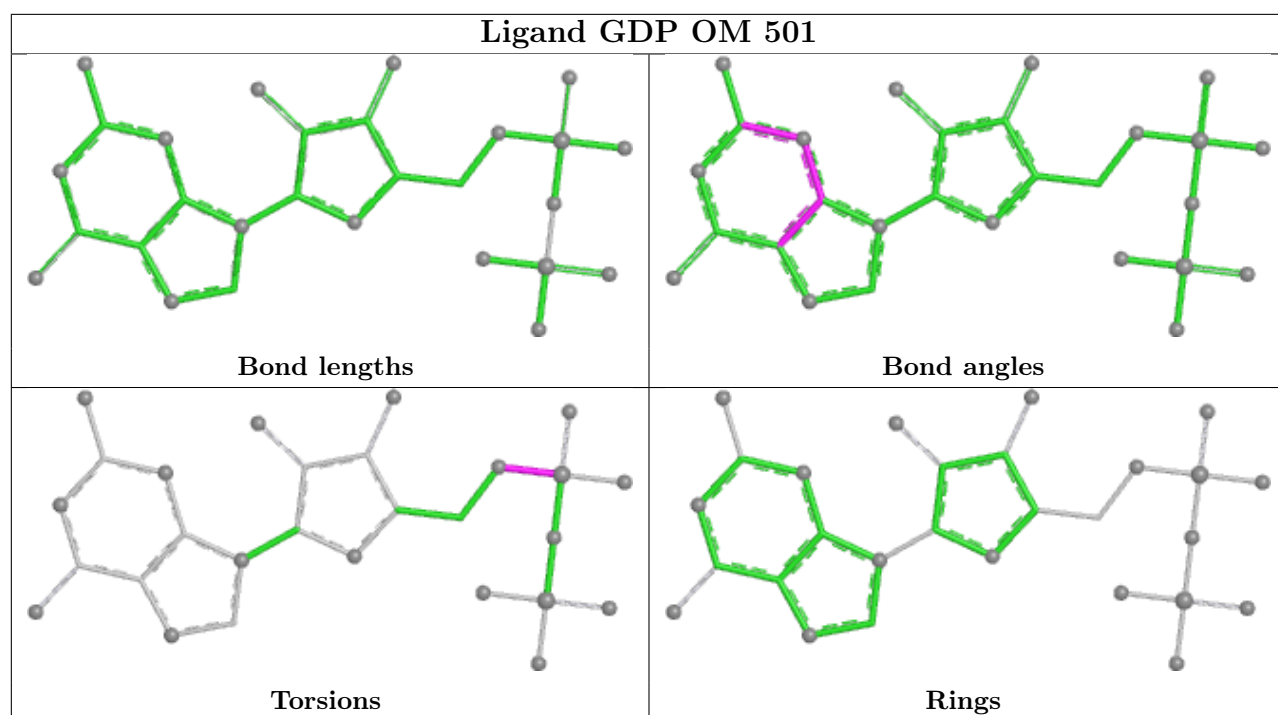


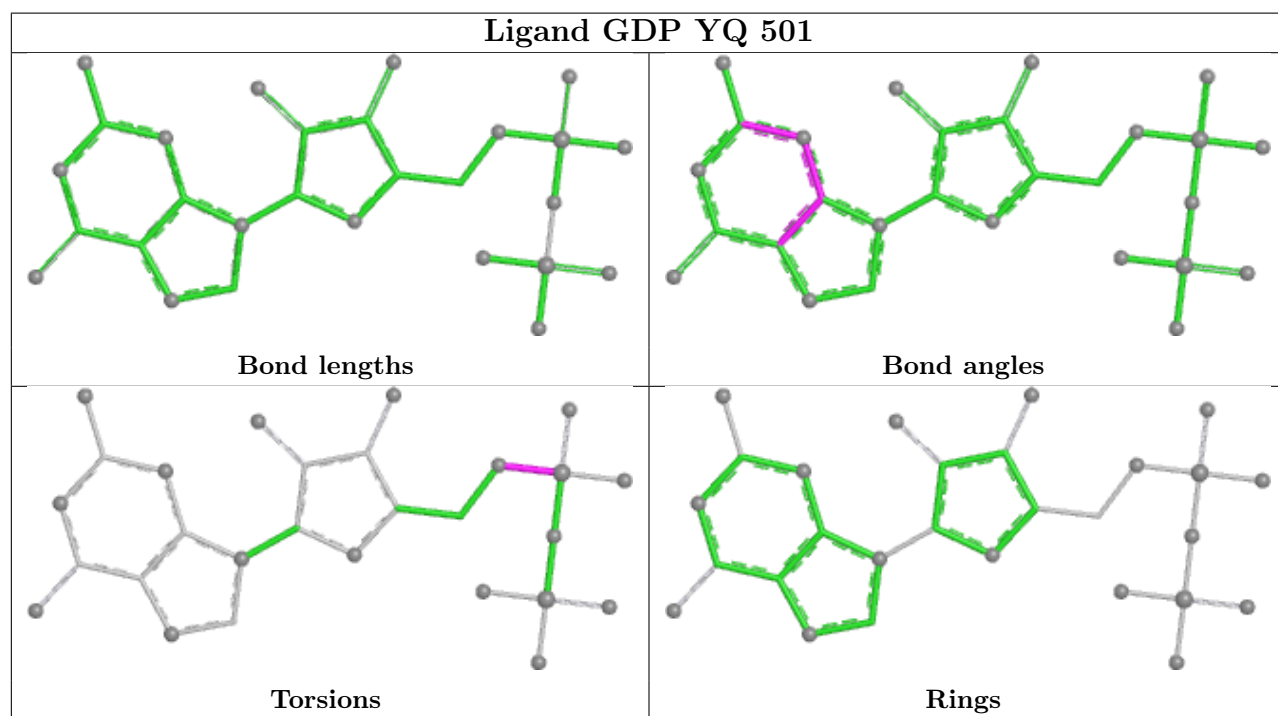
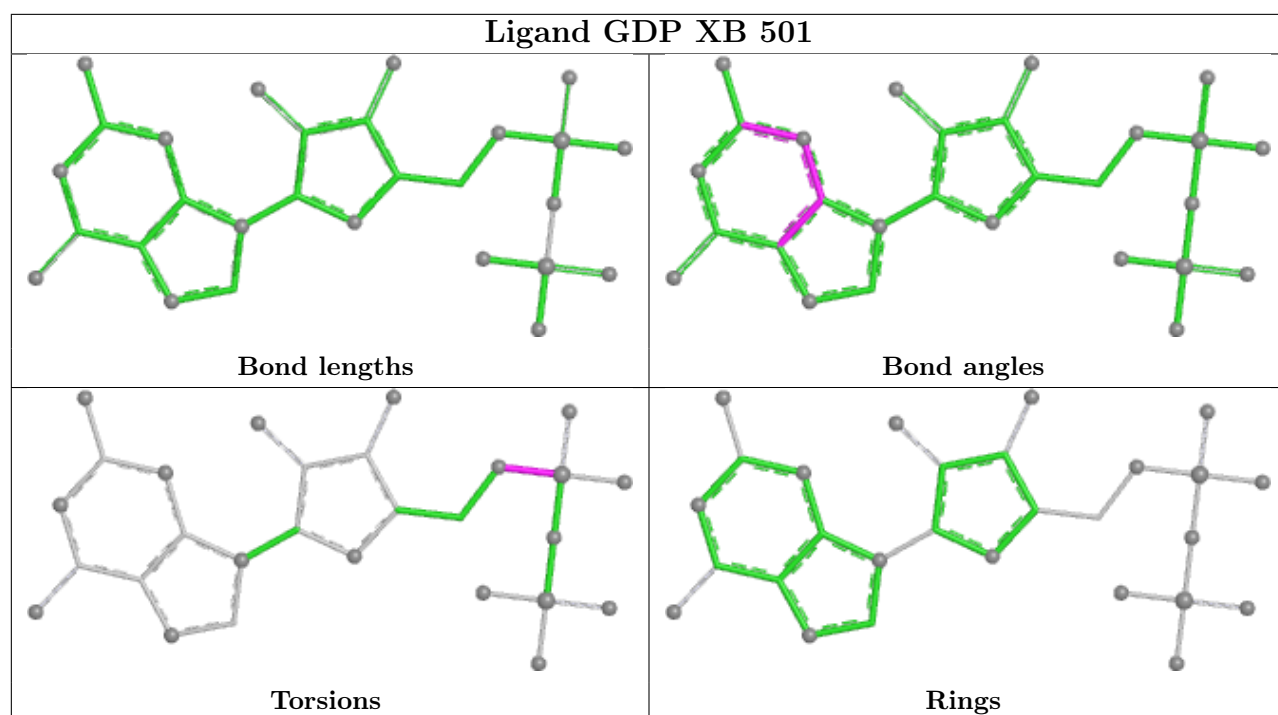
## Ligand GTP YJ 602



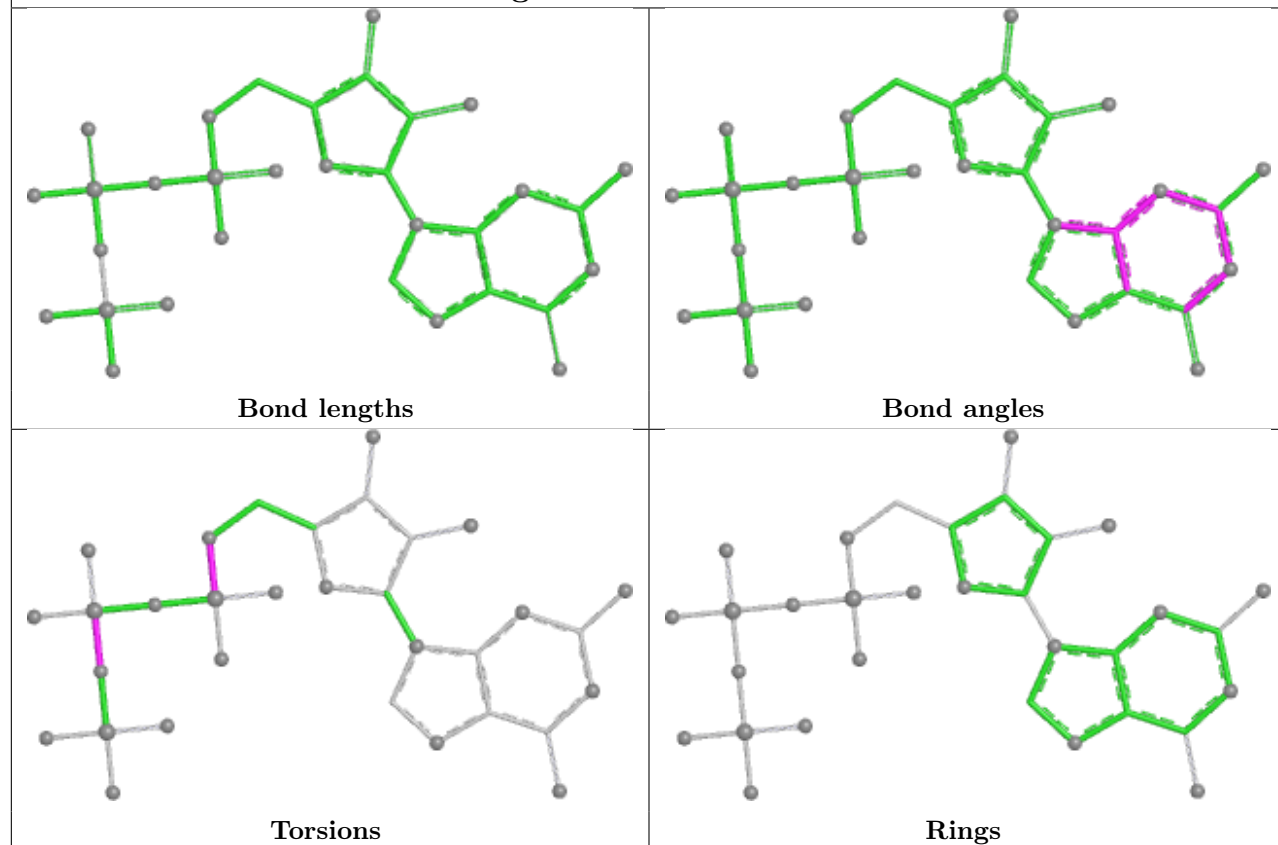




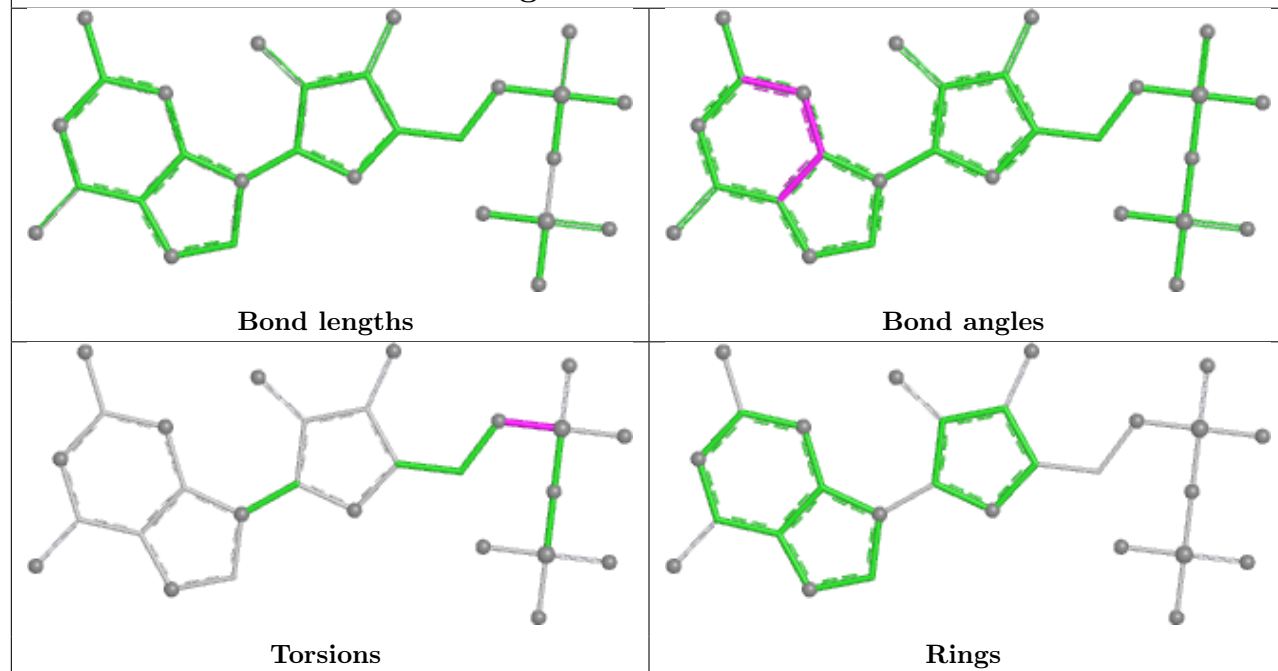




## Ligand GTP XW 602

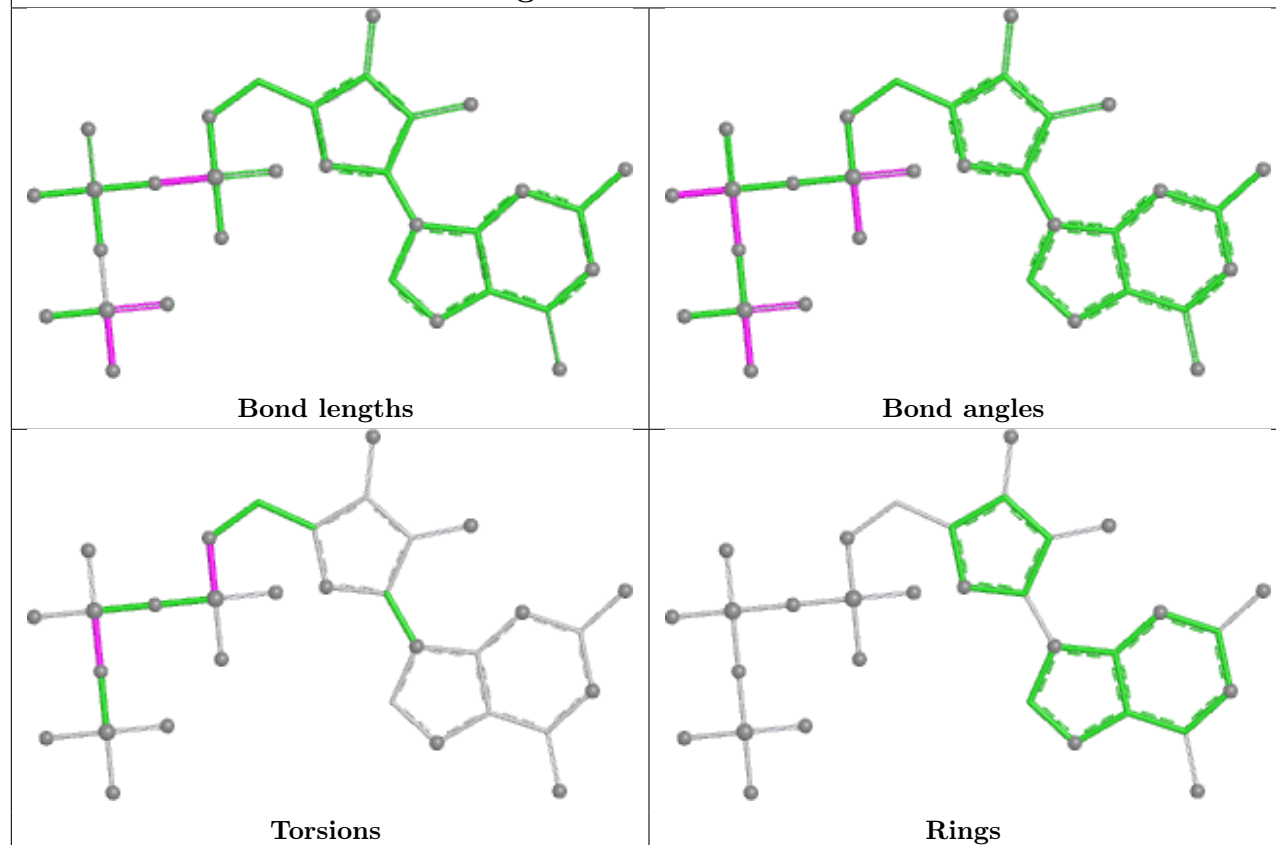


## Ligand GDP LY 501

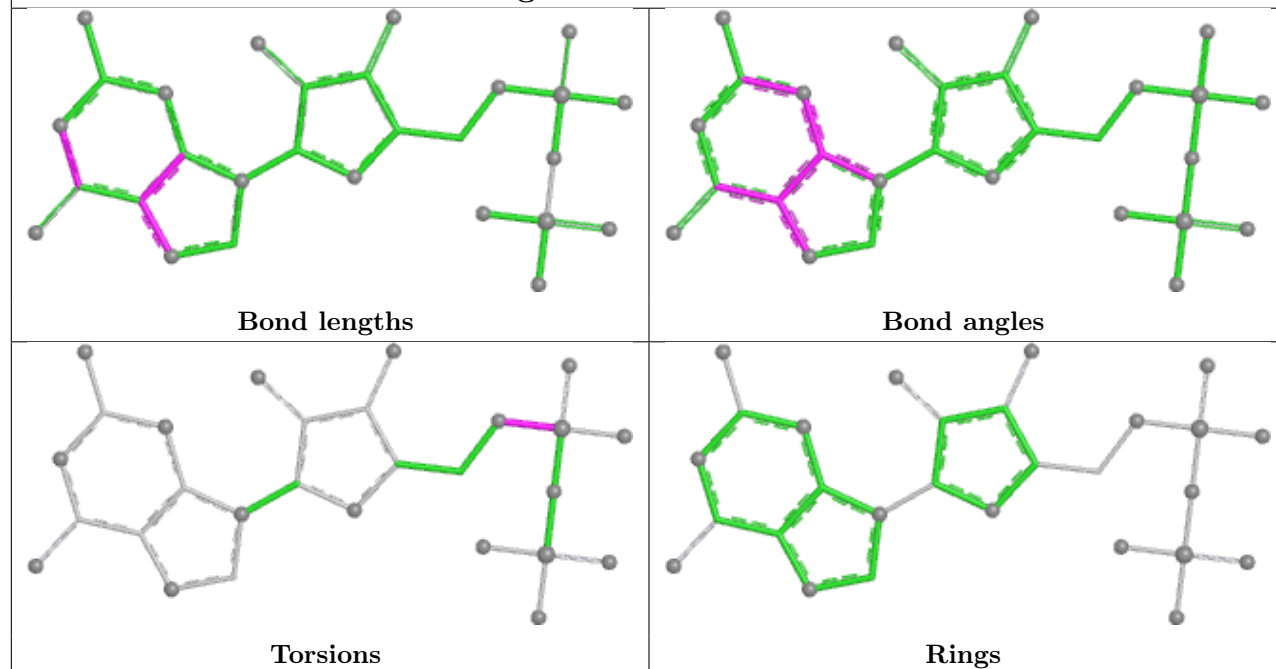


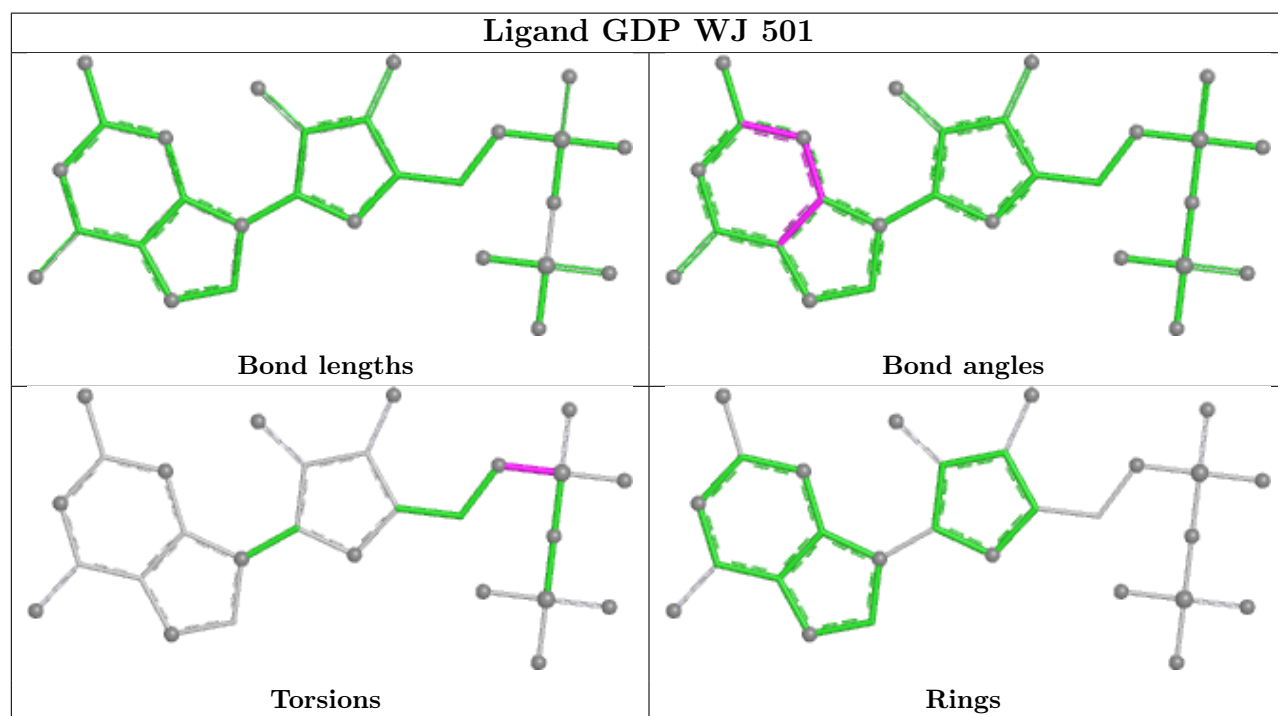
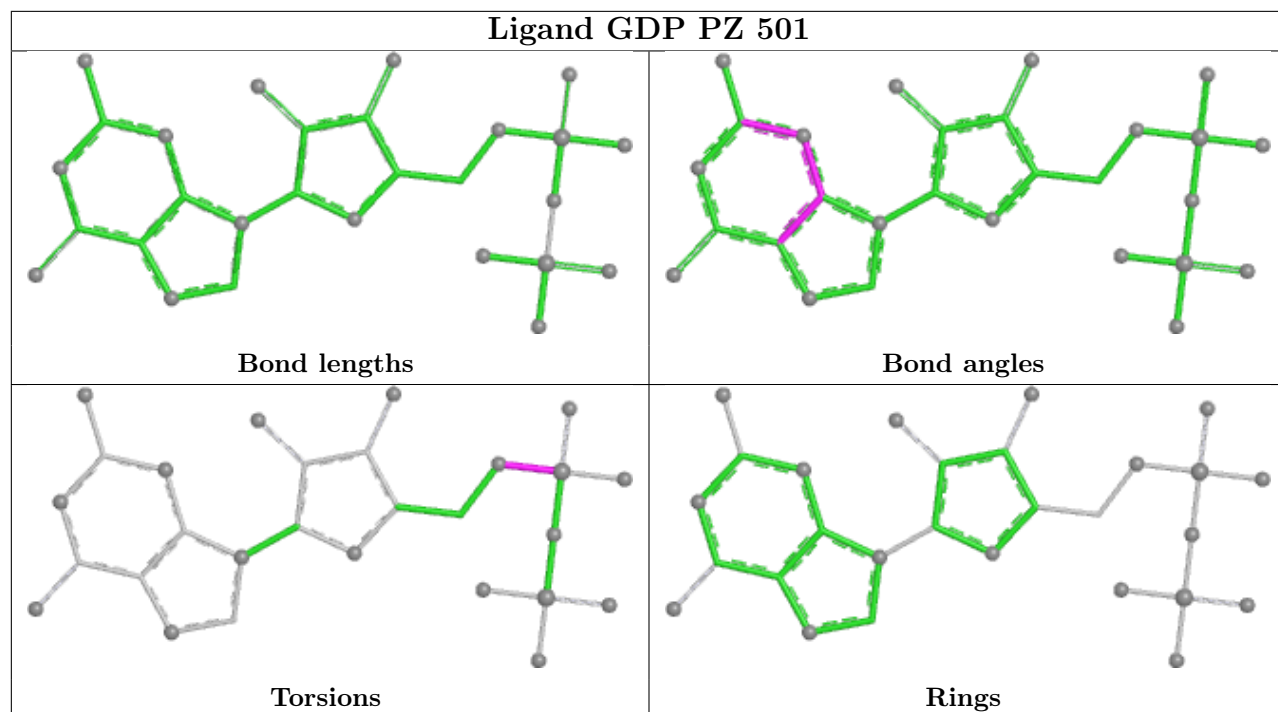


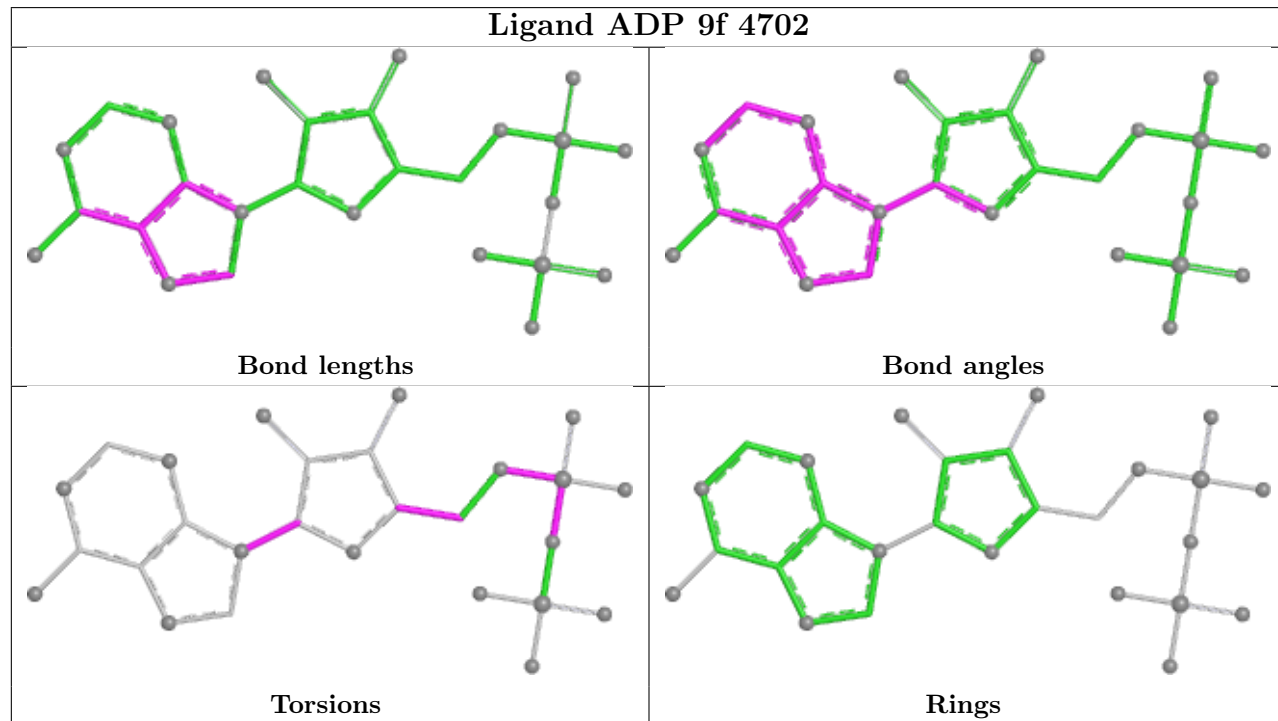
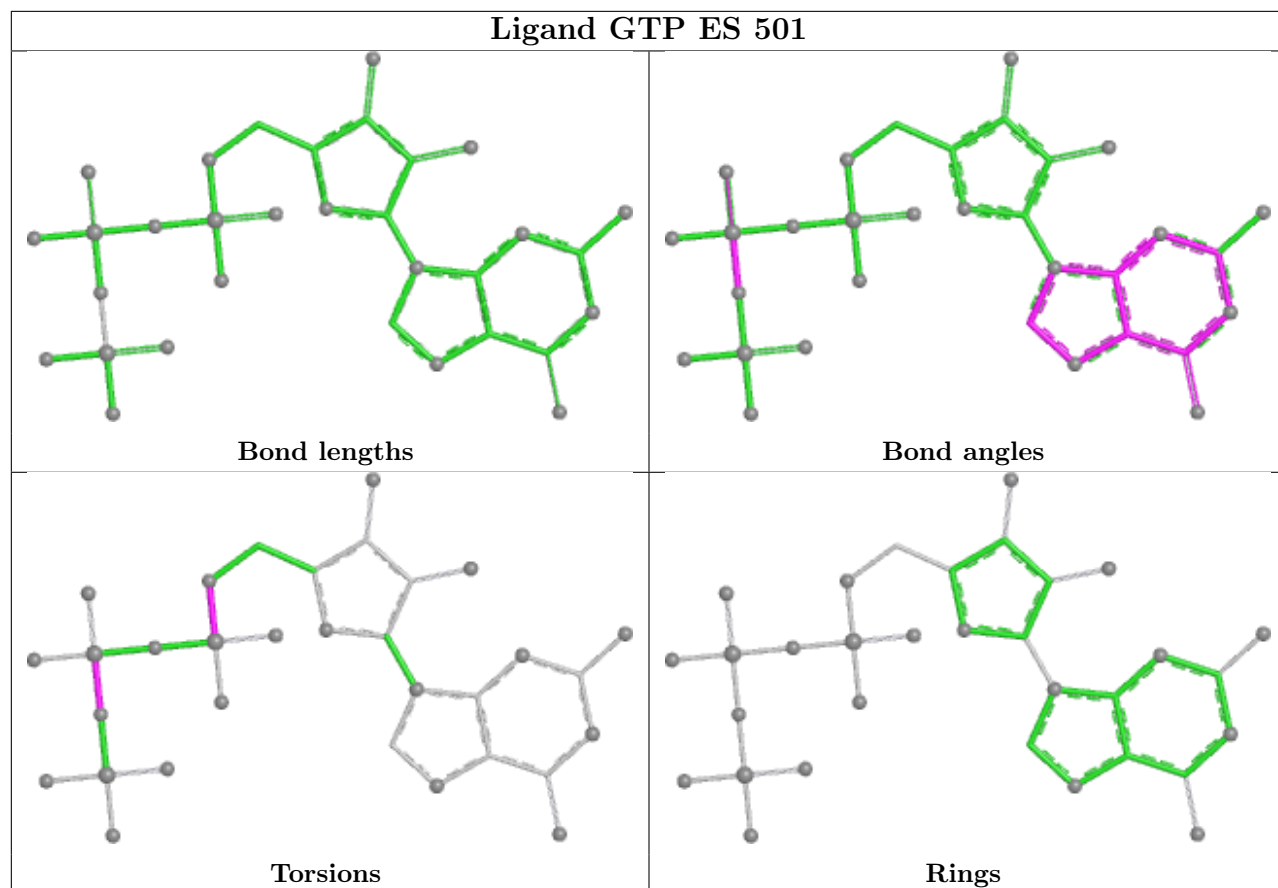
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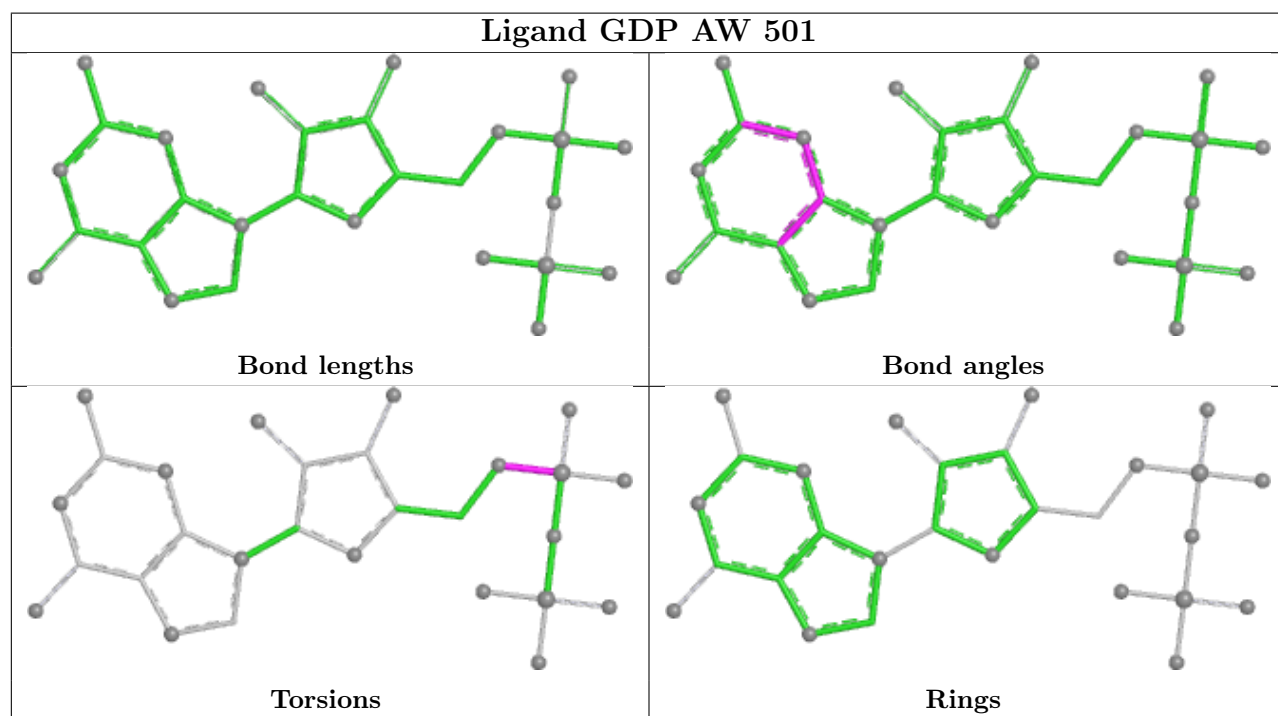
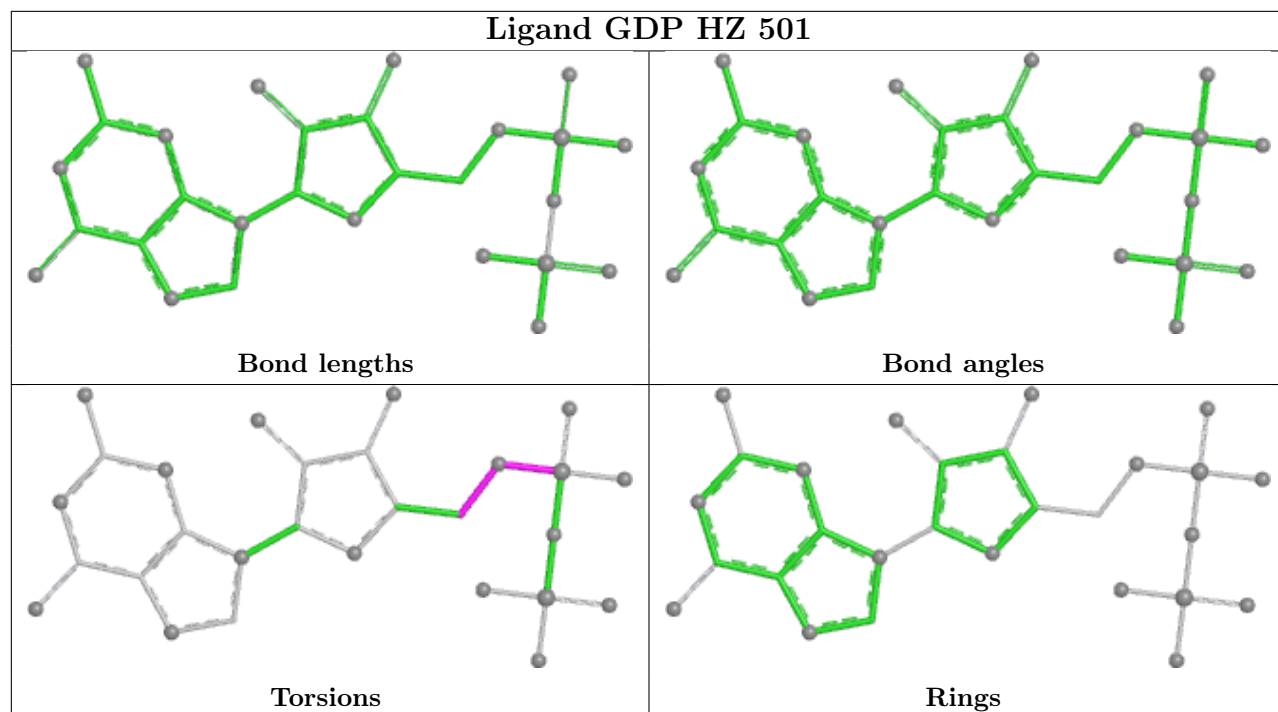


## Ligand GDP HL 501

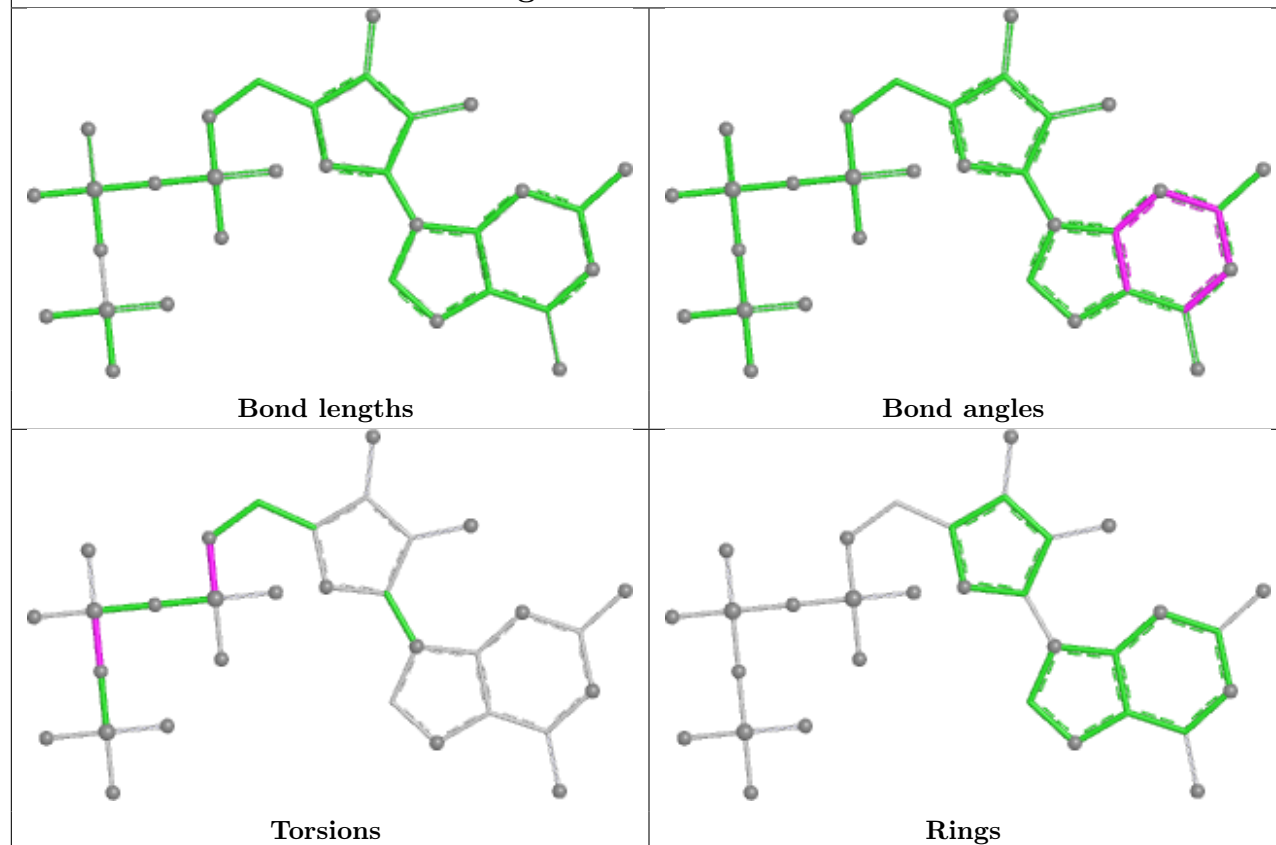




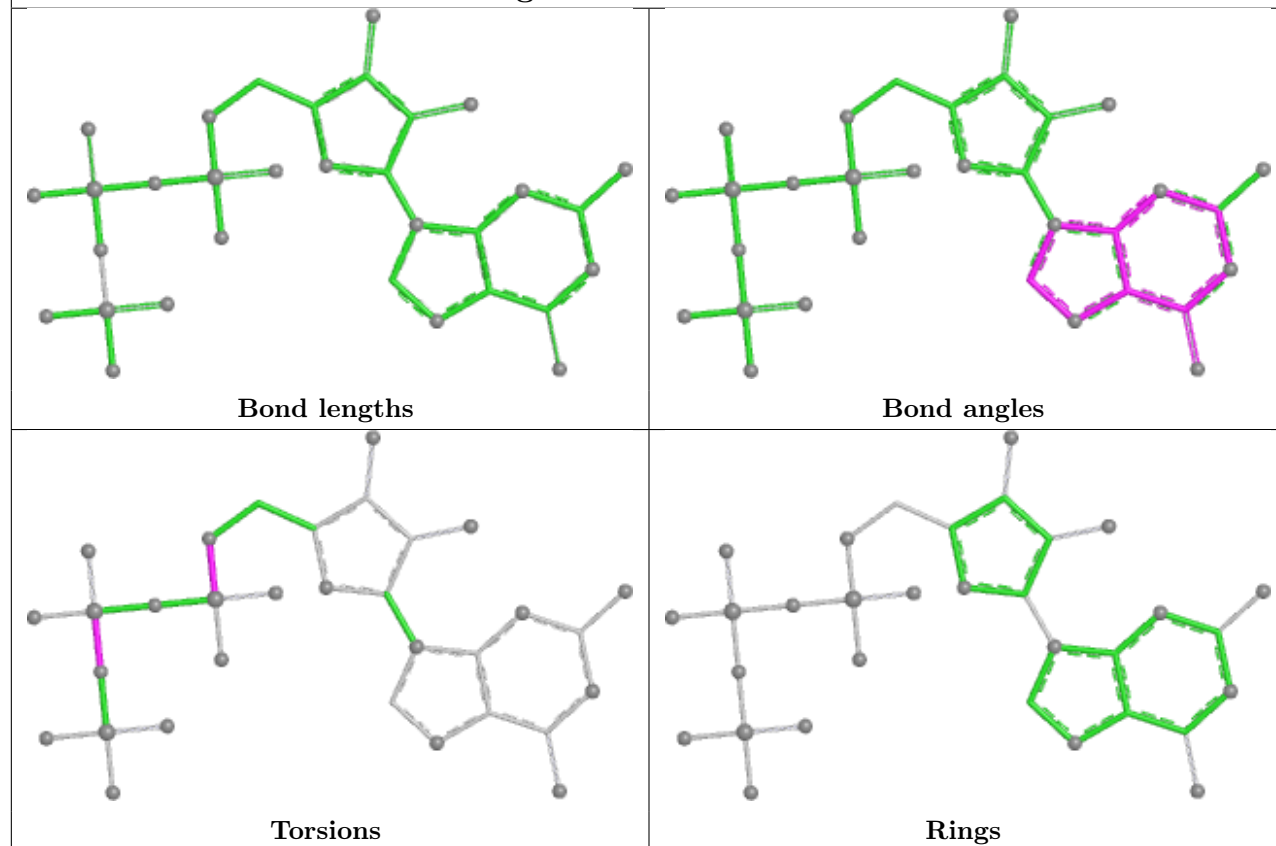


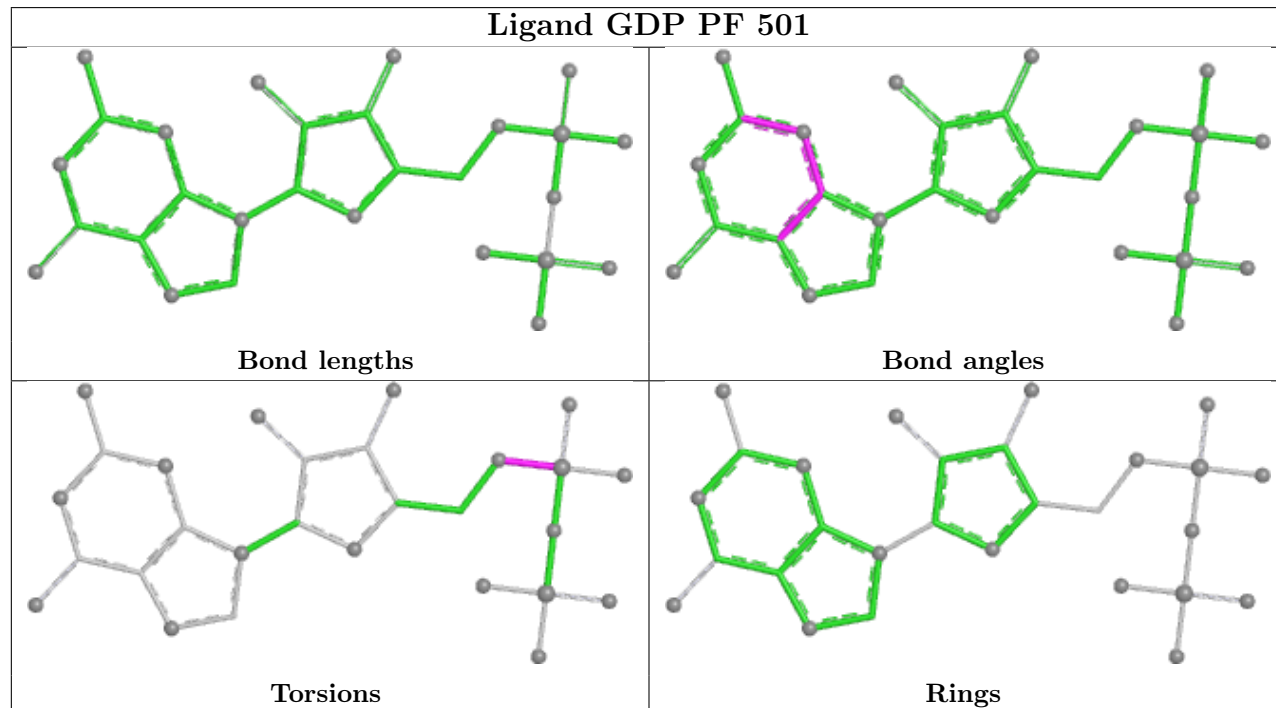
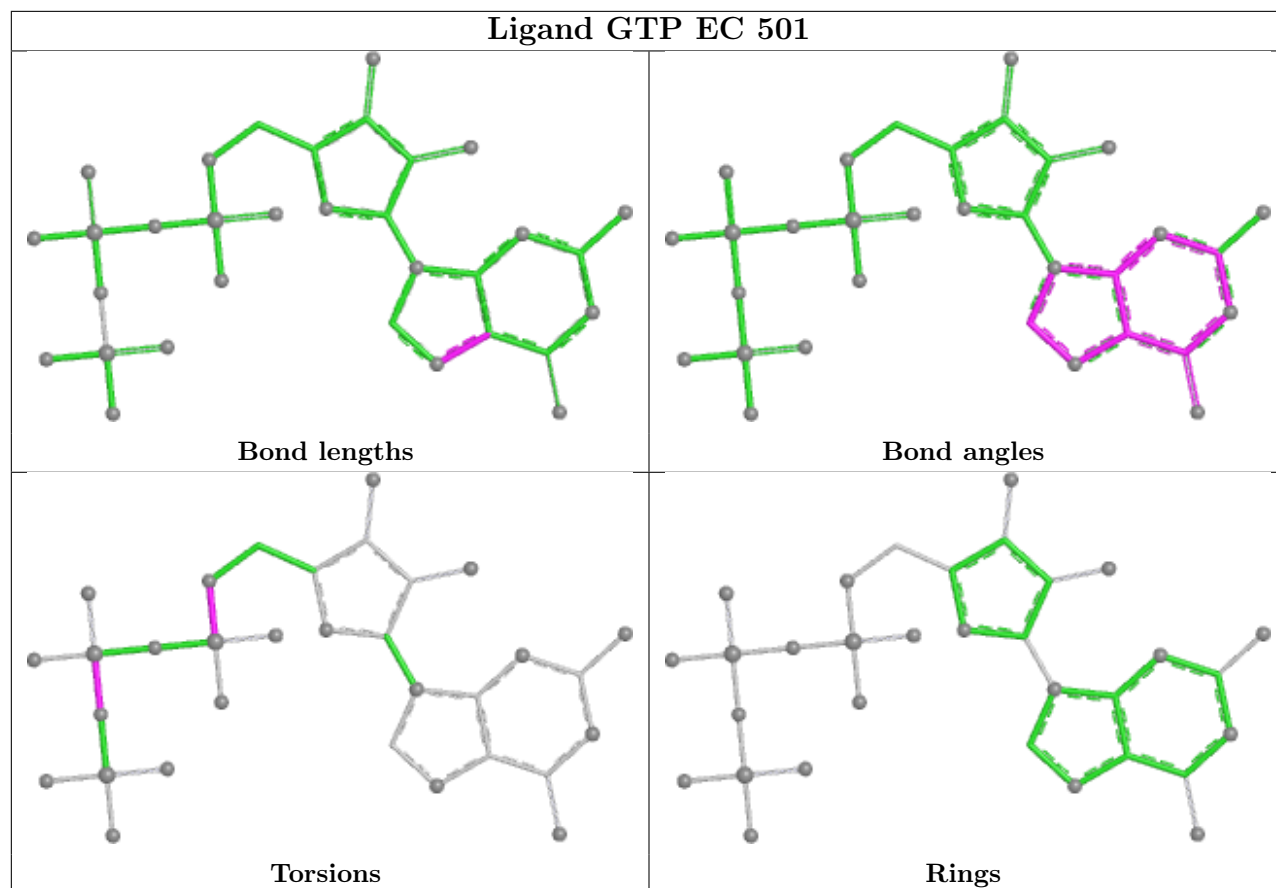


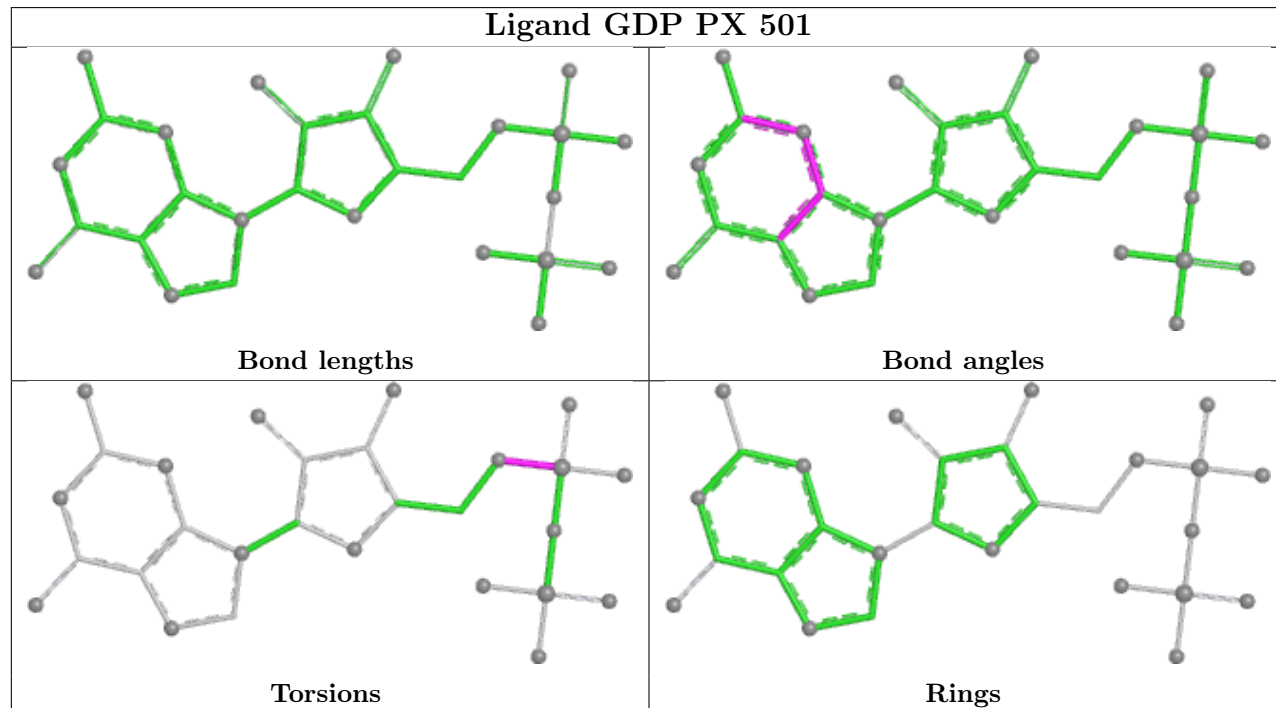
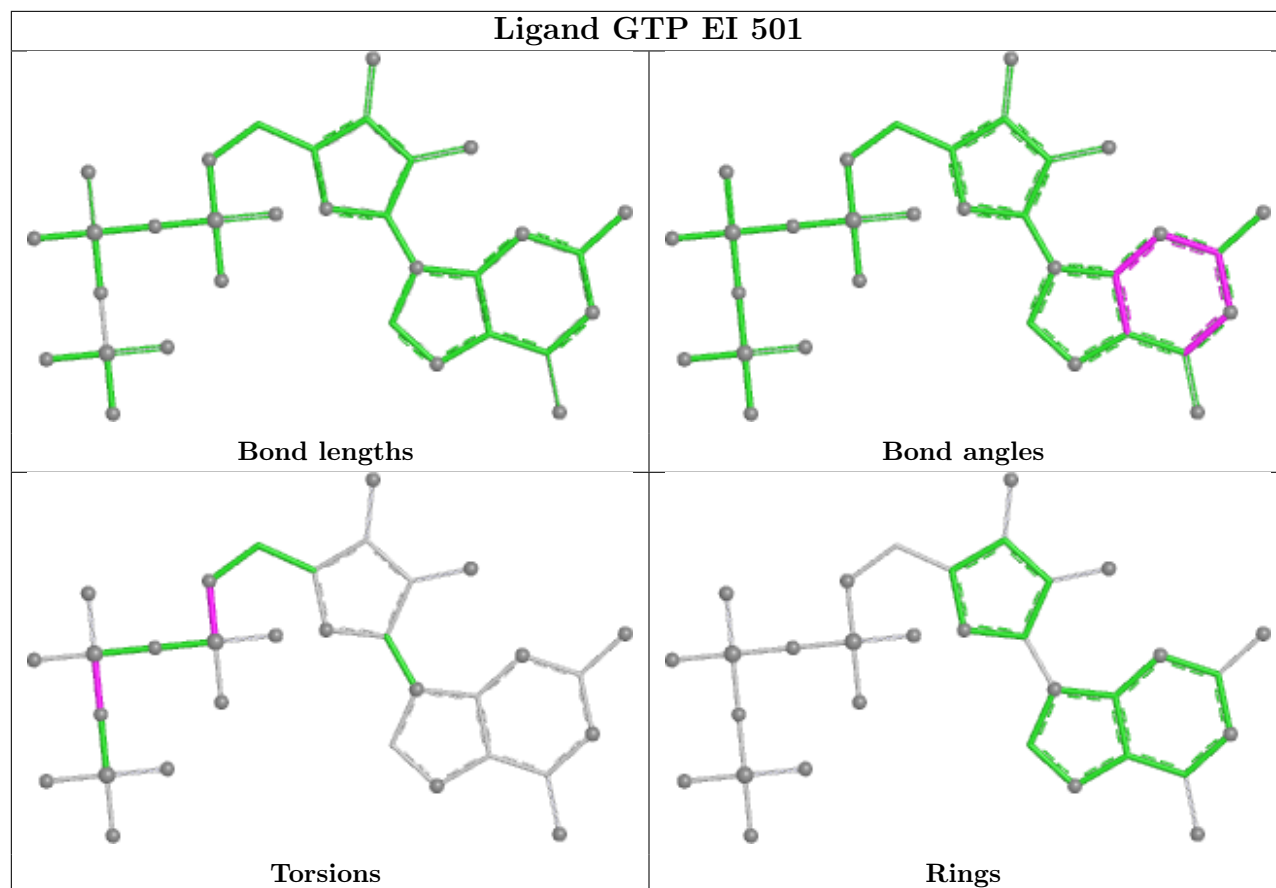
## Ligand GTP EG 501

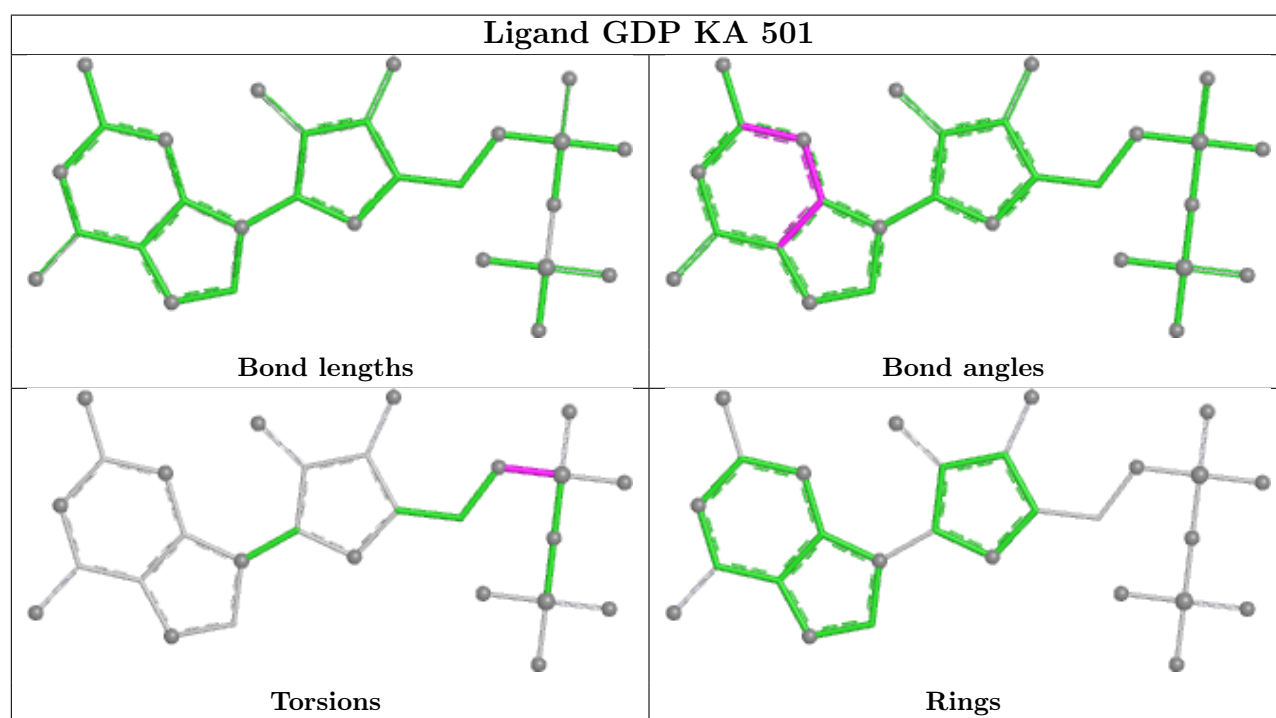
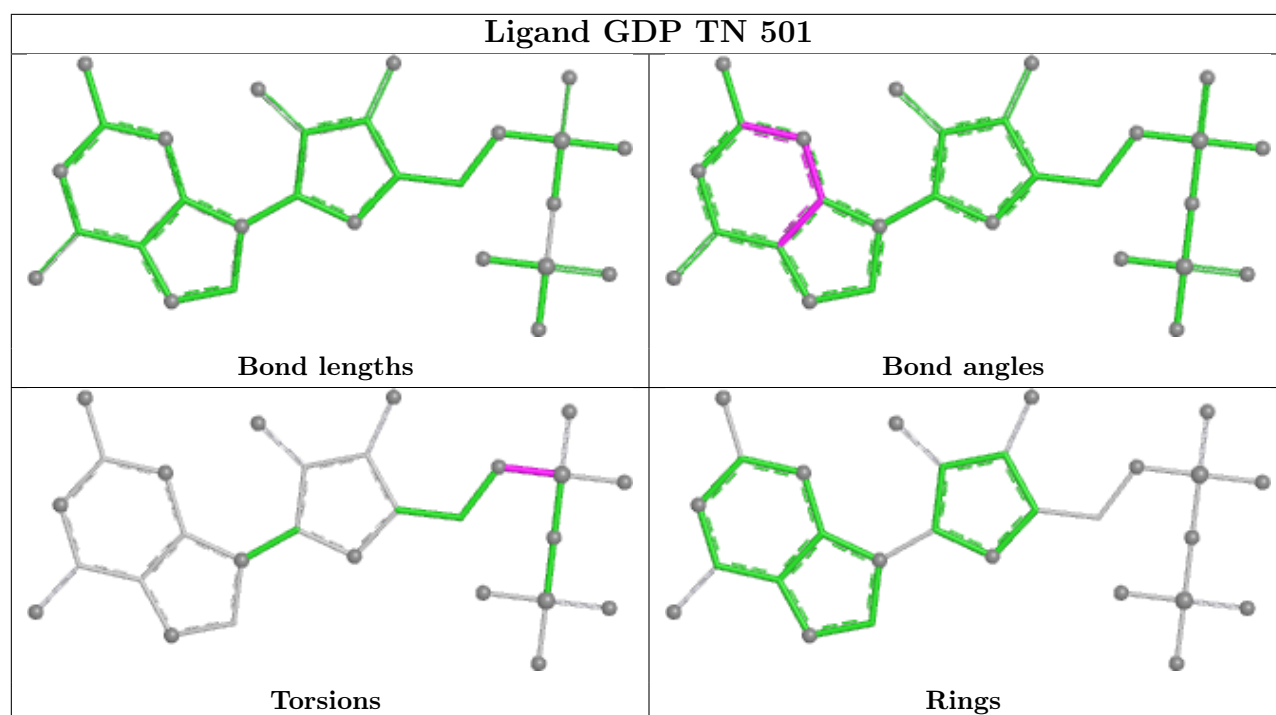


## Ligand GTP DO 501

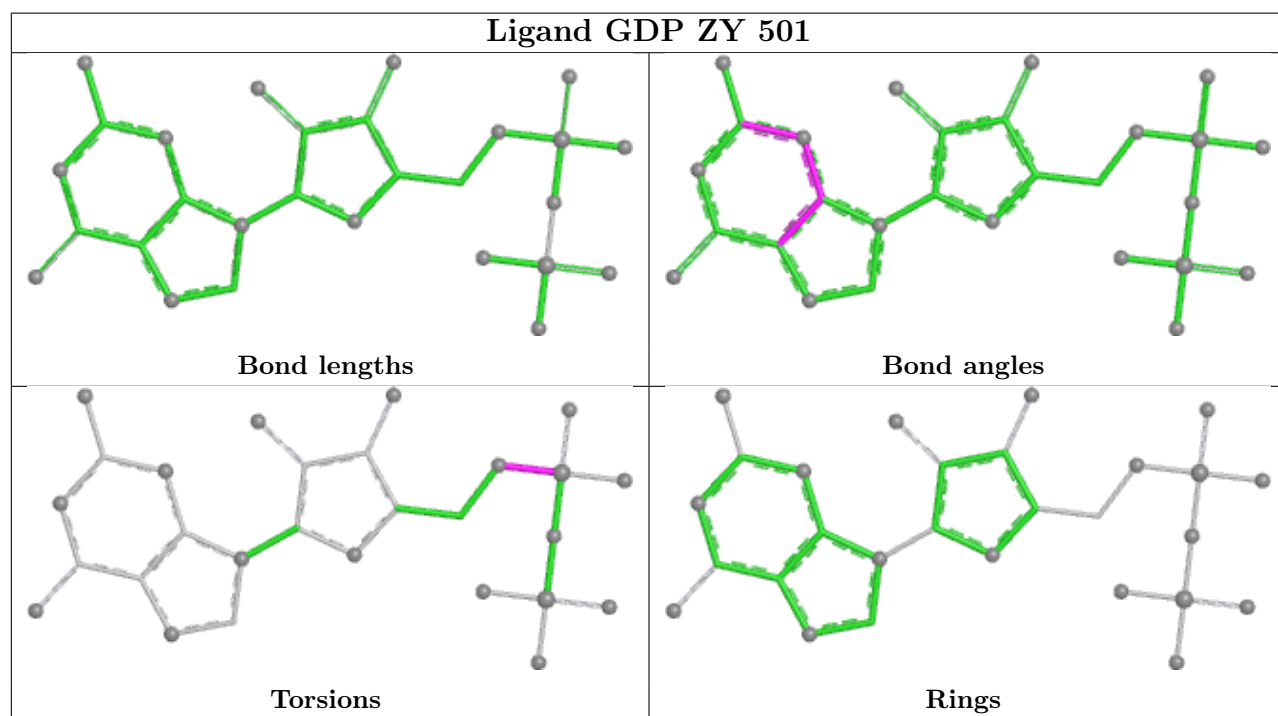
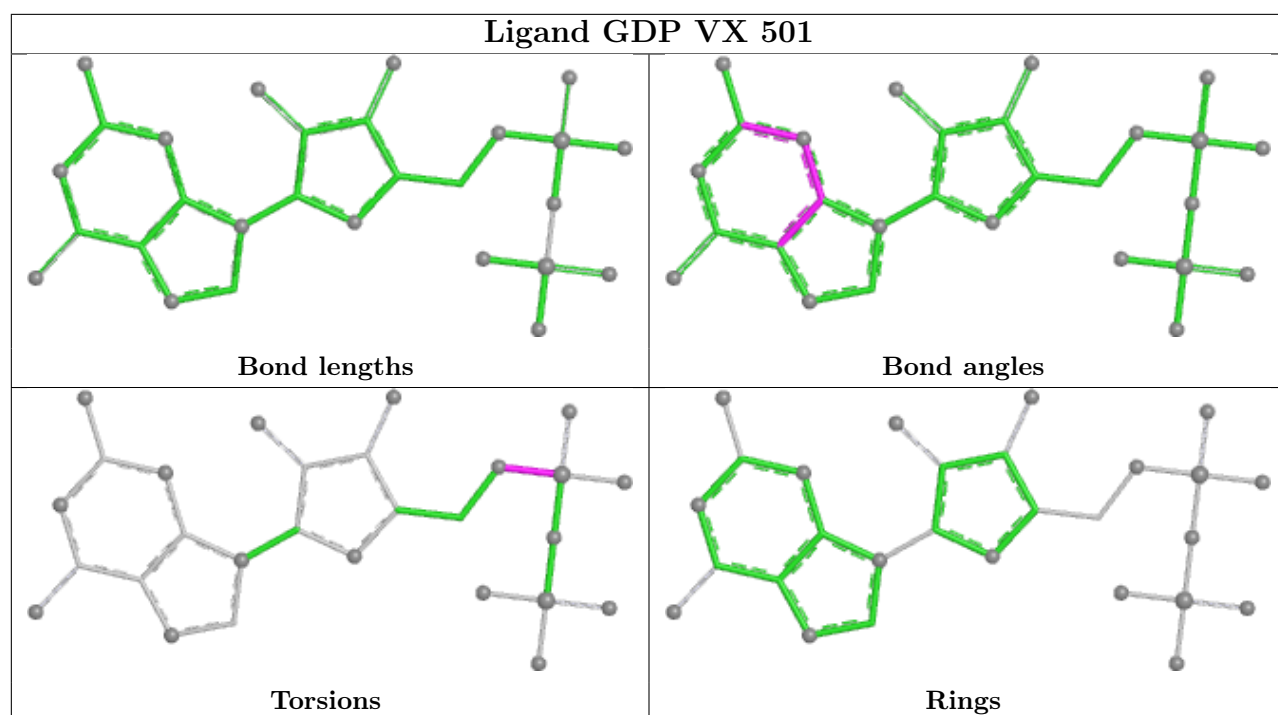


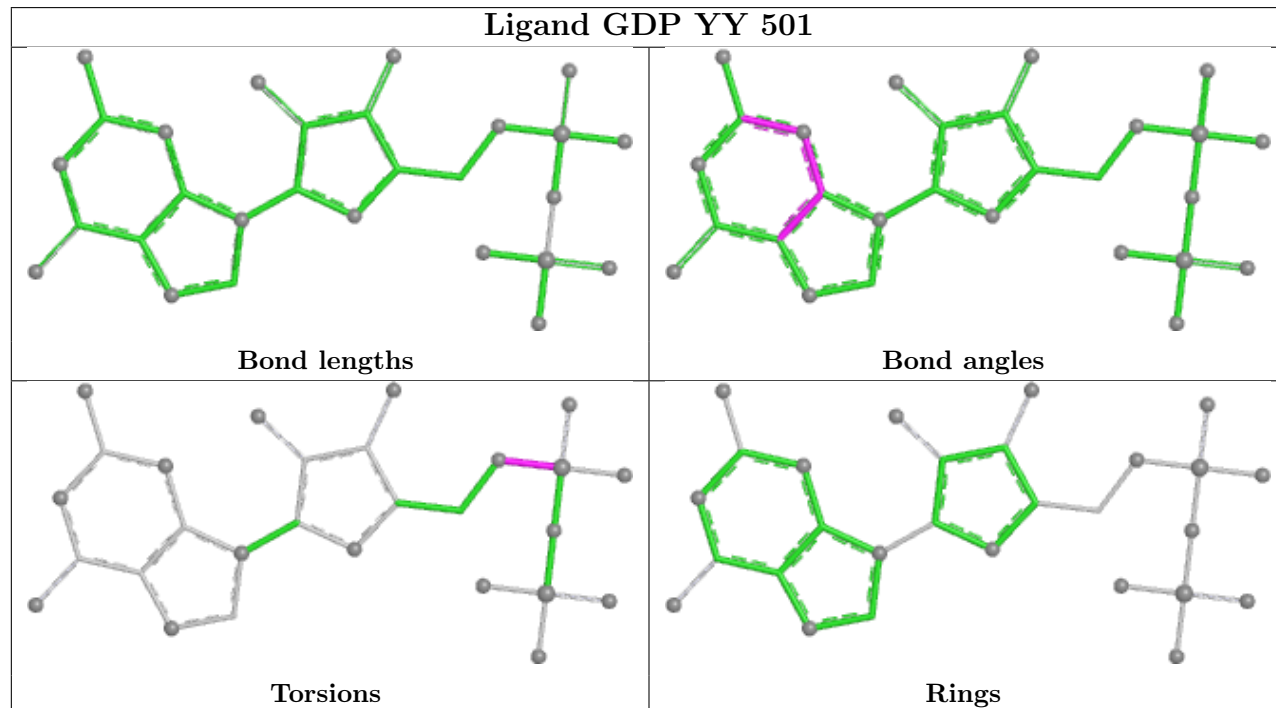
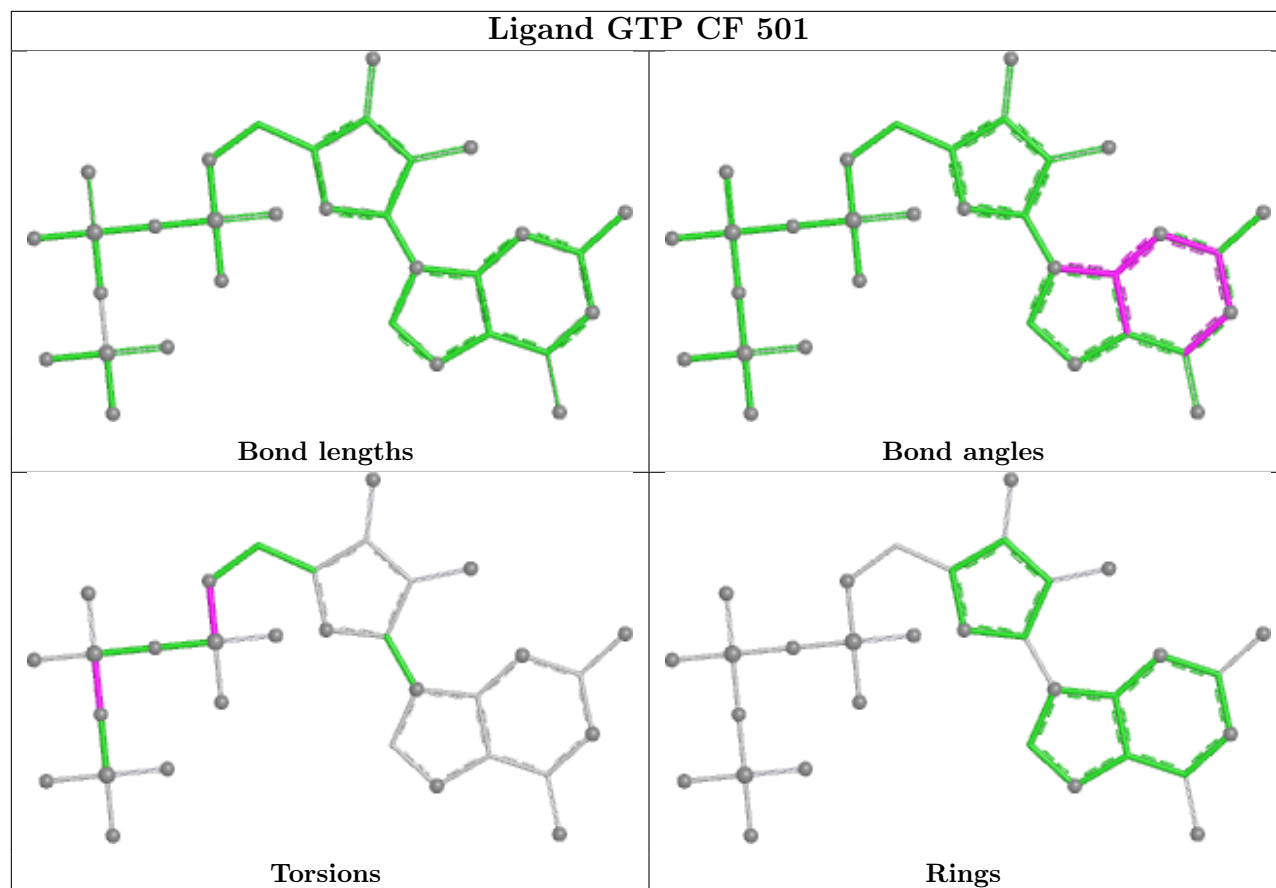


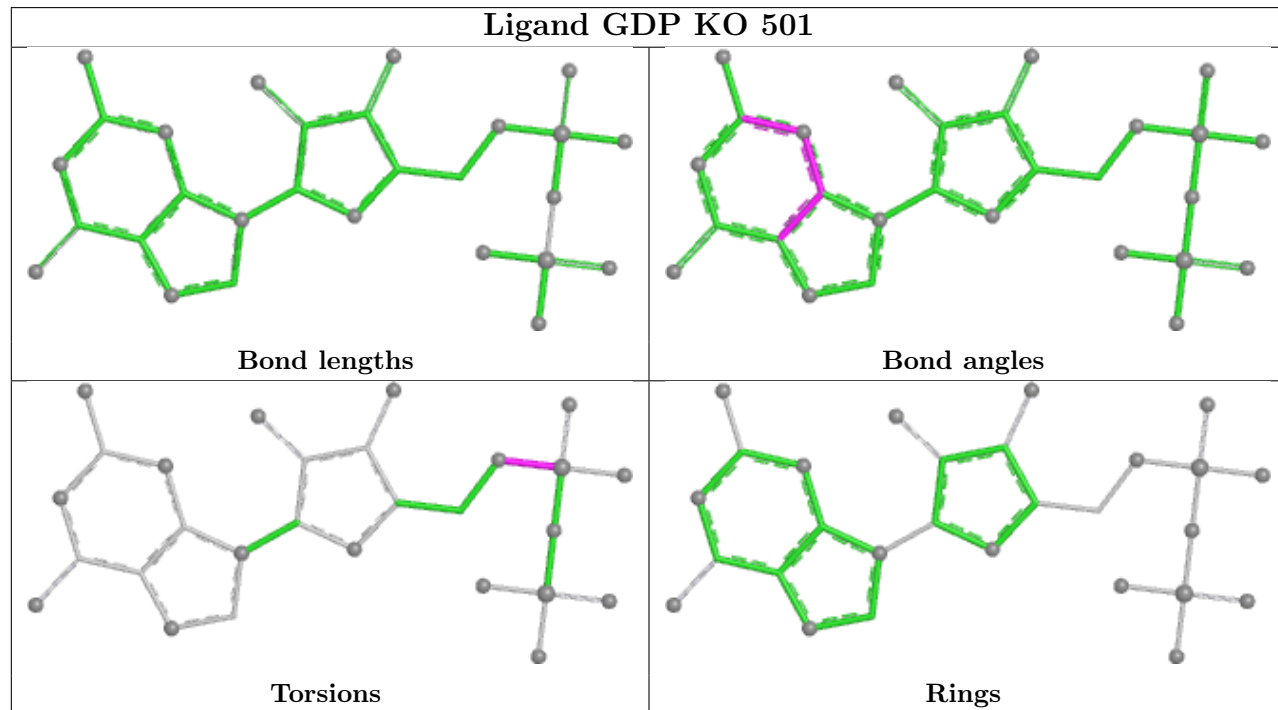
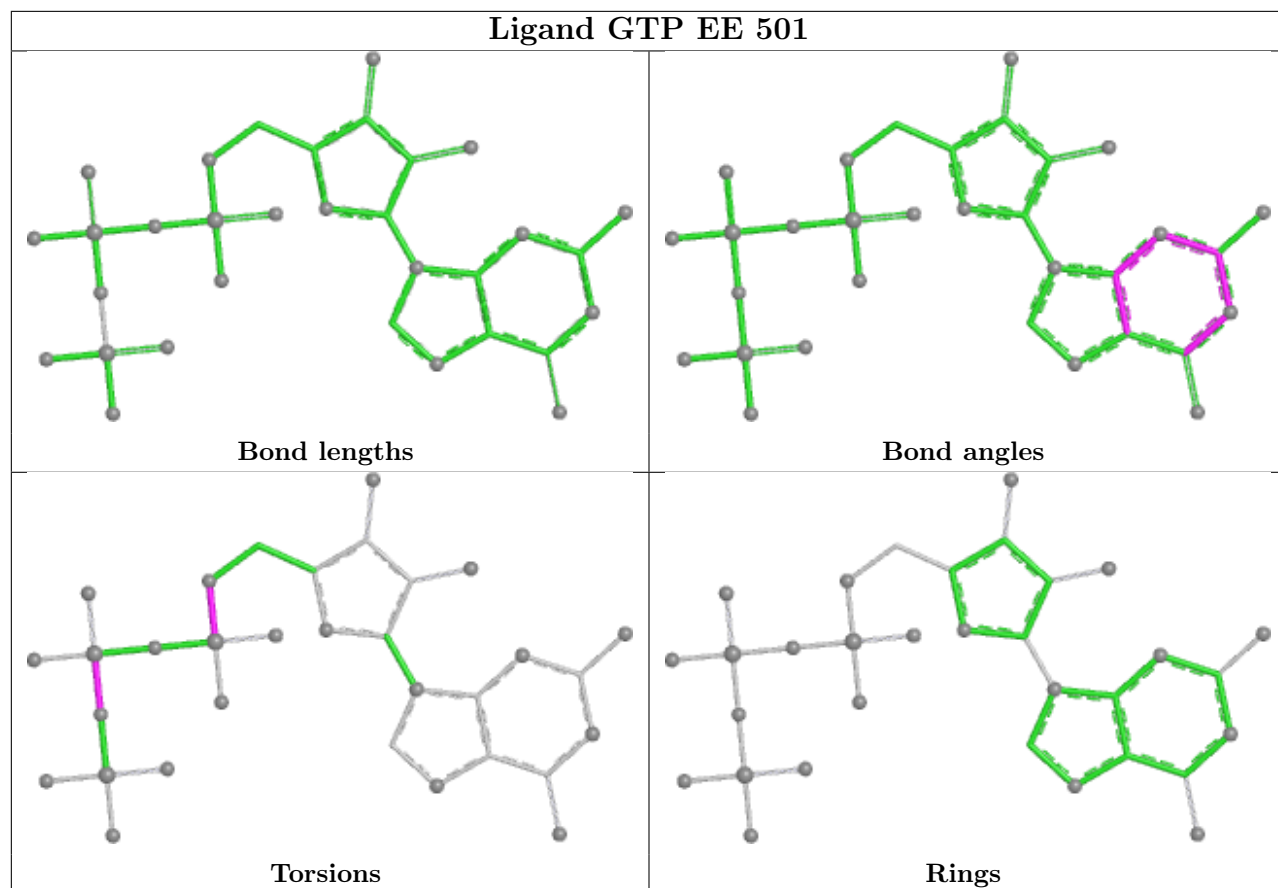


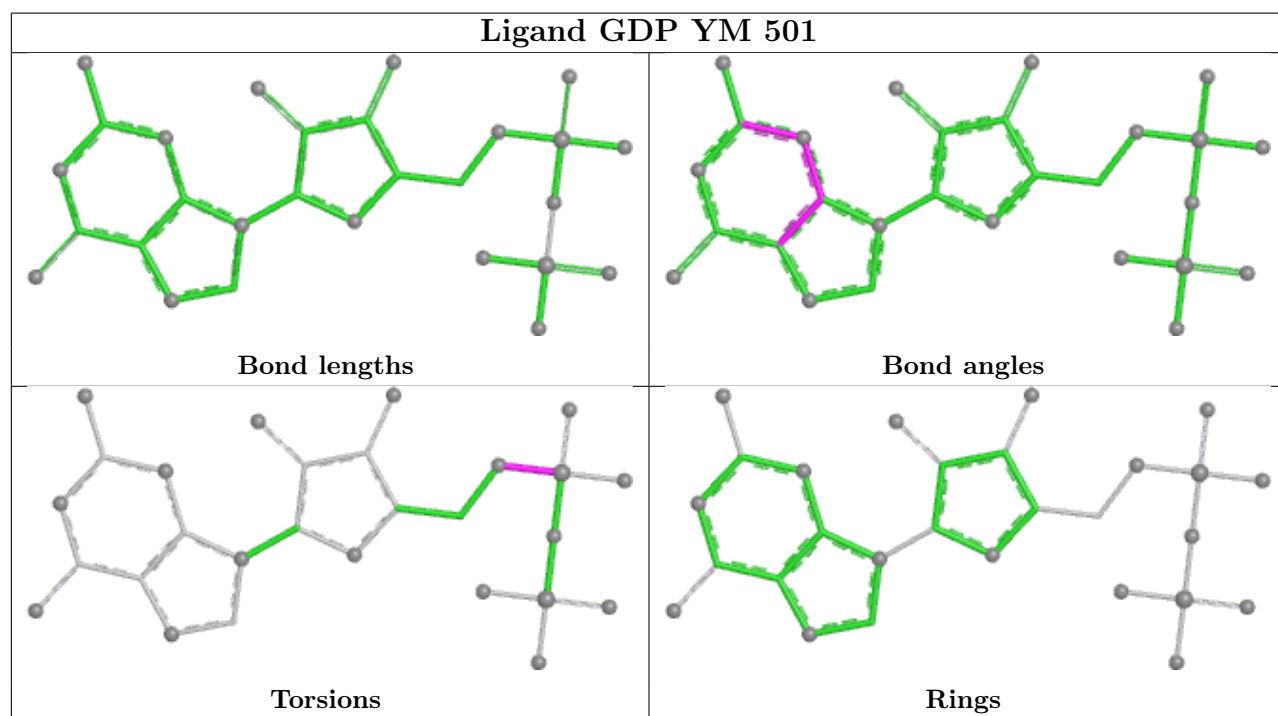
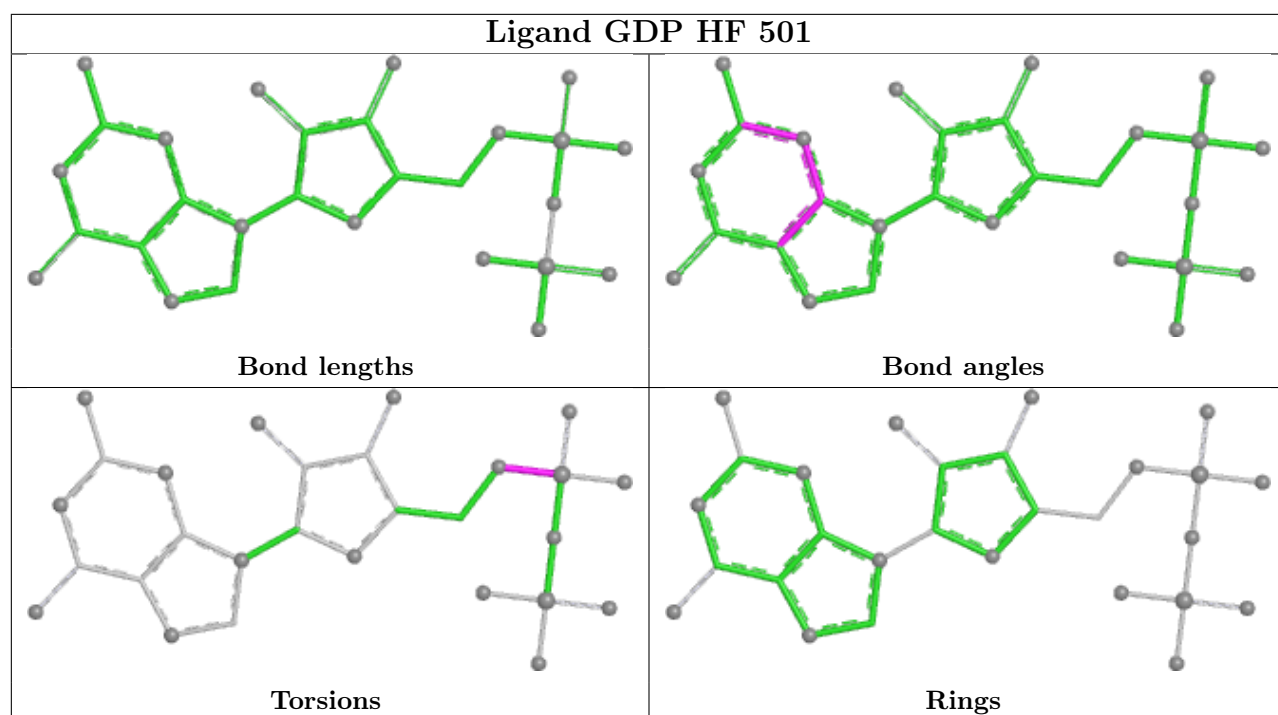




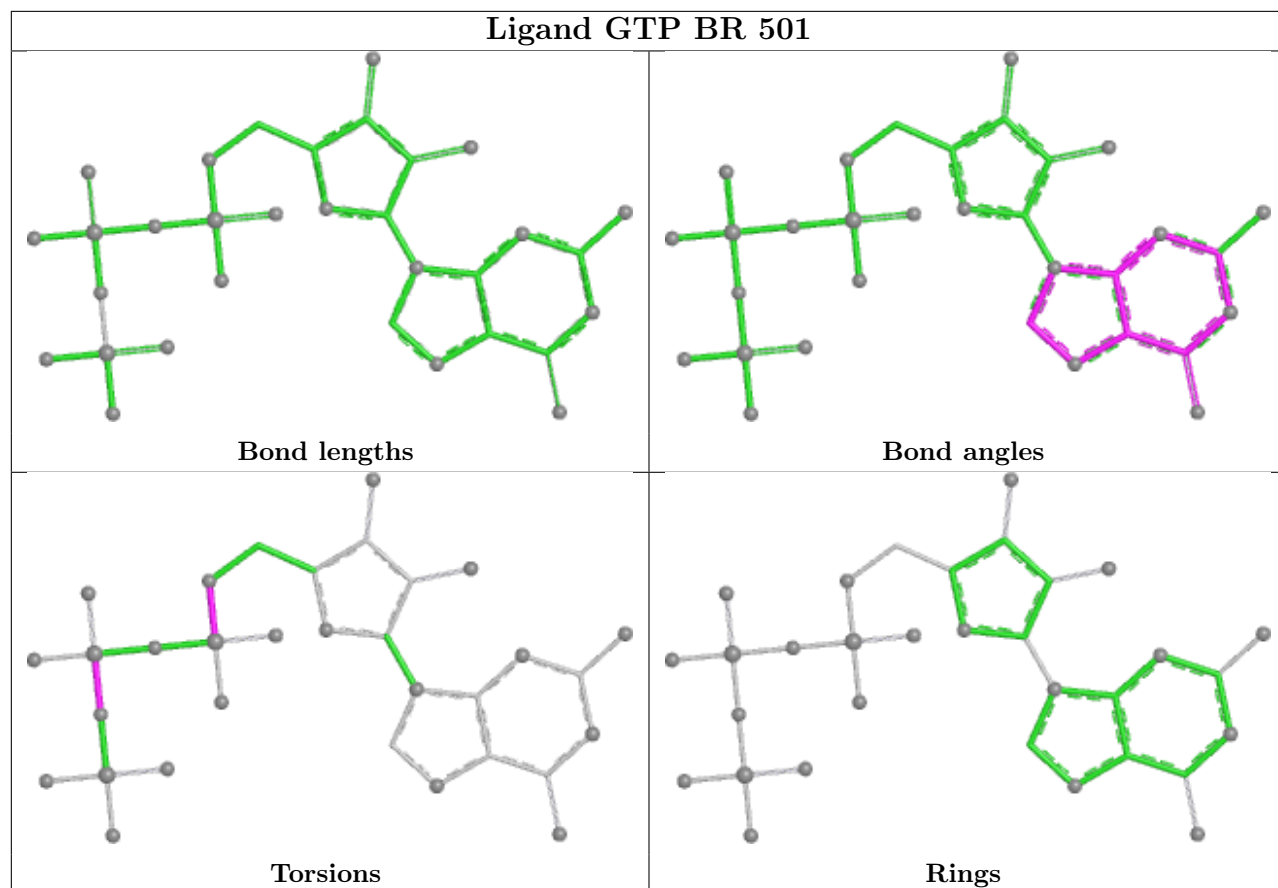




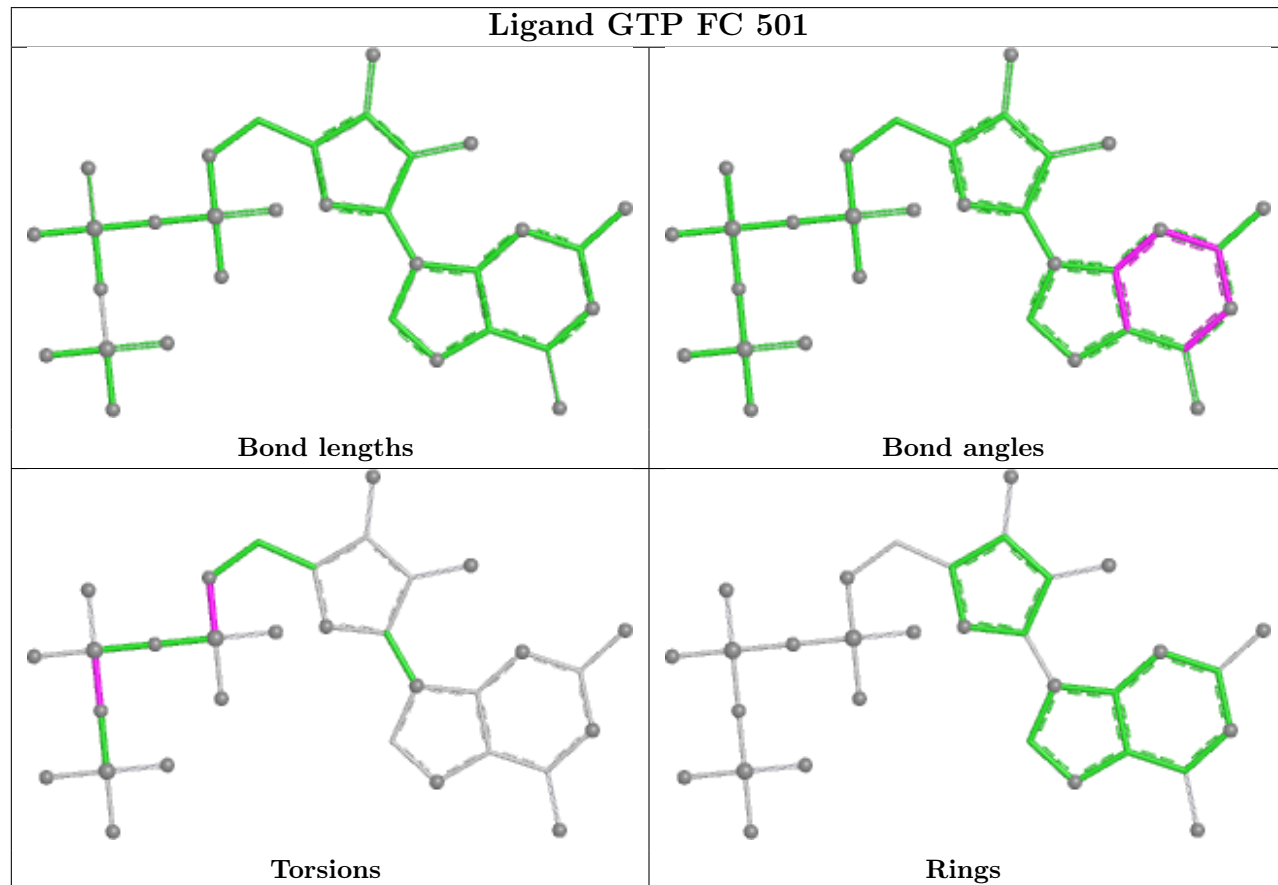




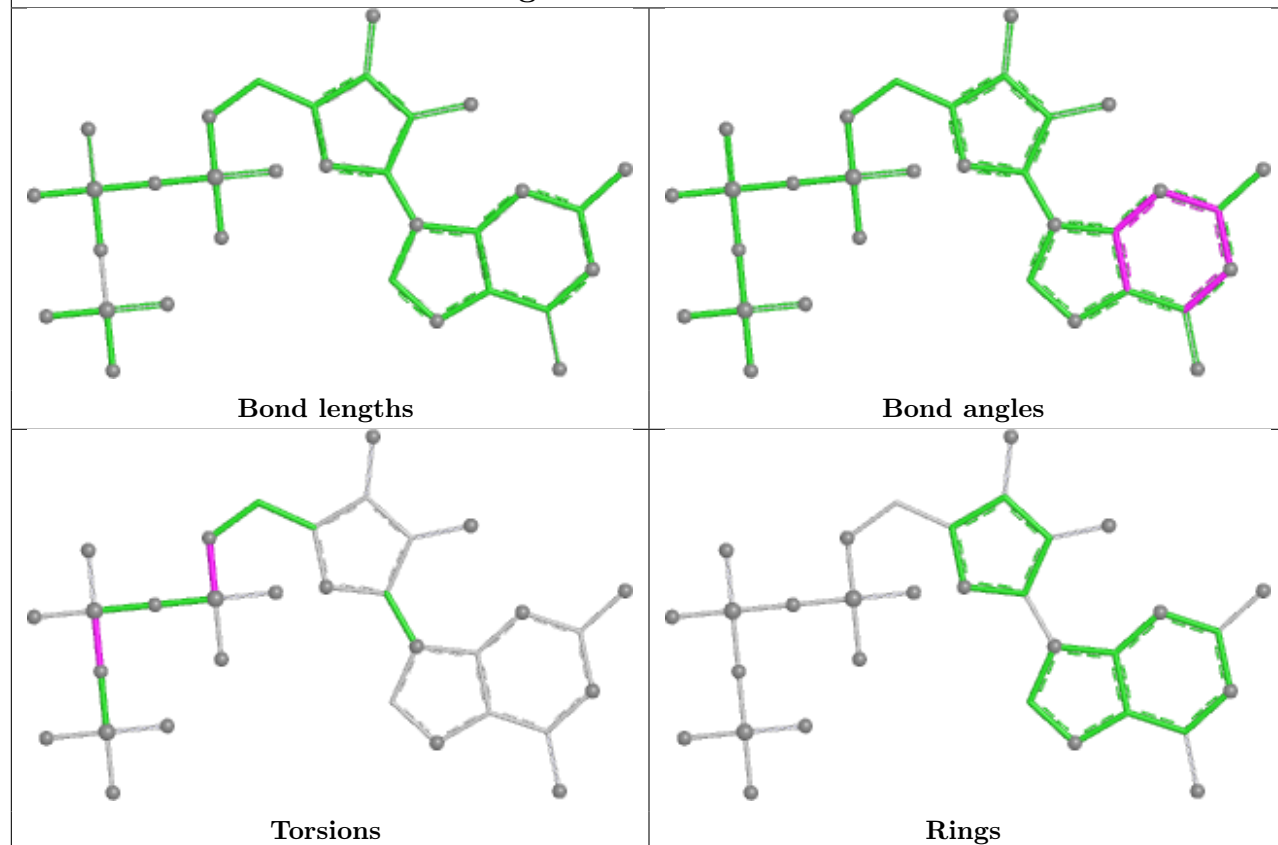
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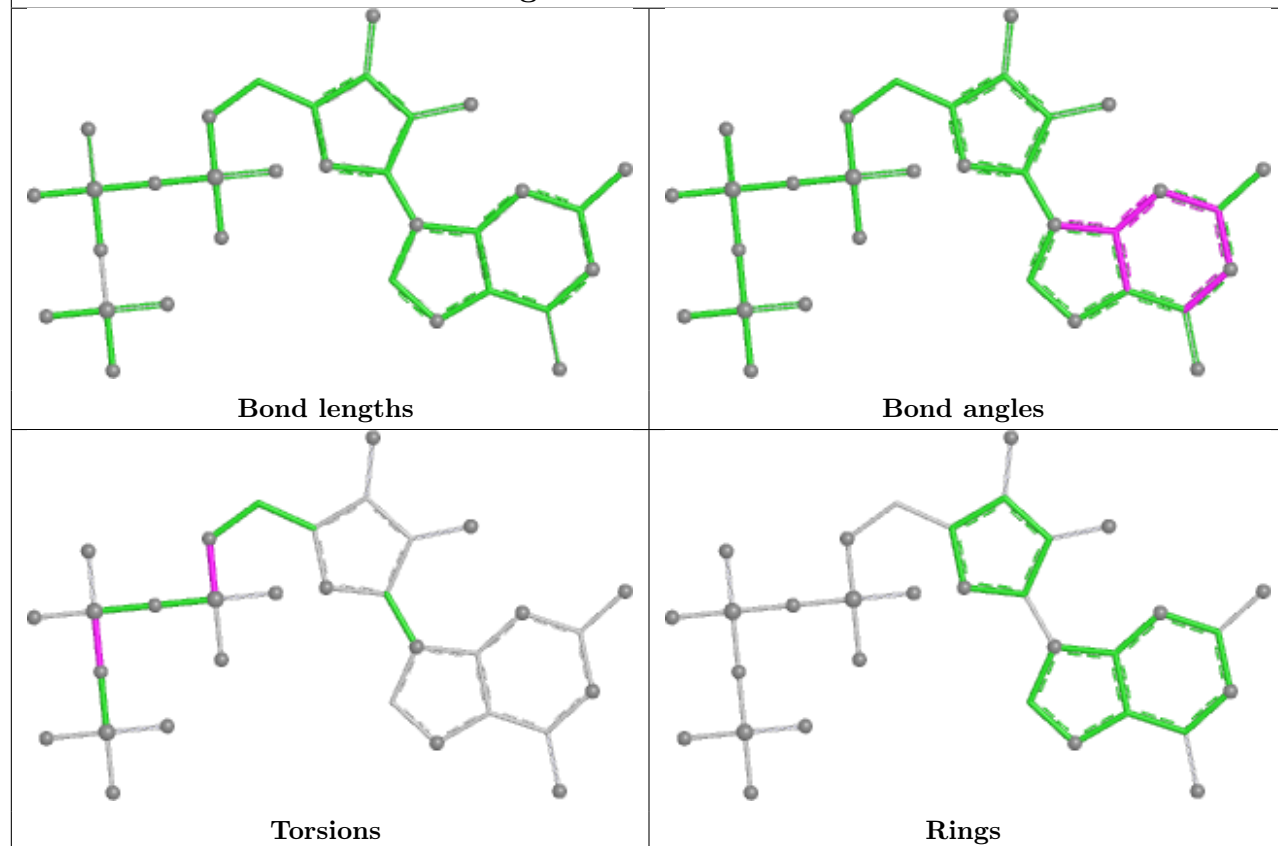
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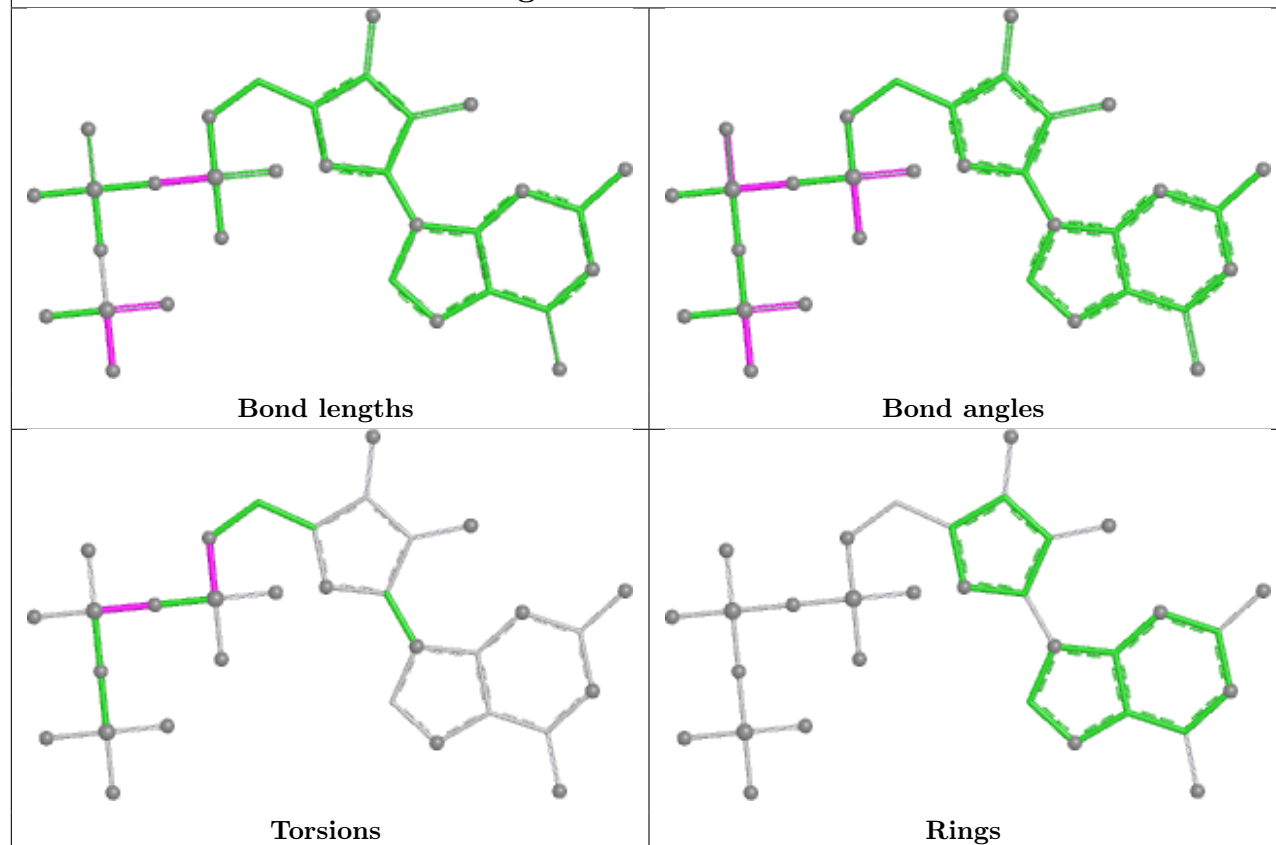
## Ligand GTP UF 501



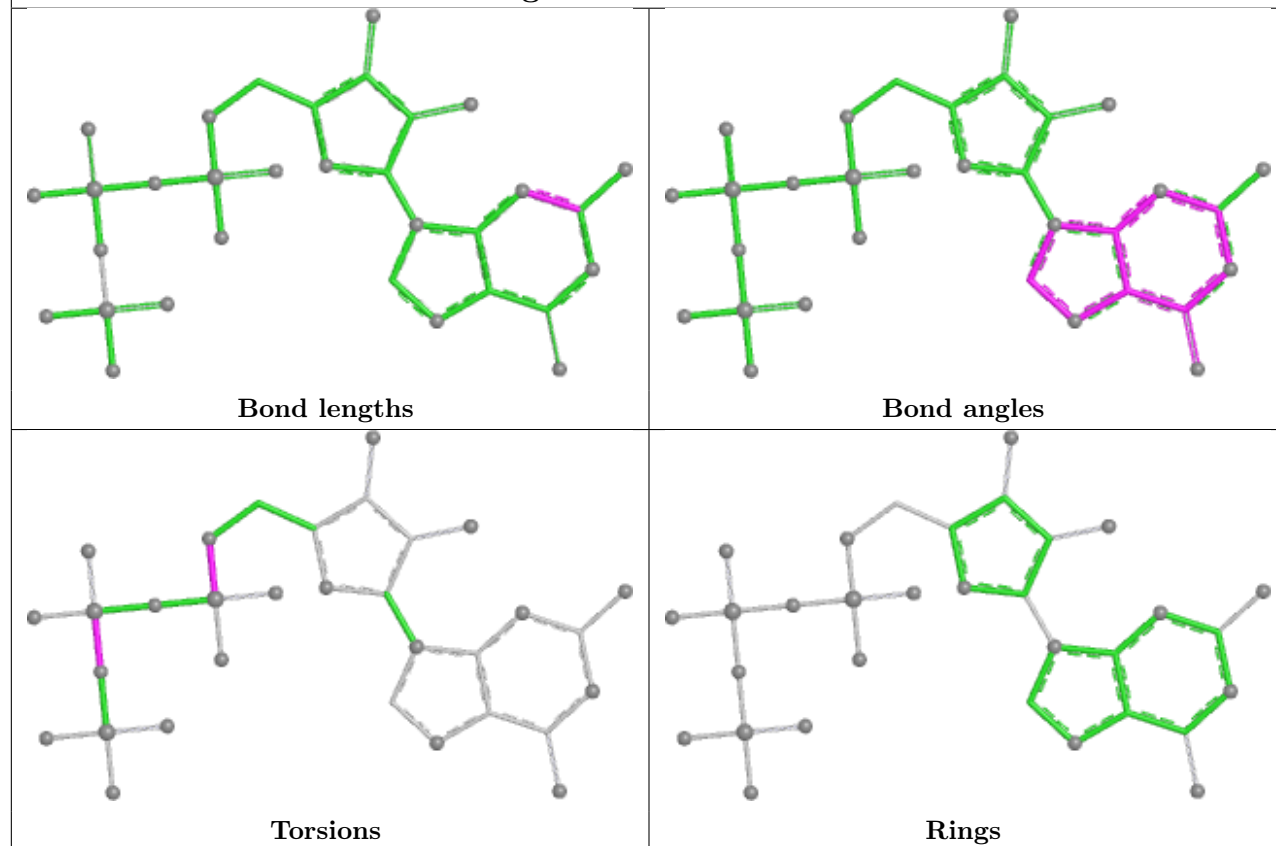
## Ligand GTP GS 602



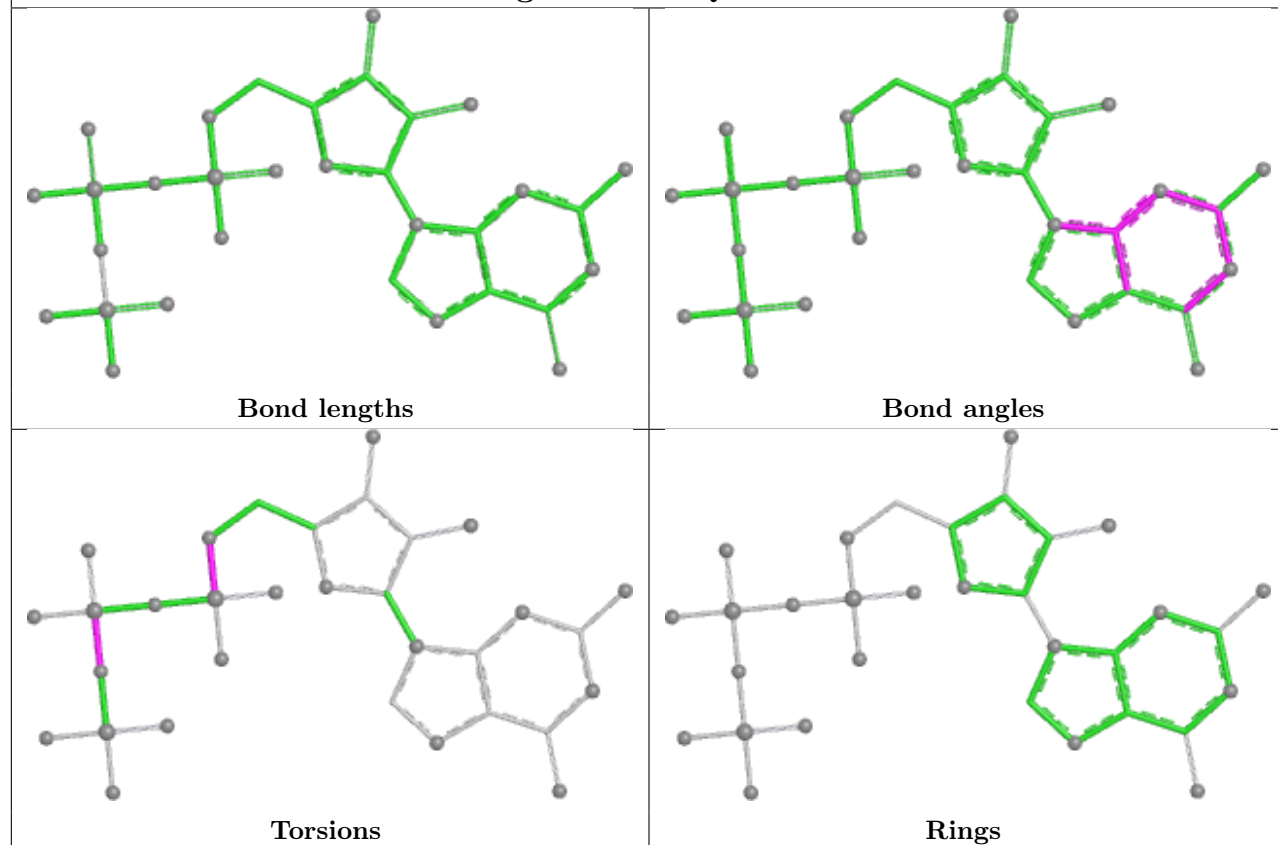
## Ligand GTP TX 602



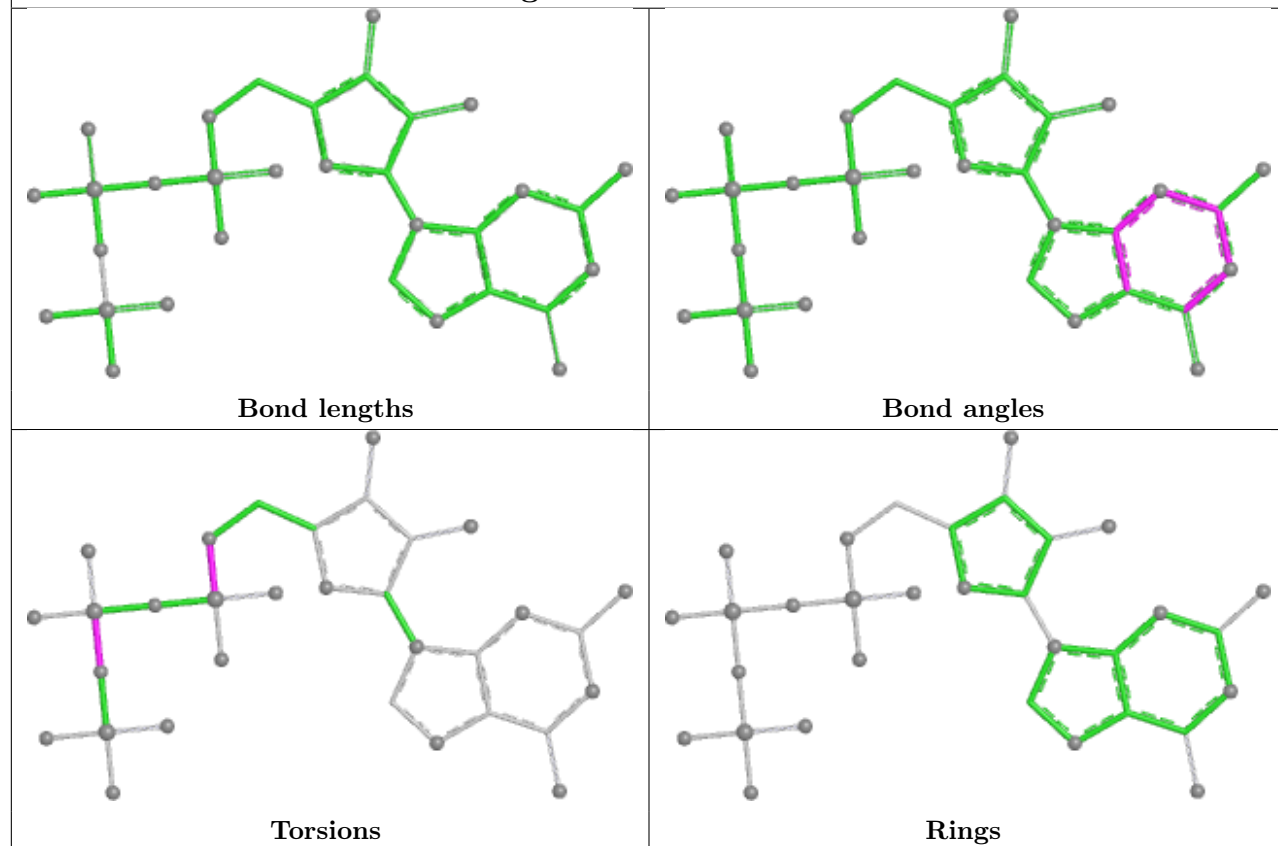
## Ligand GTP JP 602



## Ligand GTP QU 602

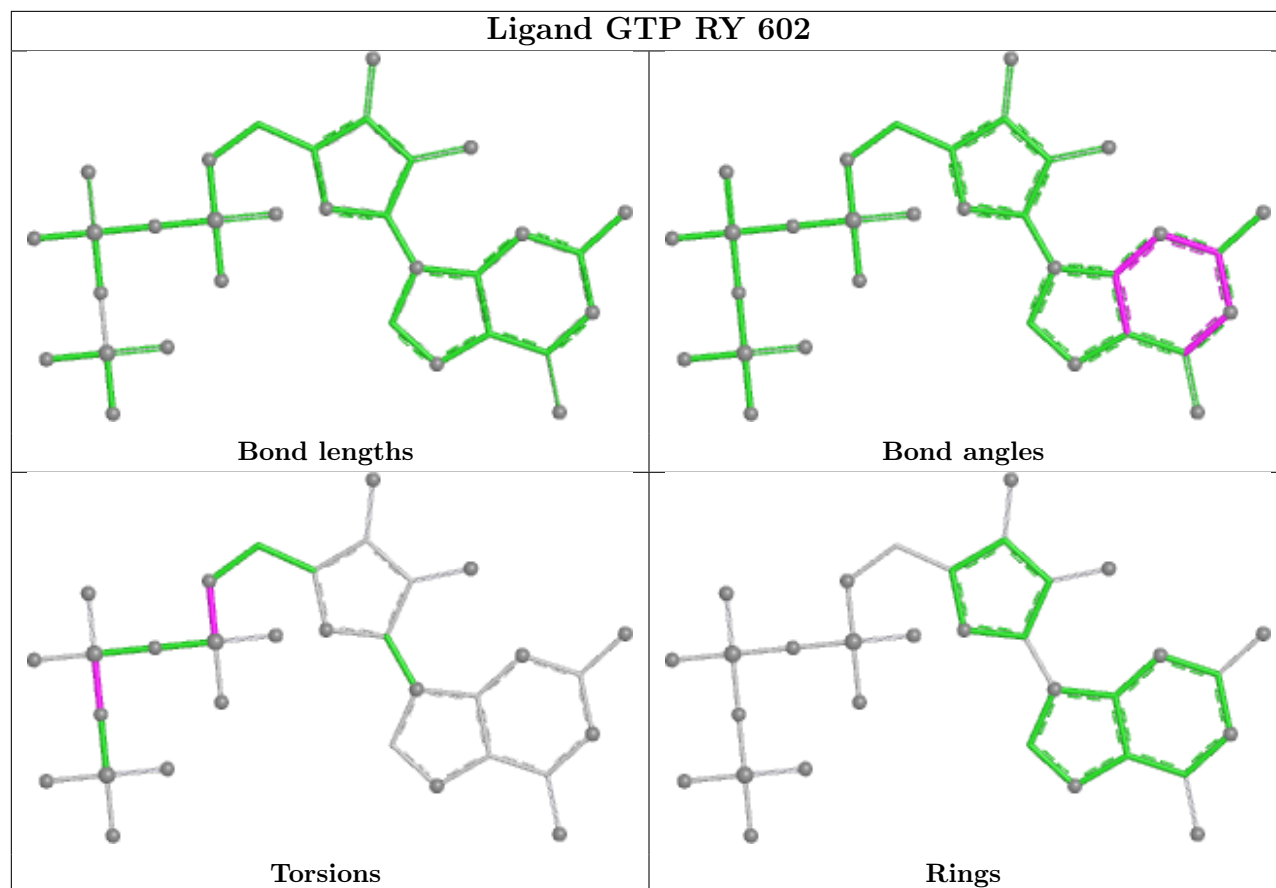


## Ligand GTP OJ 602

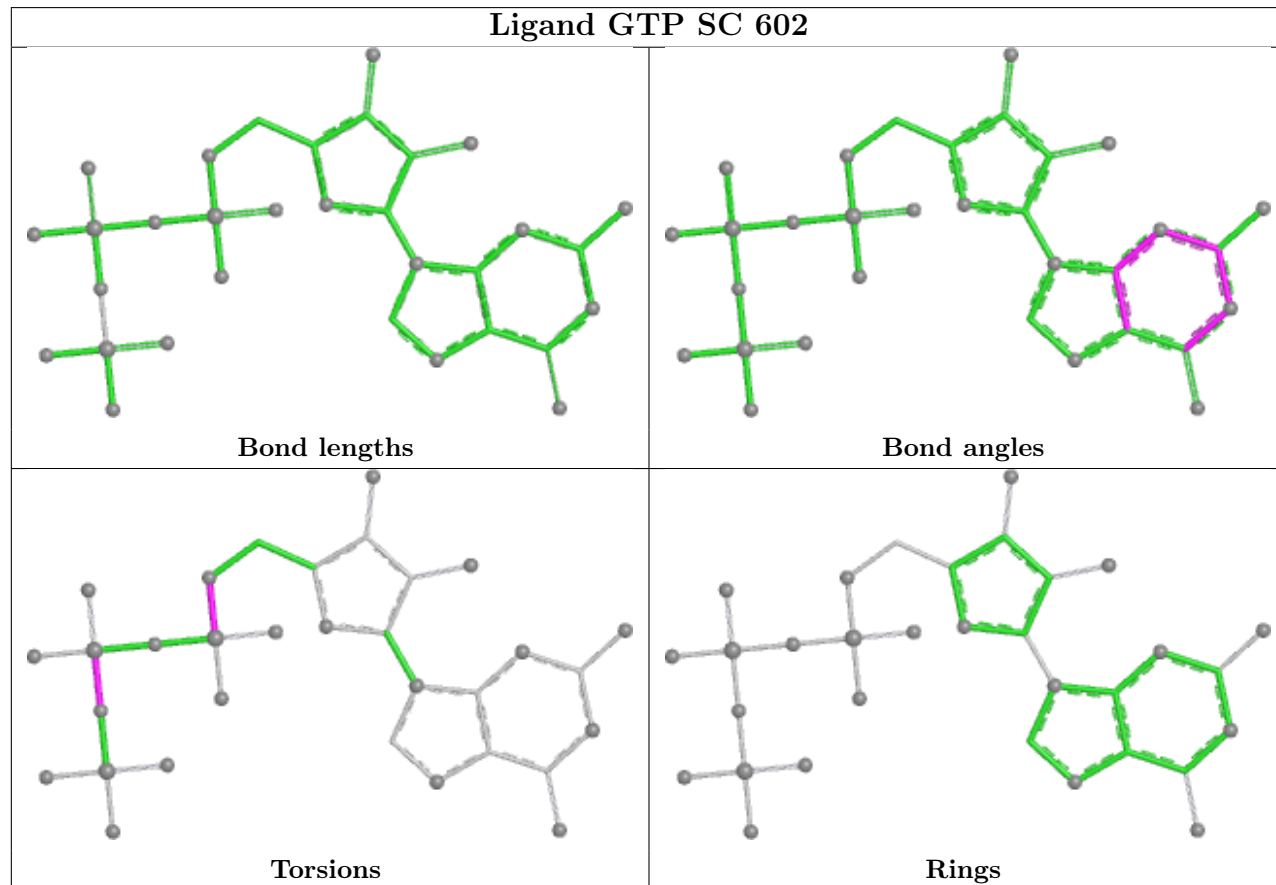




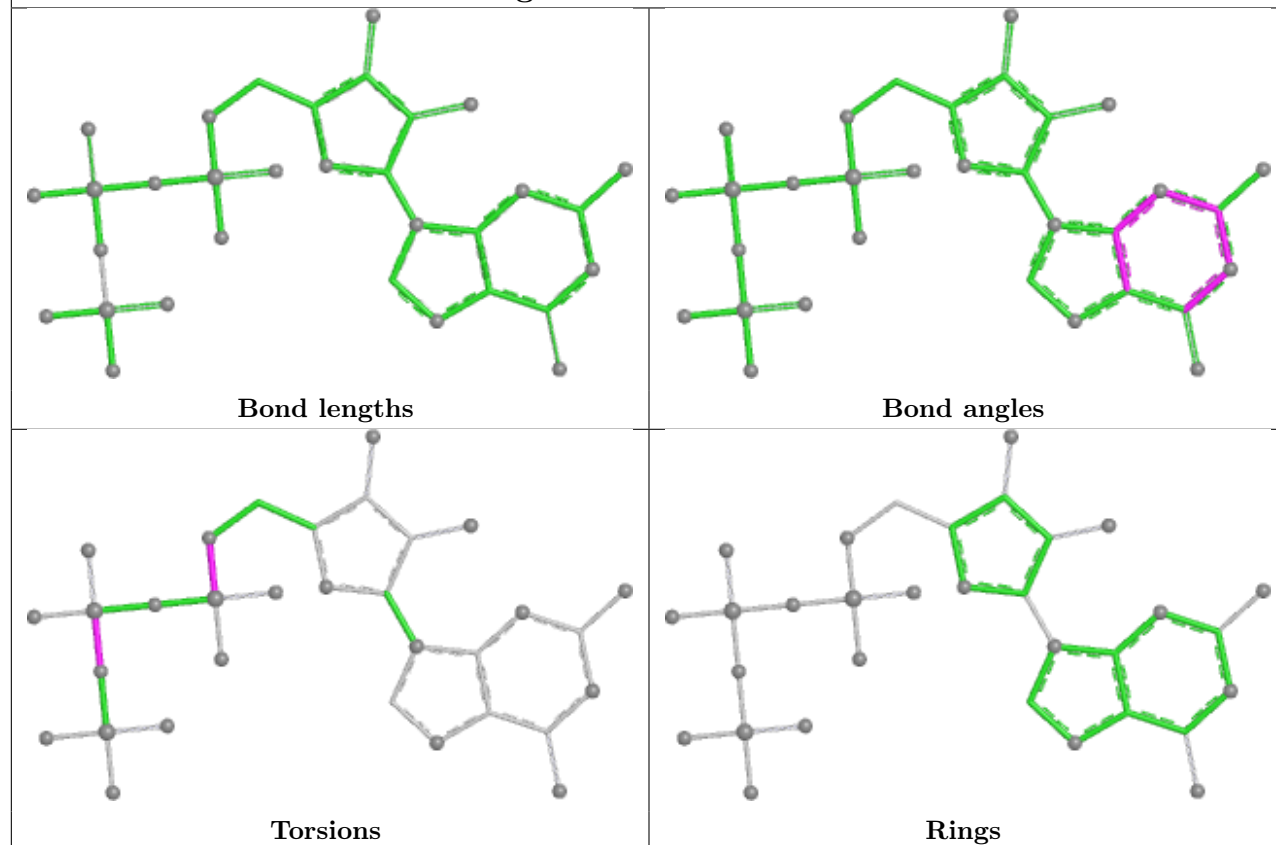
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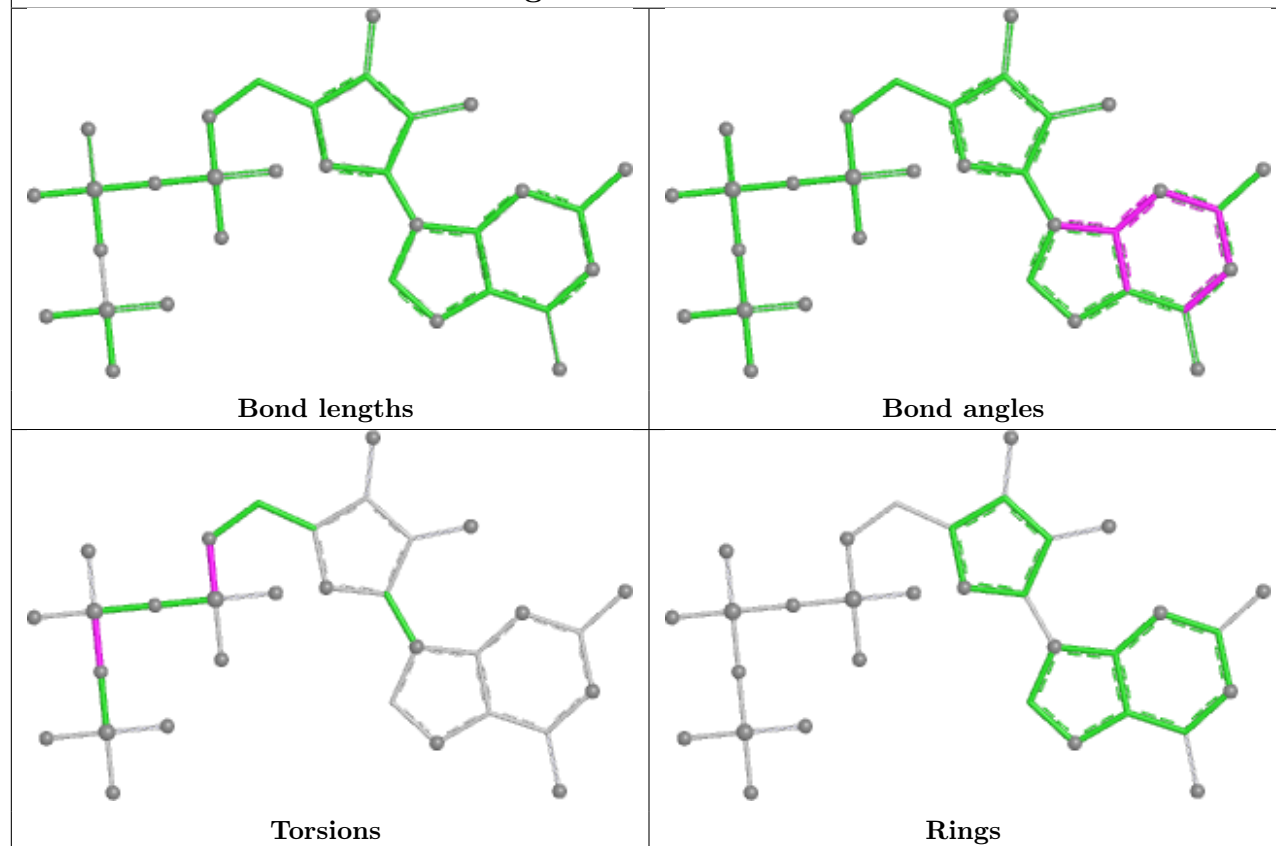
## Ligand GTP SC 602

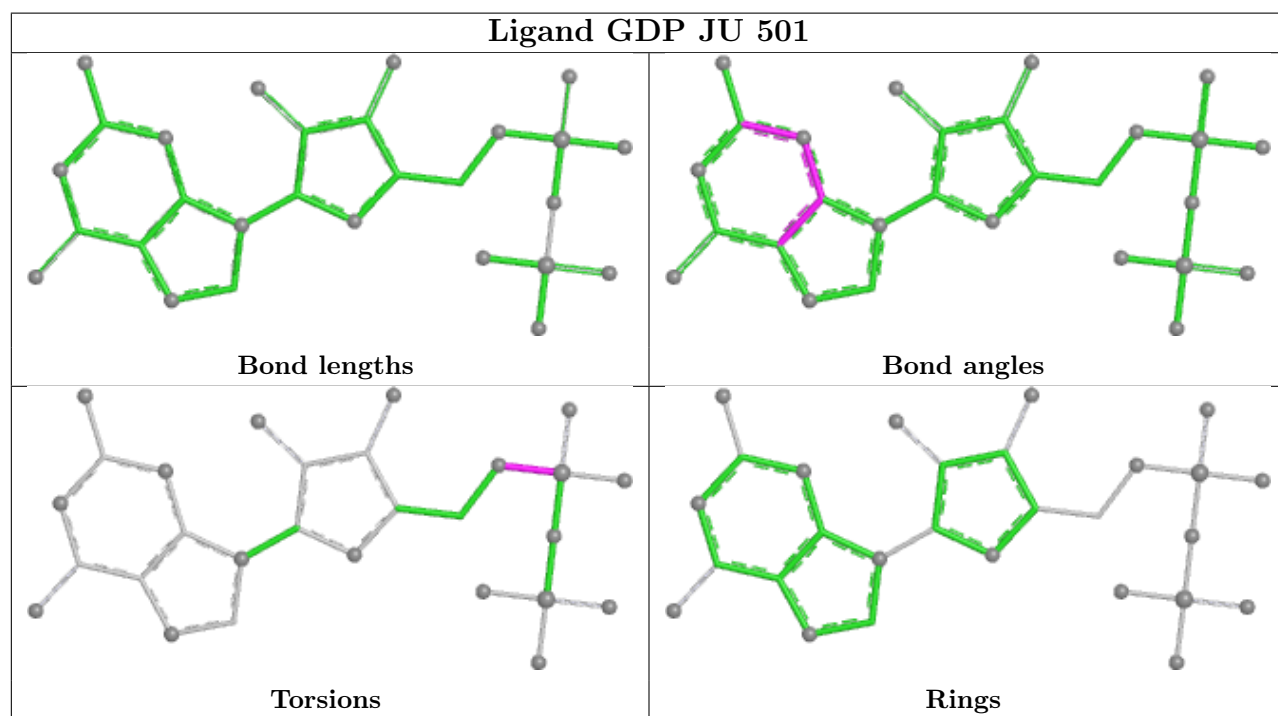
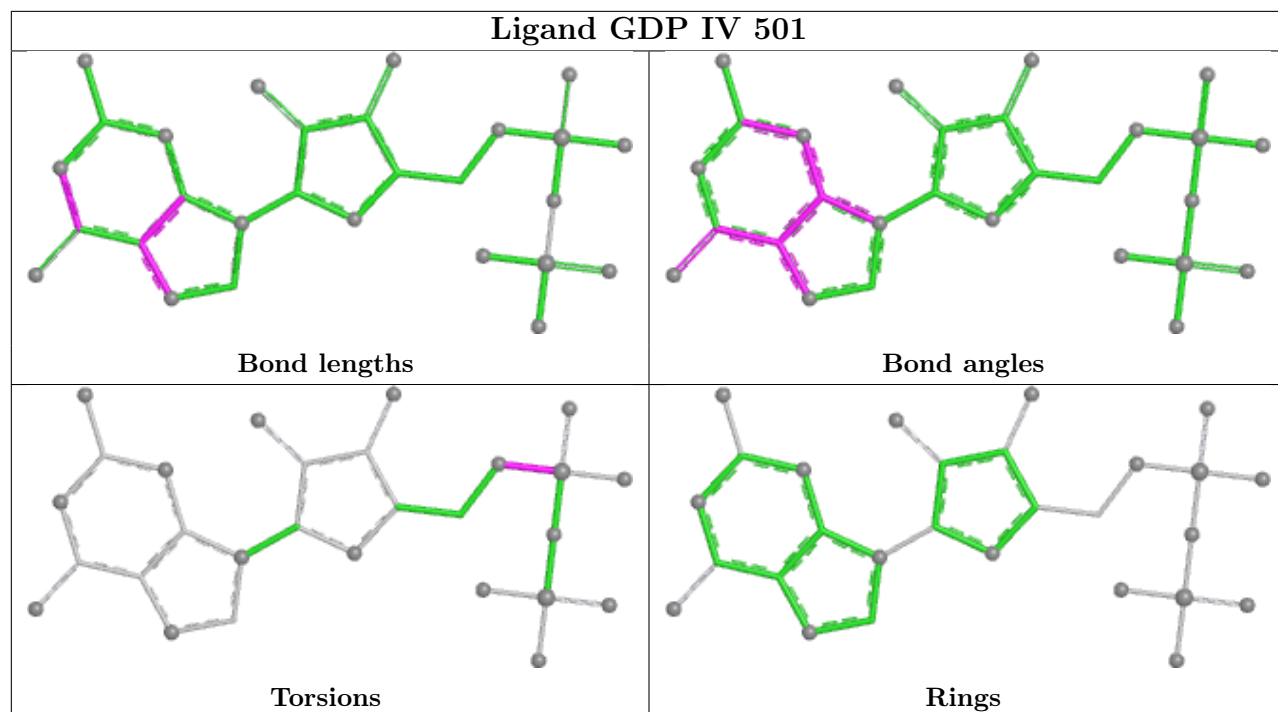


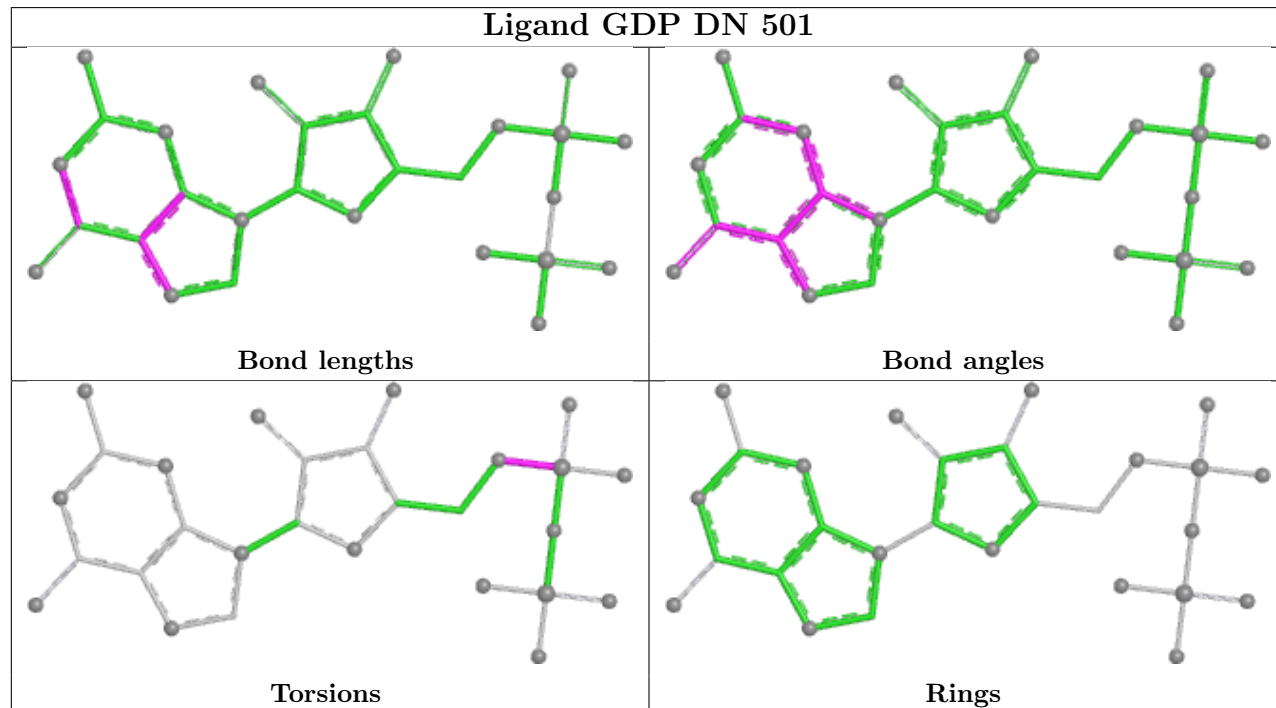
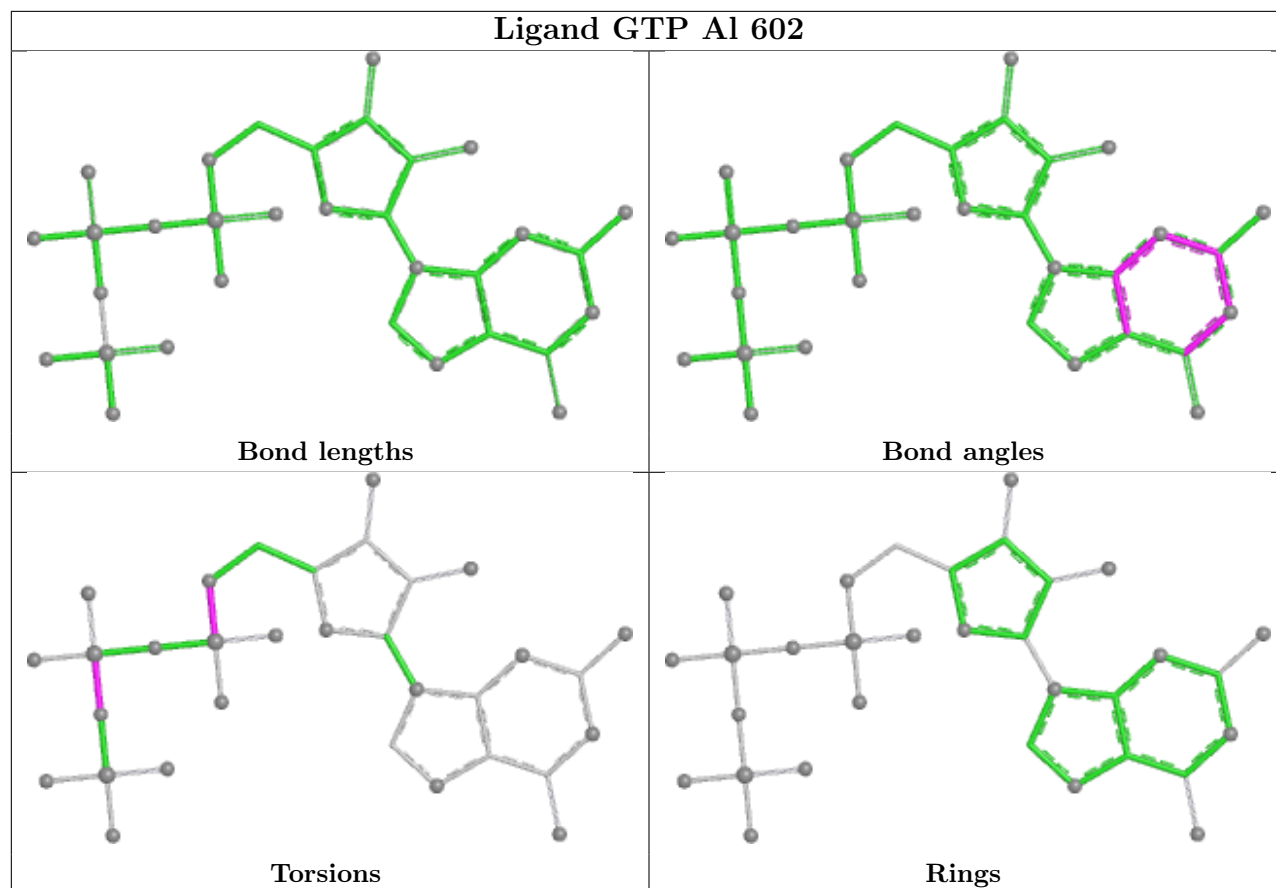
## Ligand GTP YN 501



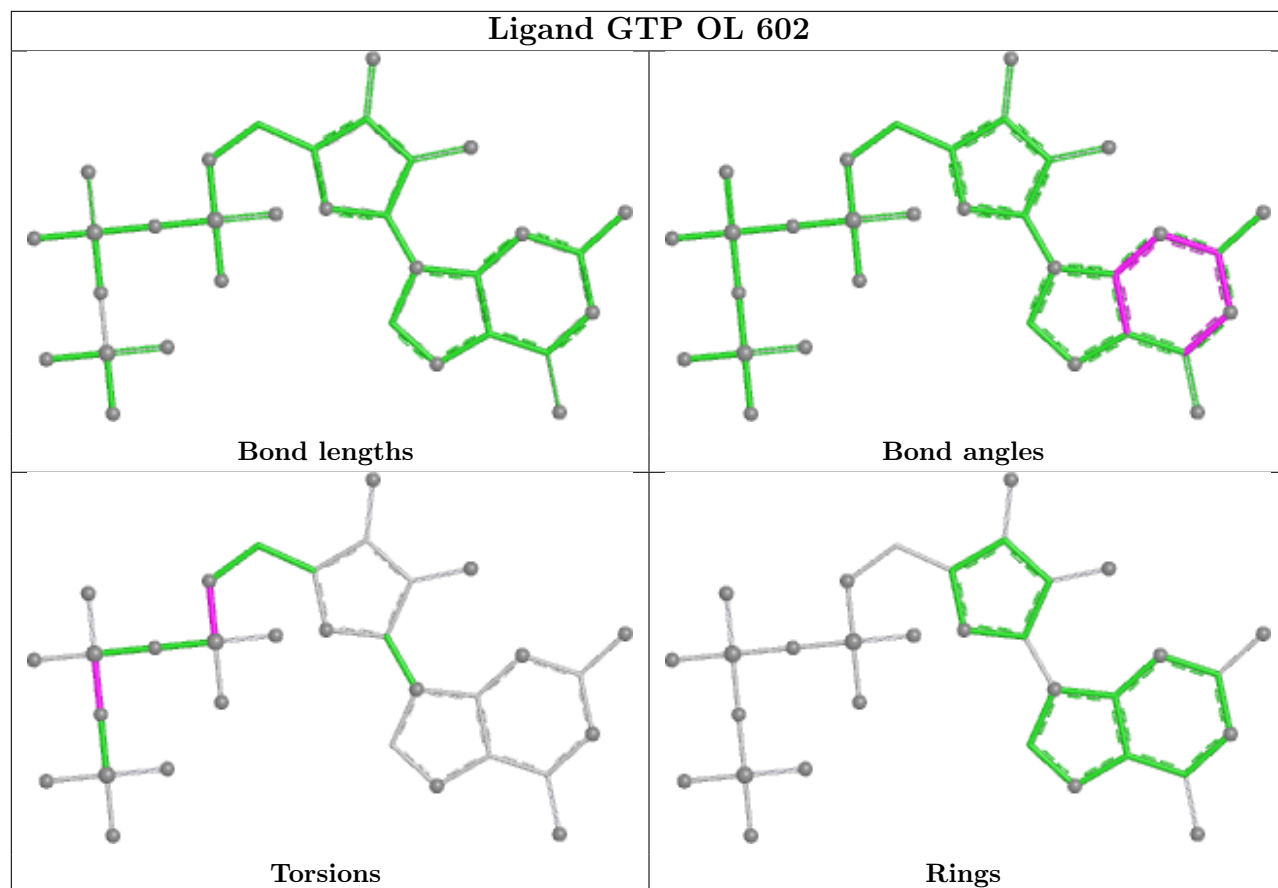
## Ligand GTP Af 501



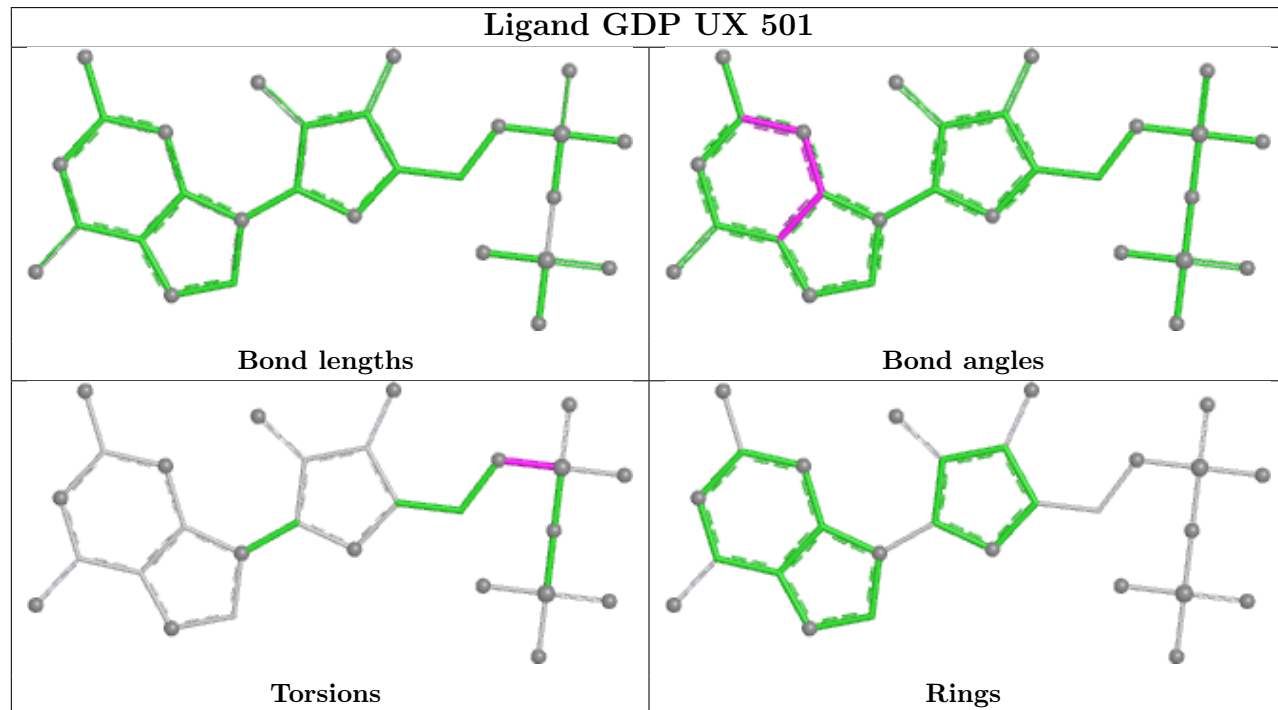


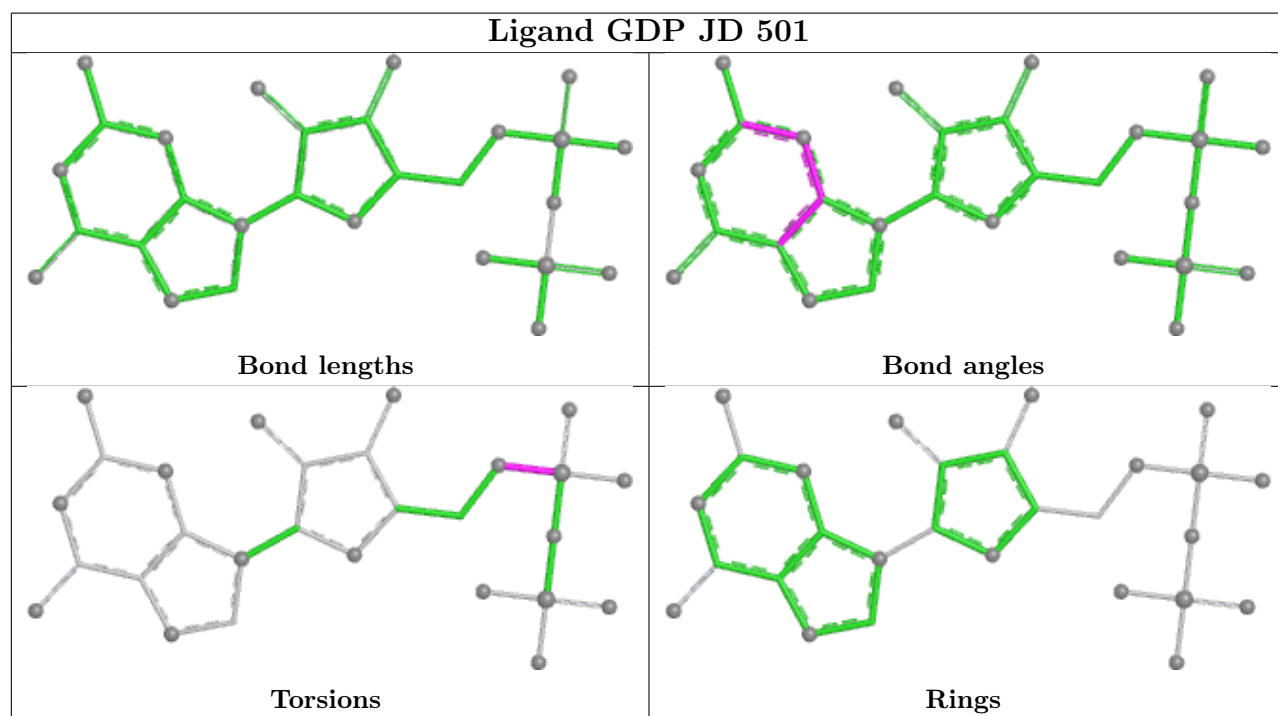
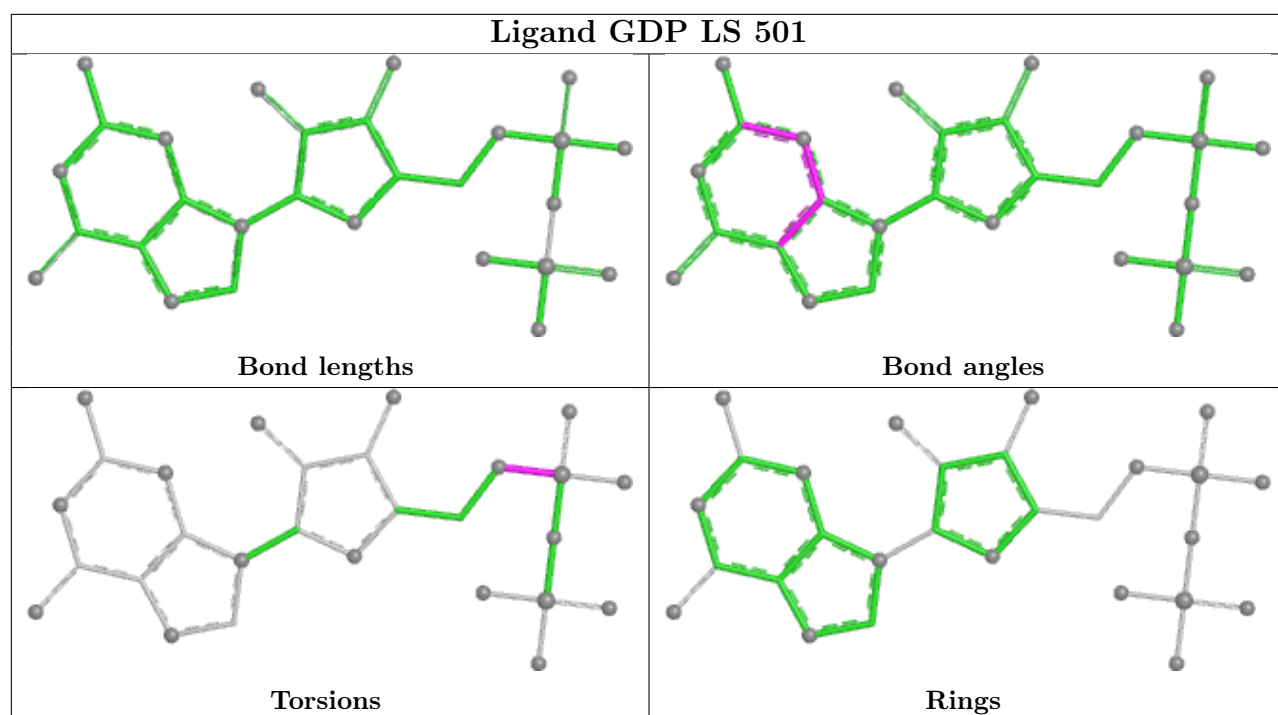


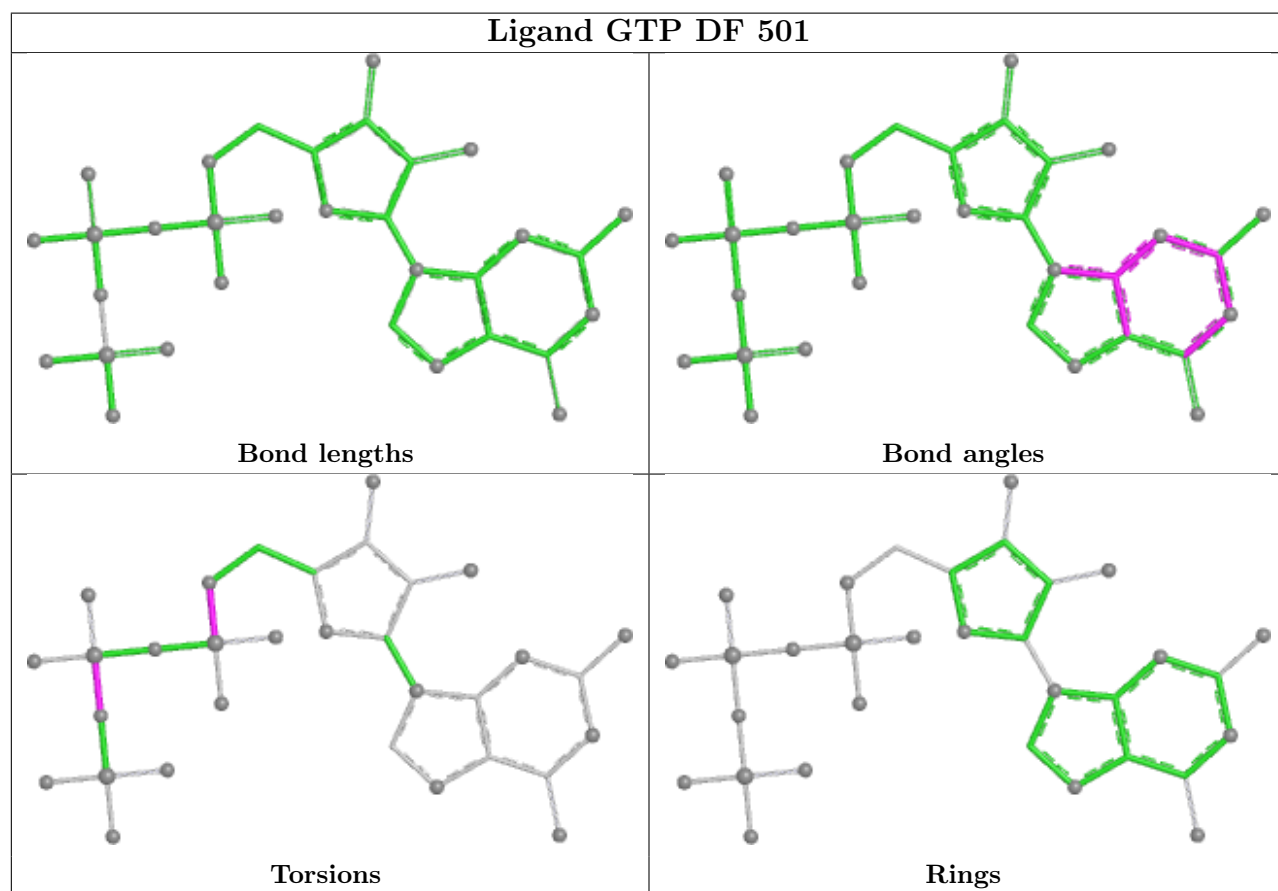
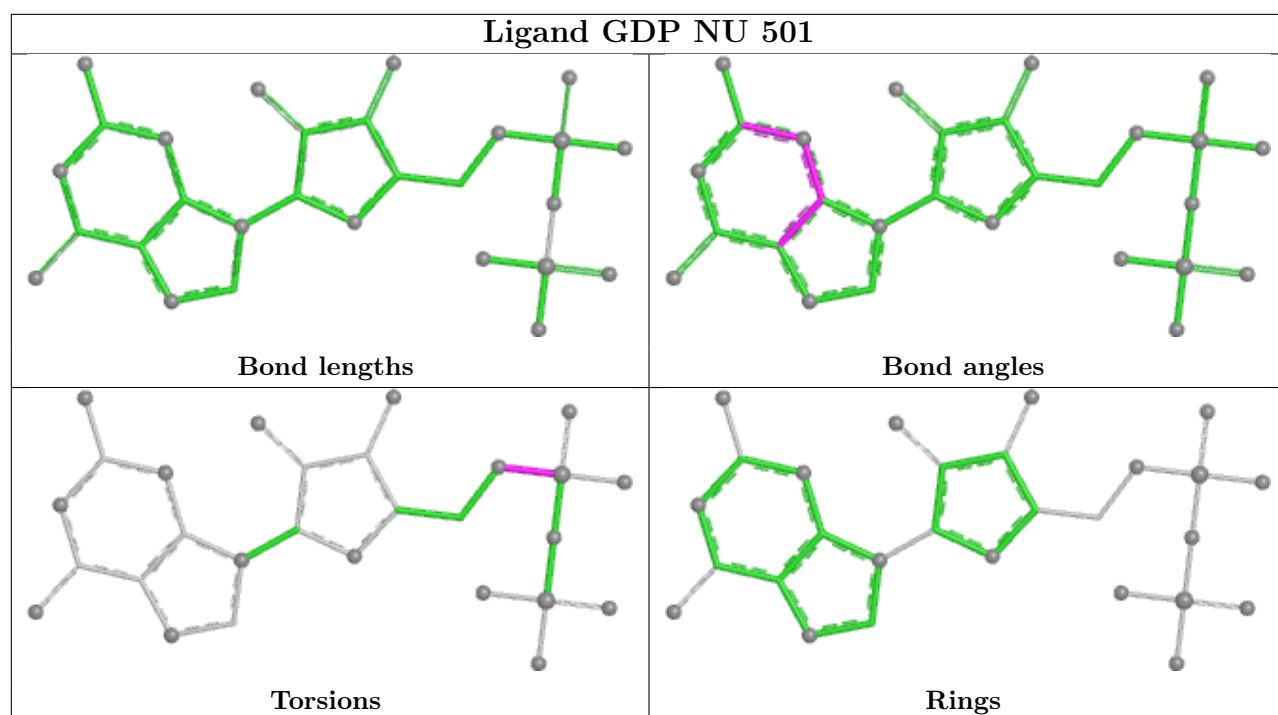
## Ligand GTP OL 602



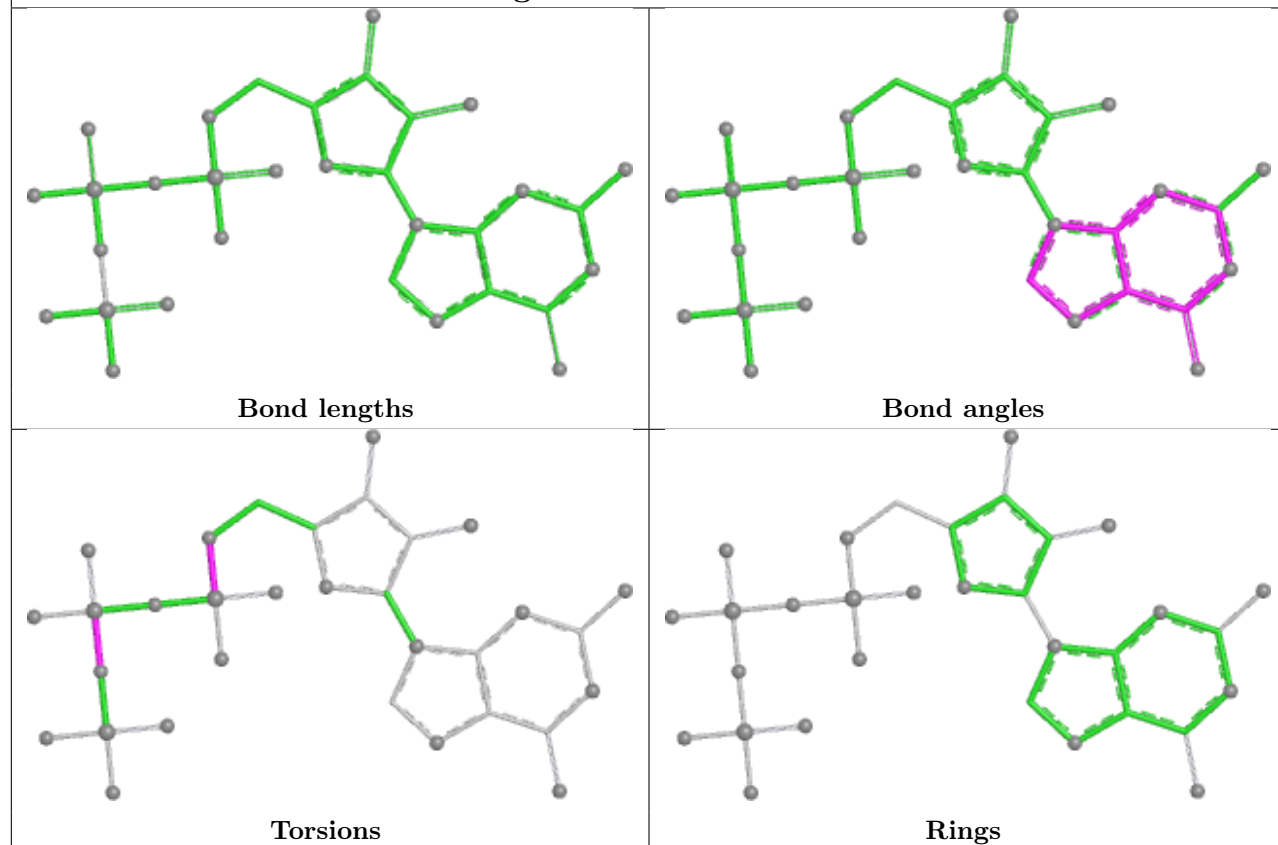
## Ligand GDP UX 501



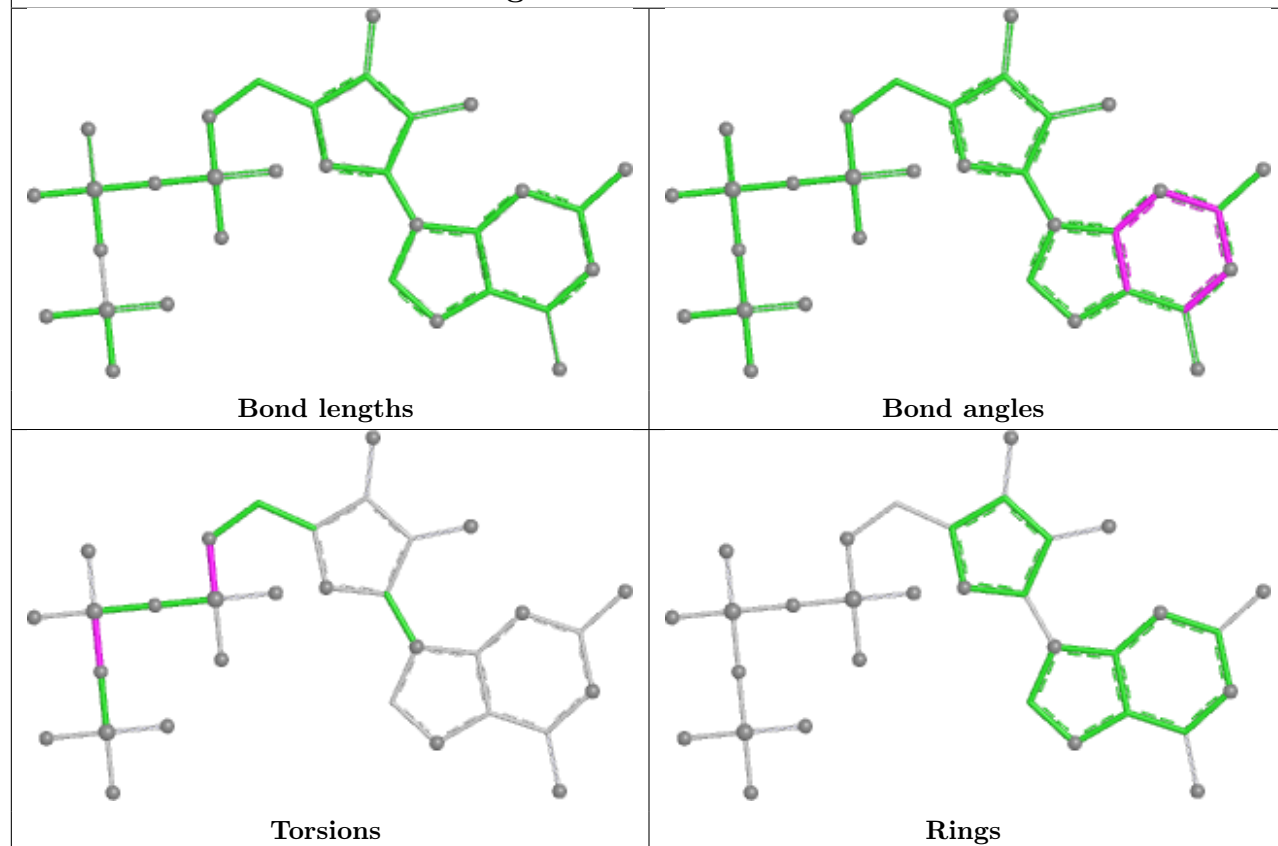




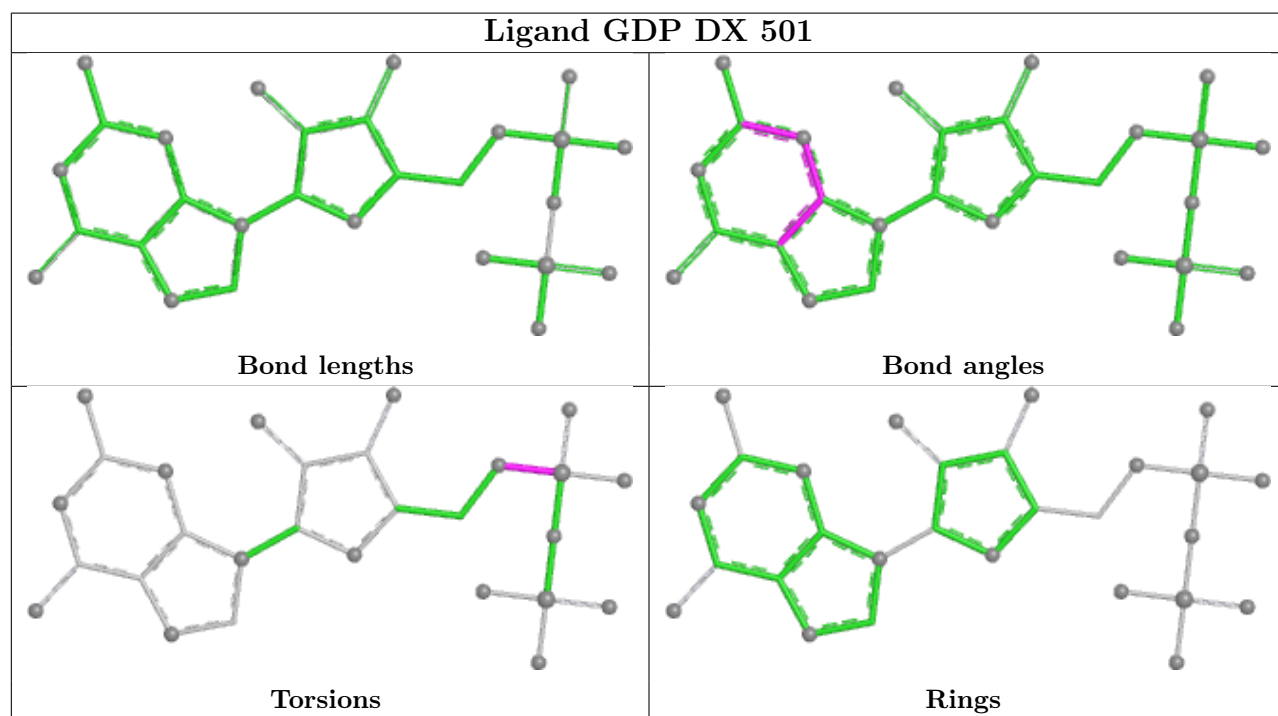
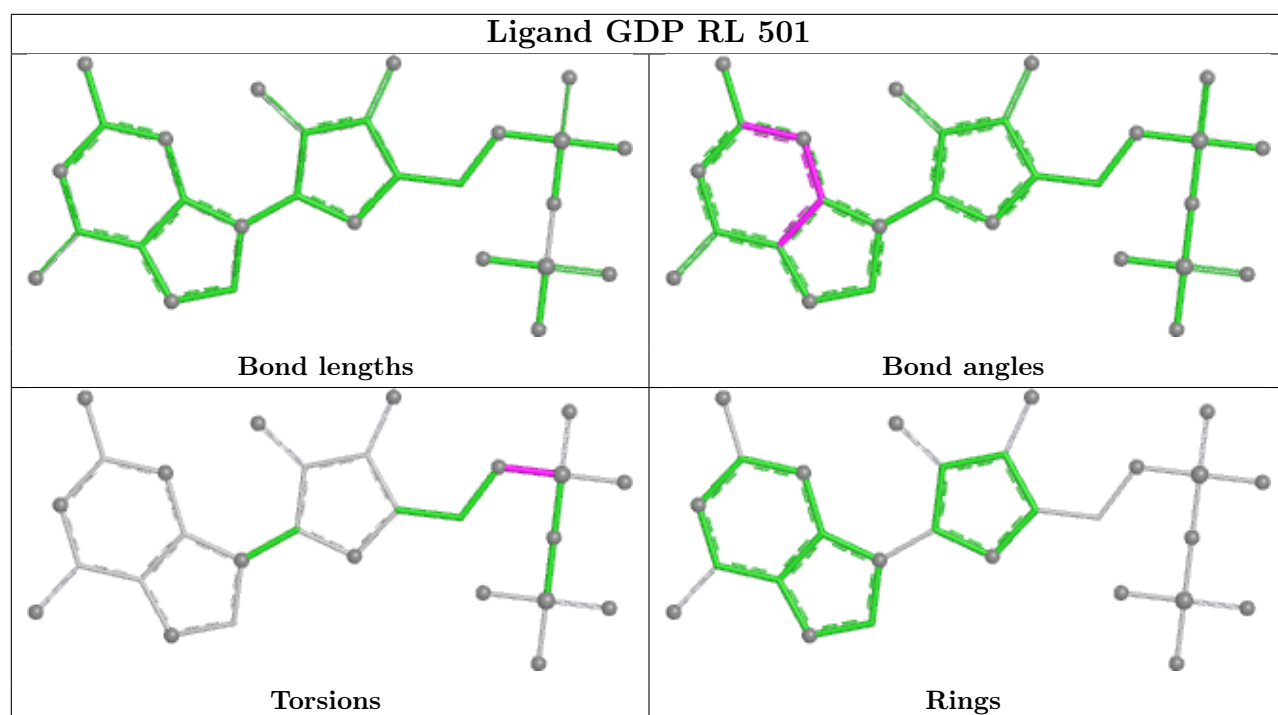
## Ligand GTP WE 602



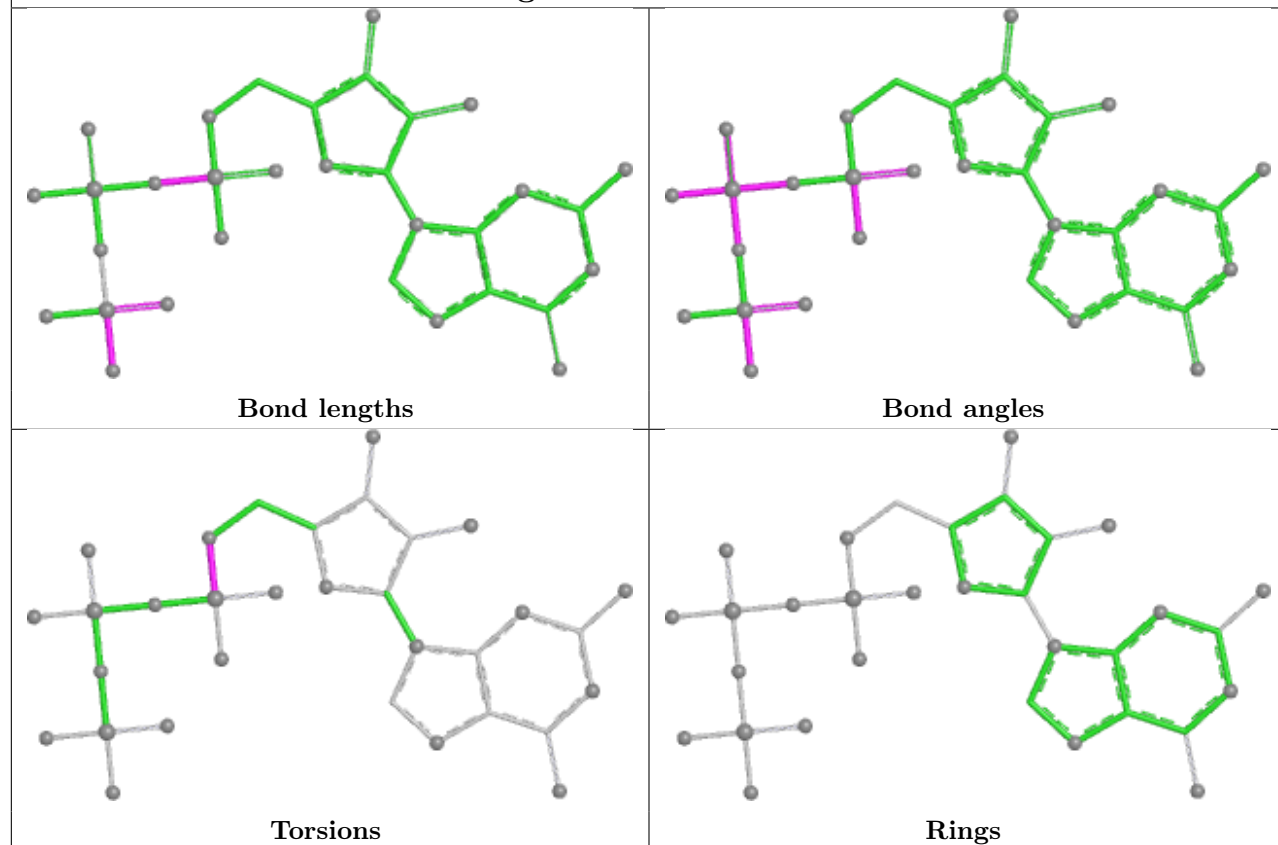
## Ligand GTP WW 501



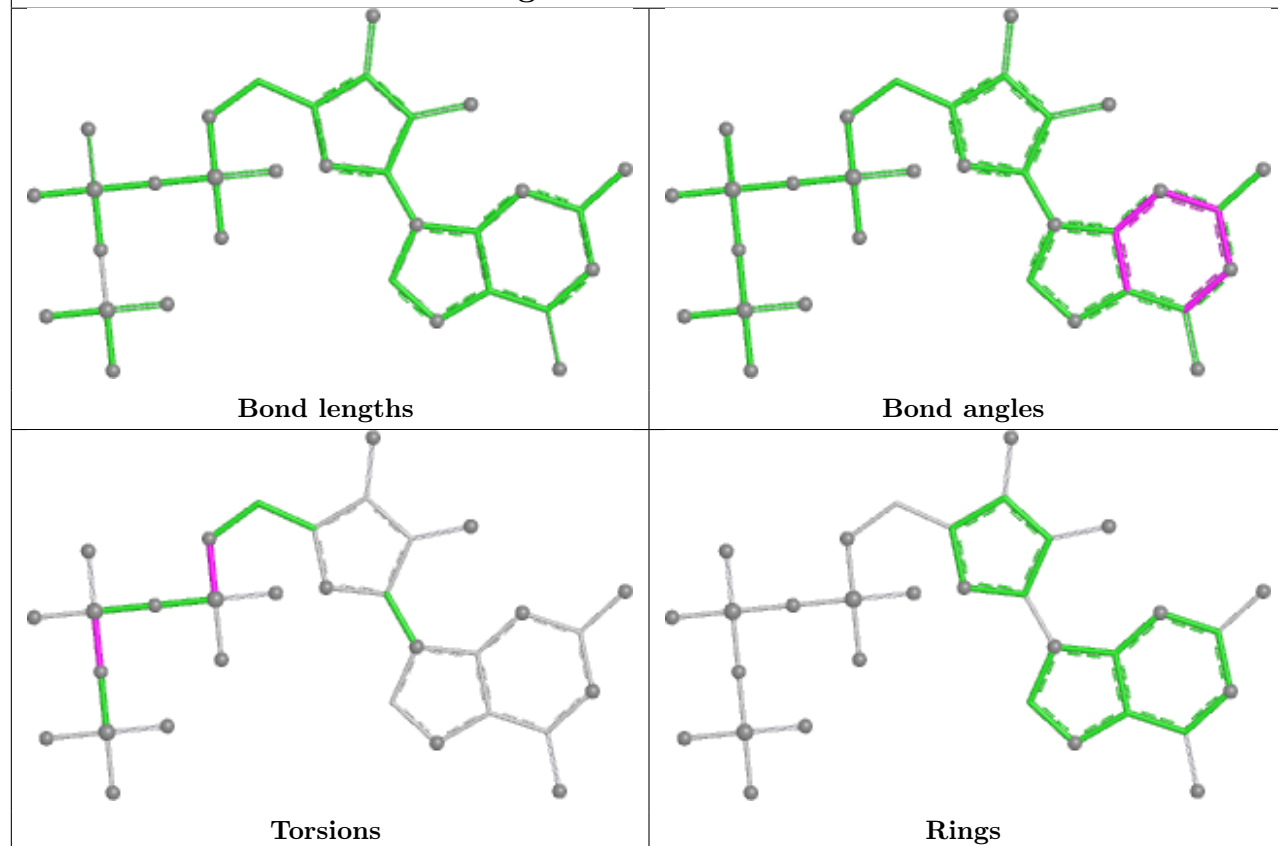


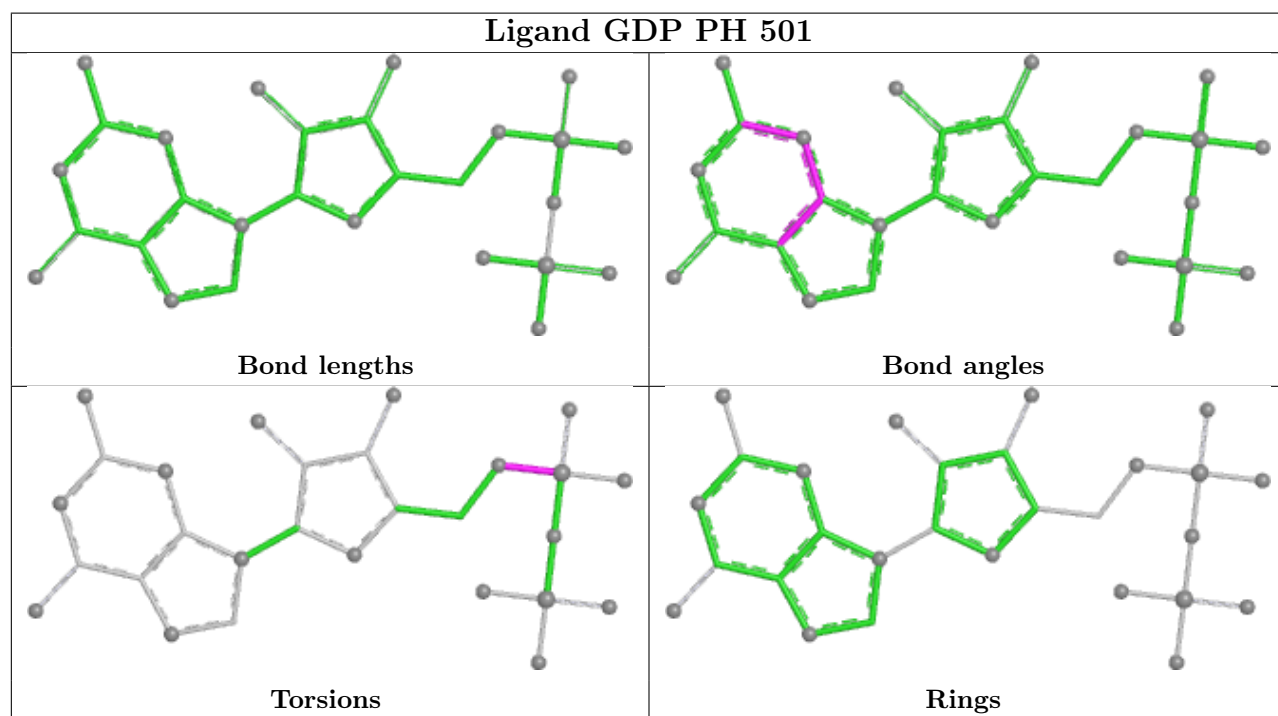
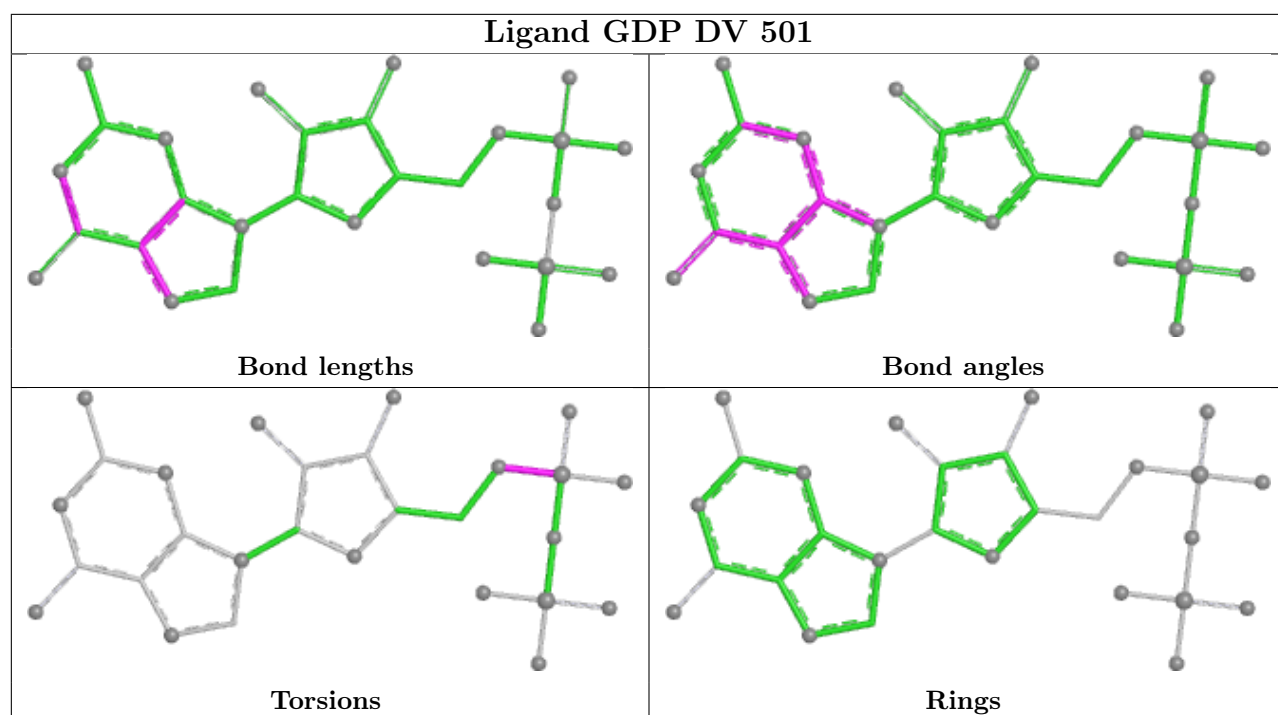


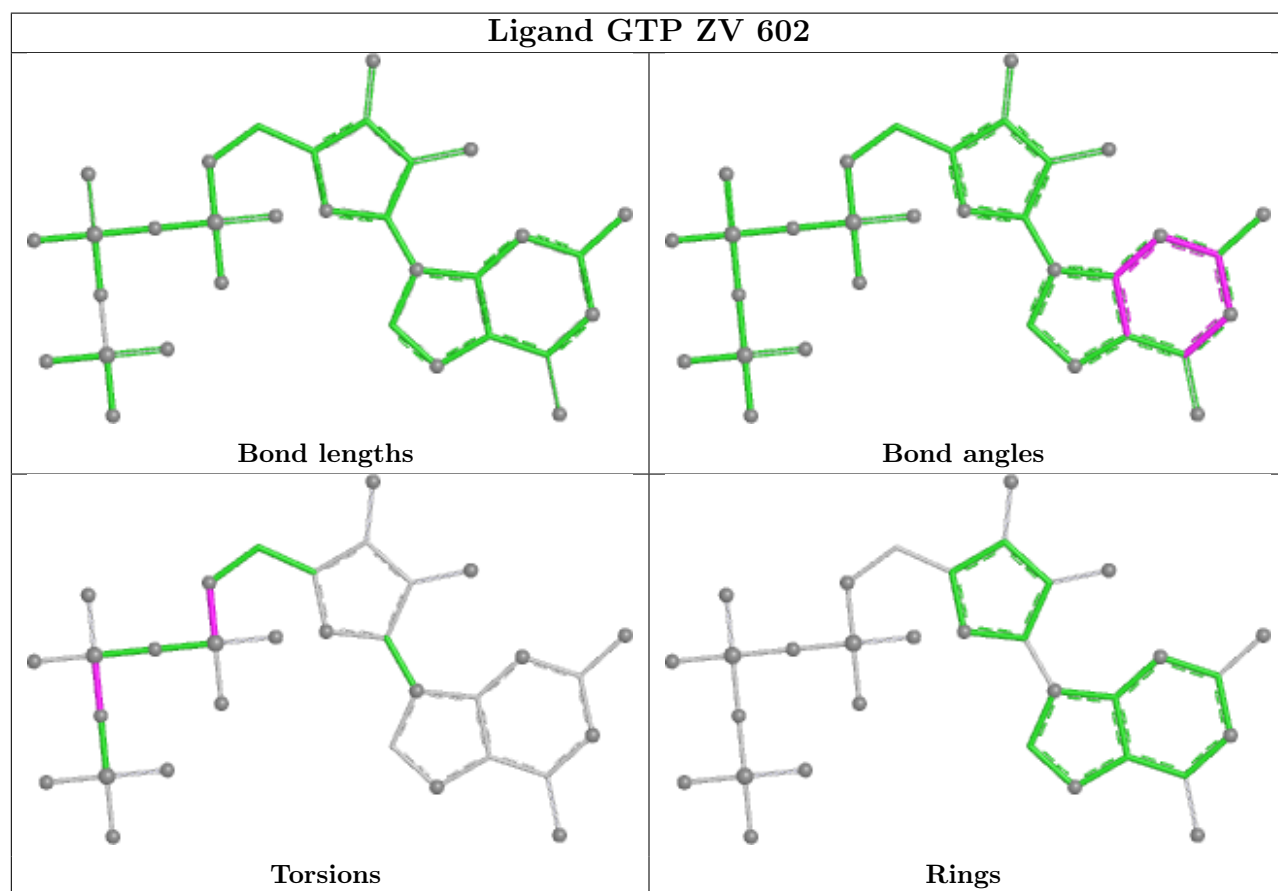
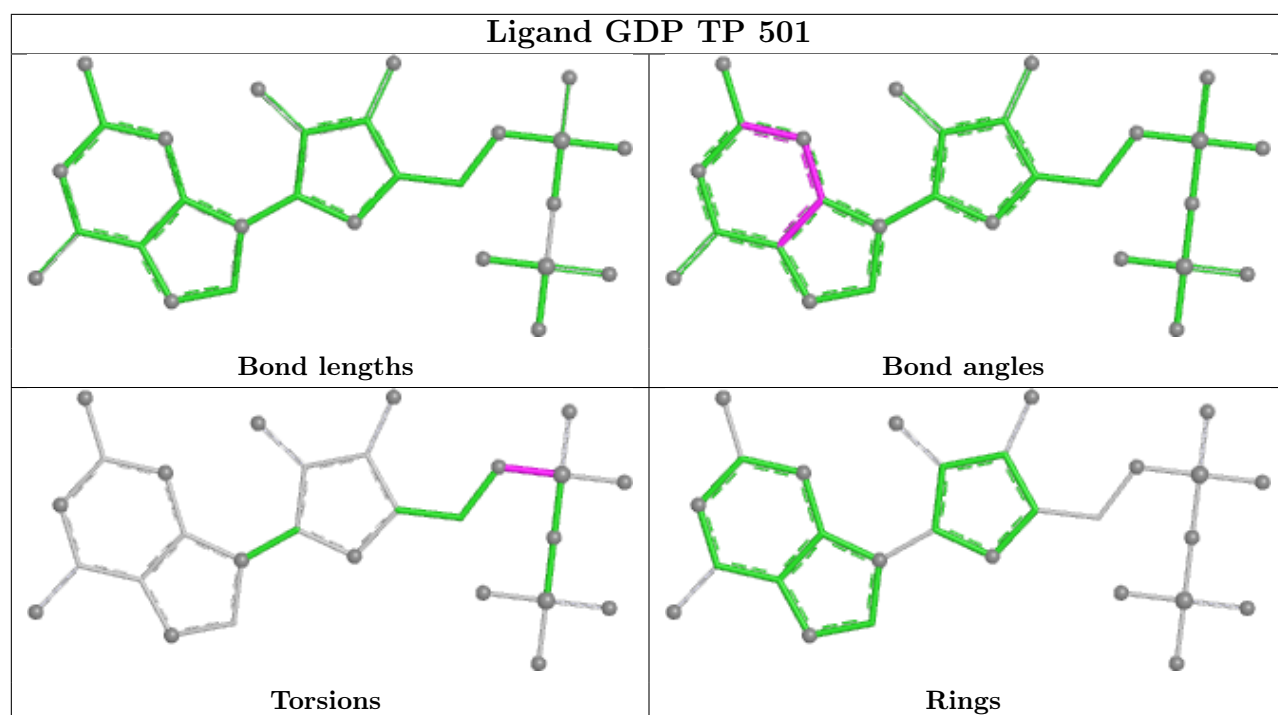
## Ligand GTP VC 501

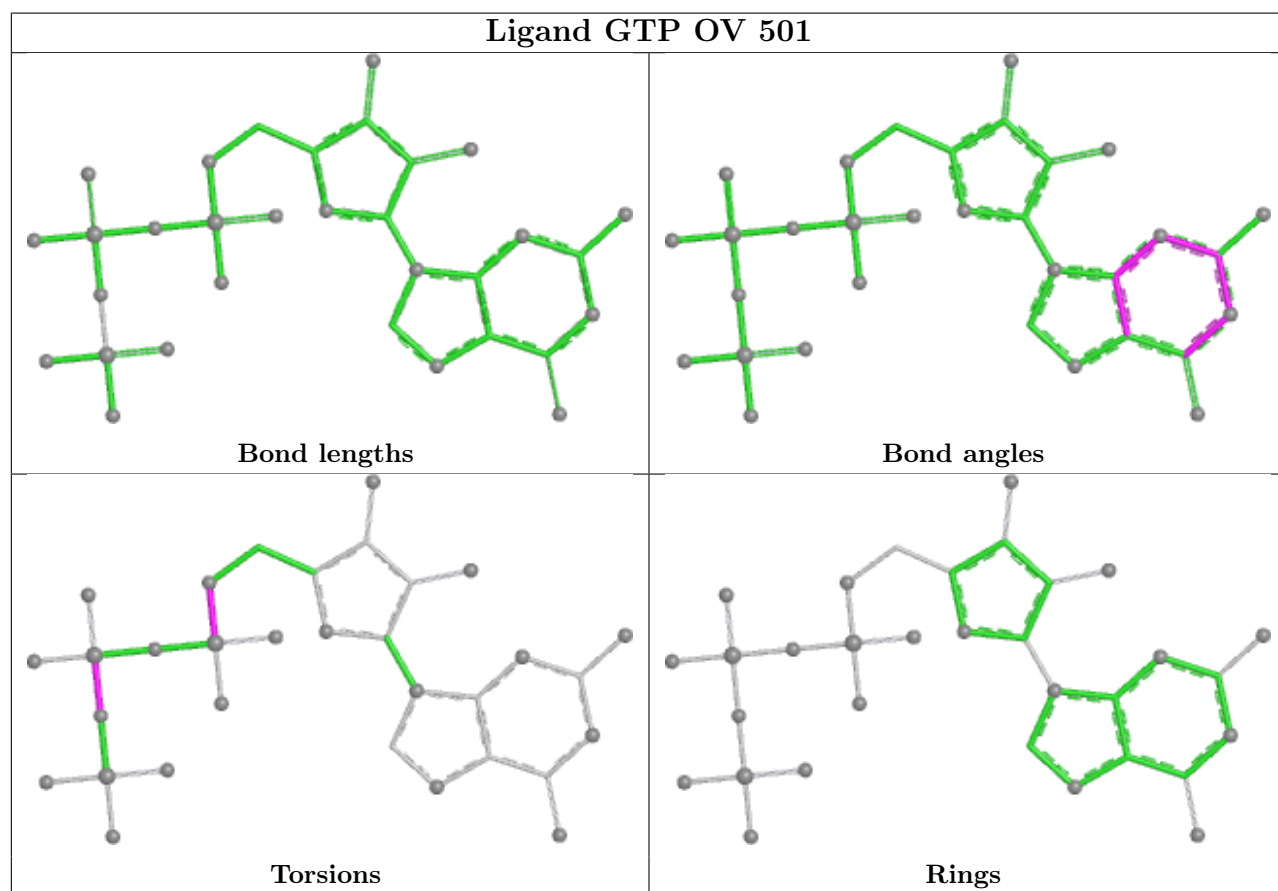
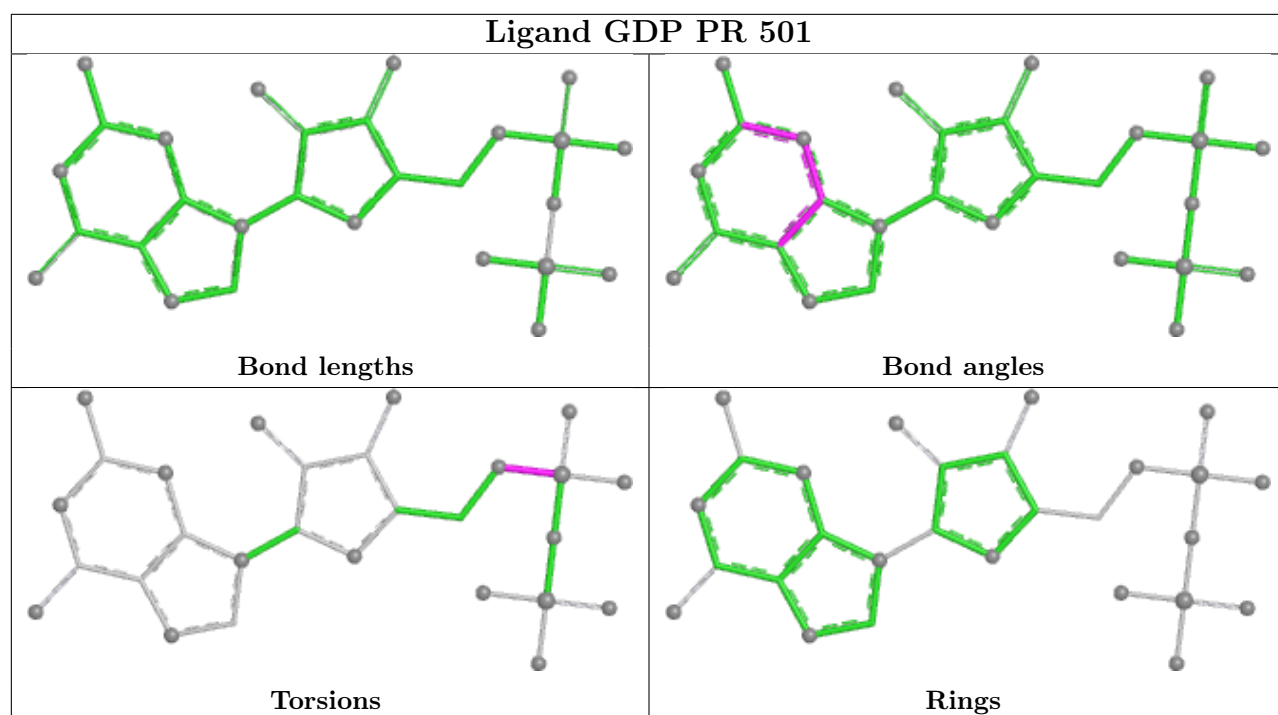


## Ligand GTP OP 501

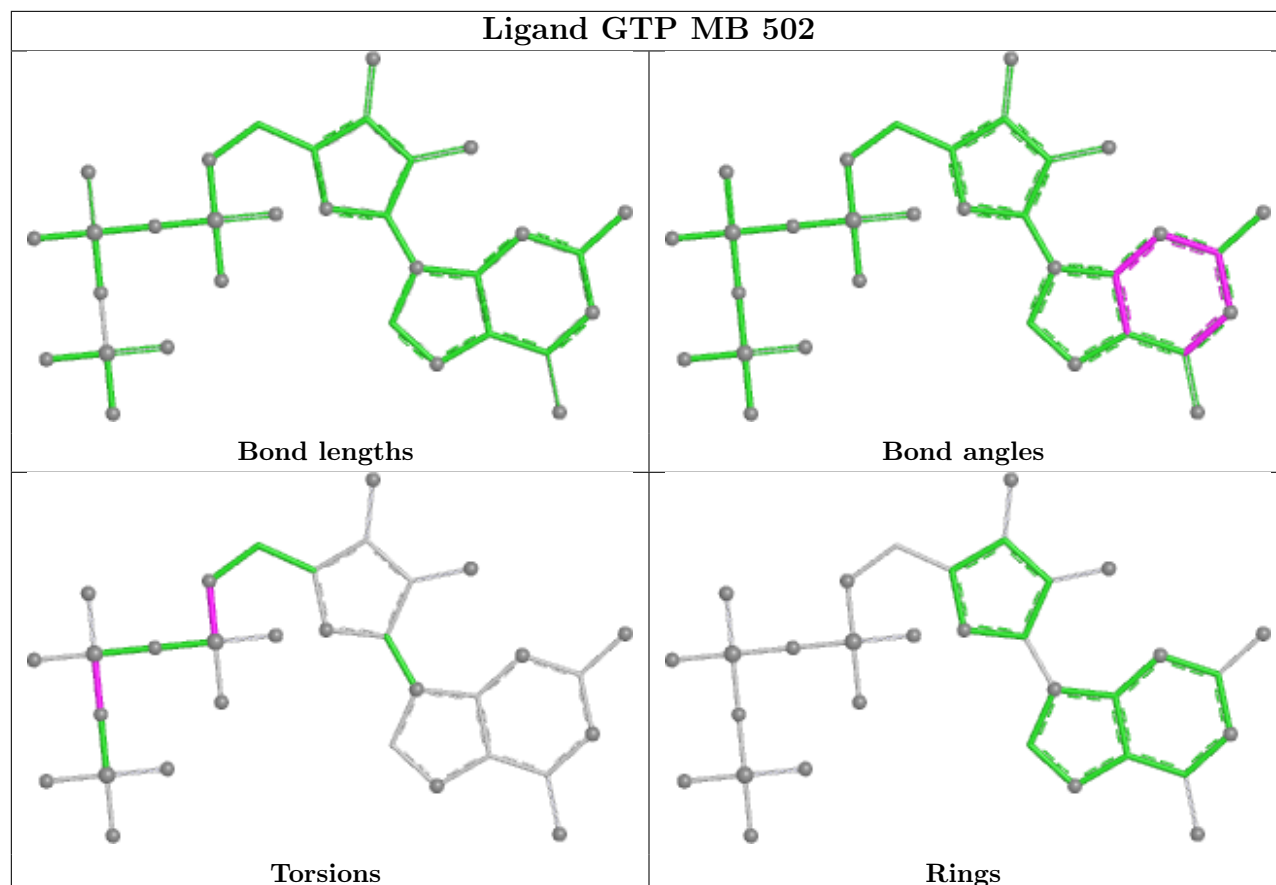




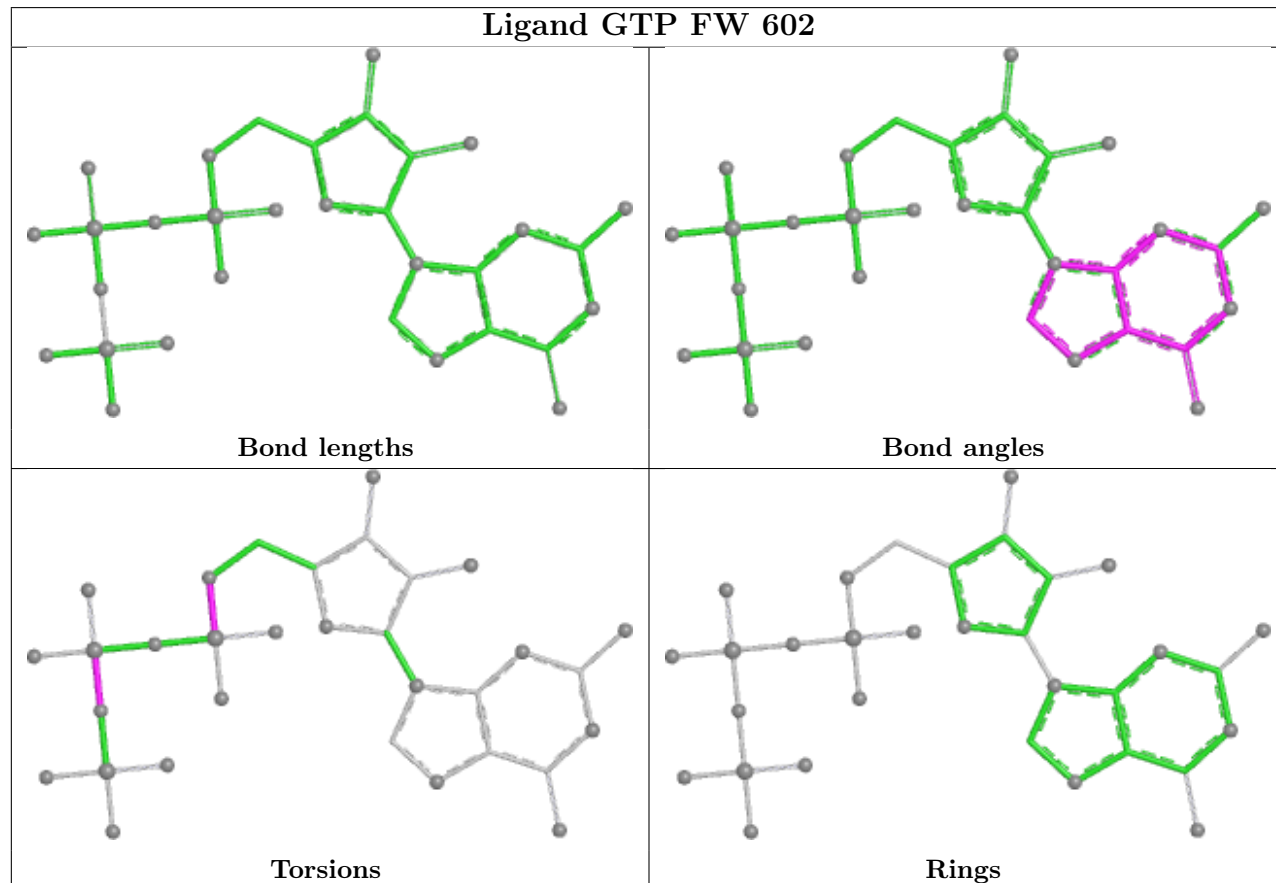


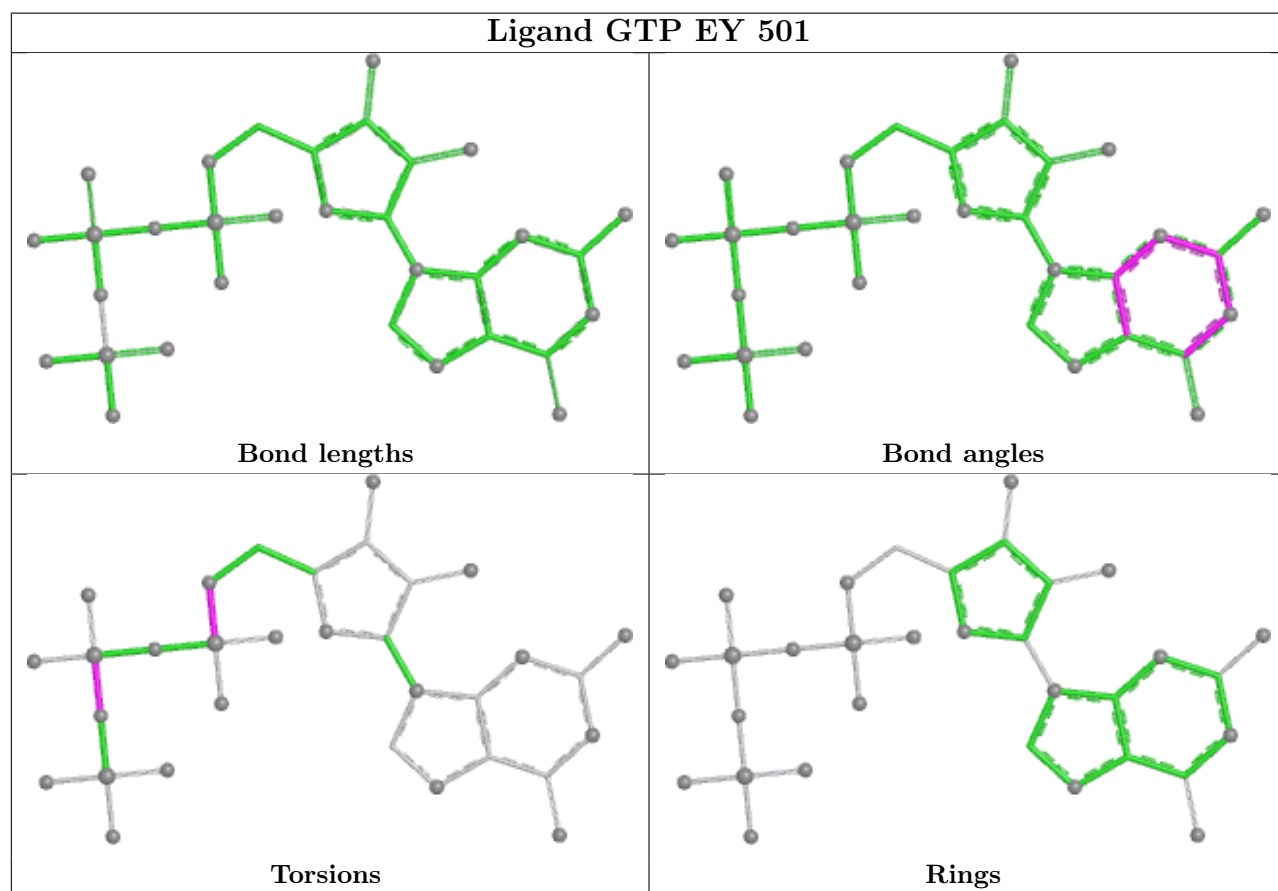
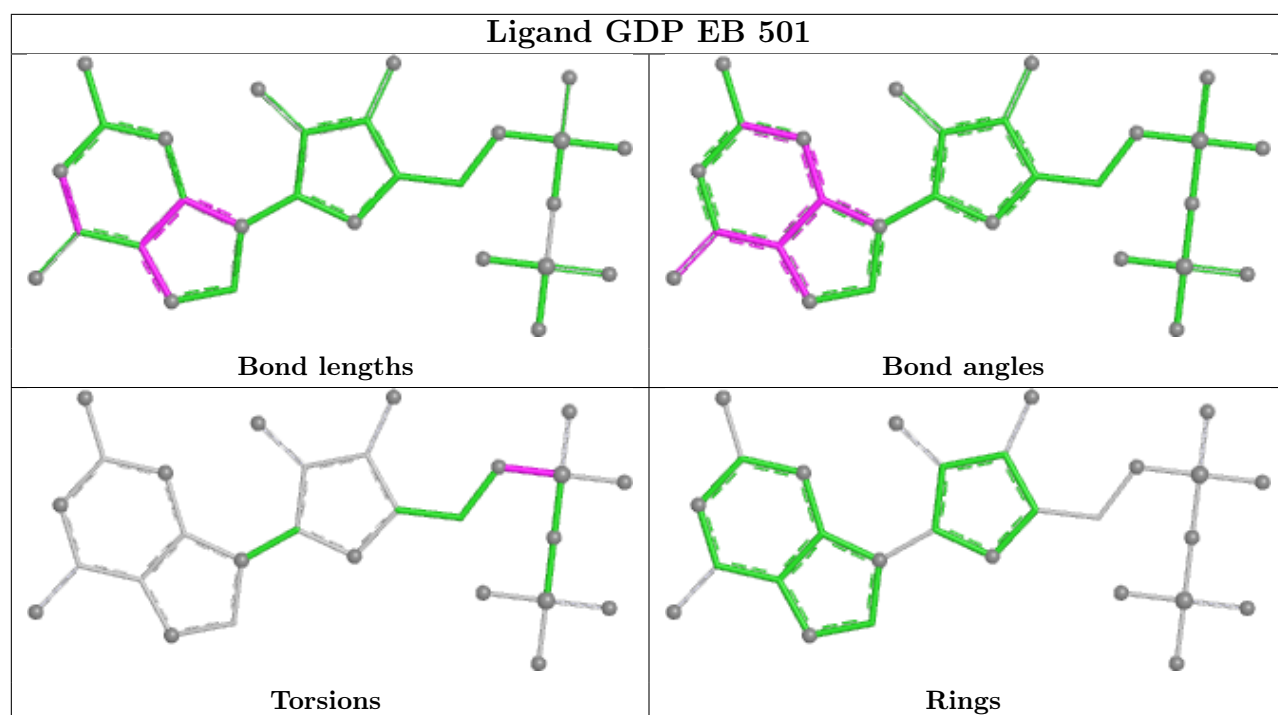


## Ligand GTP MB 502

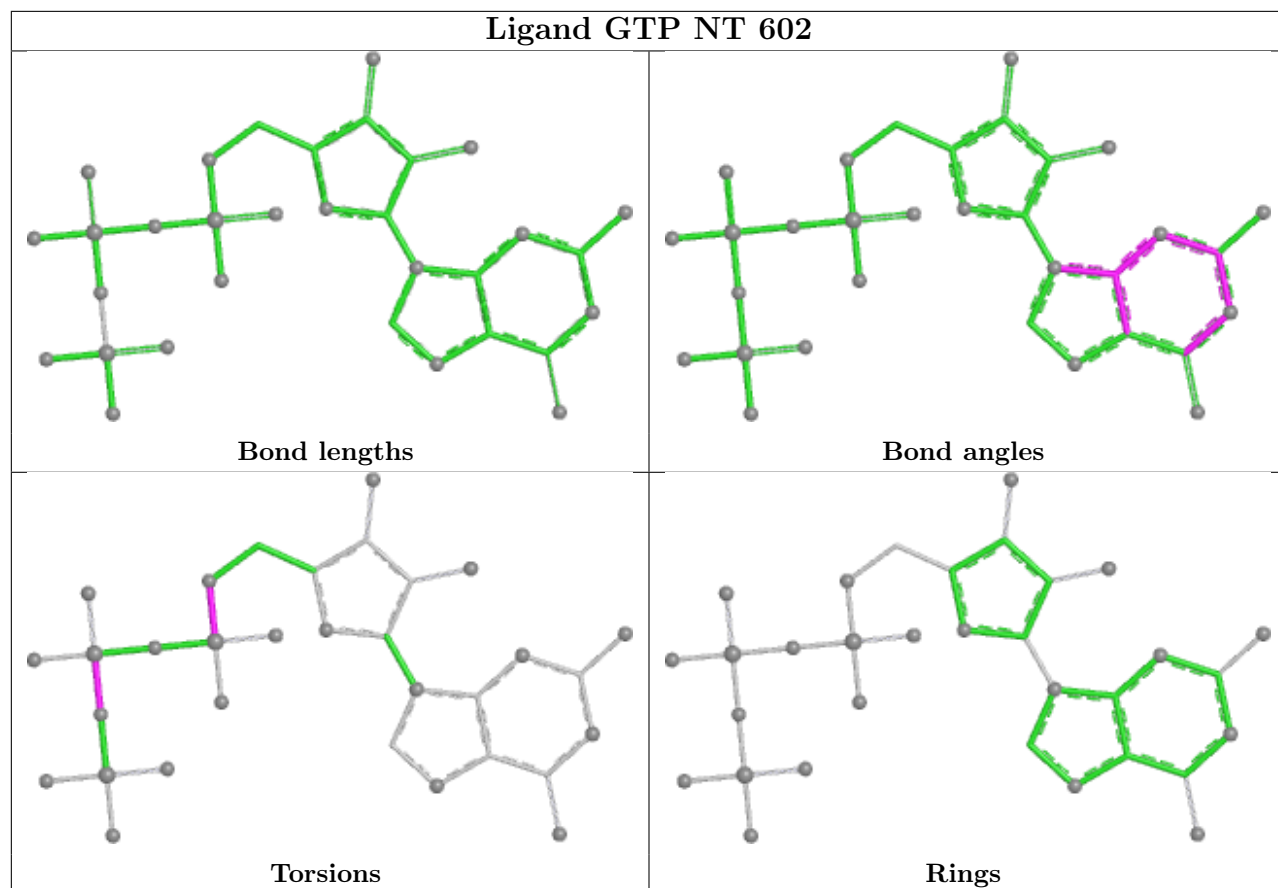


## Ligand GTP FW 602

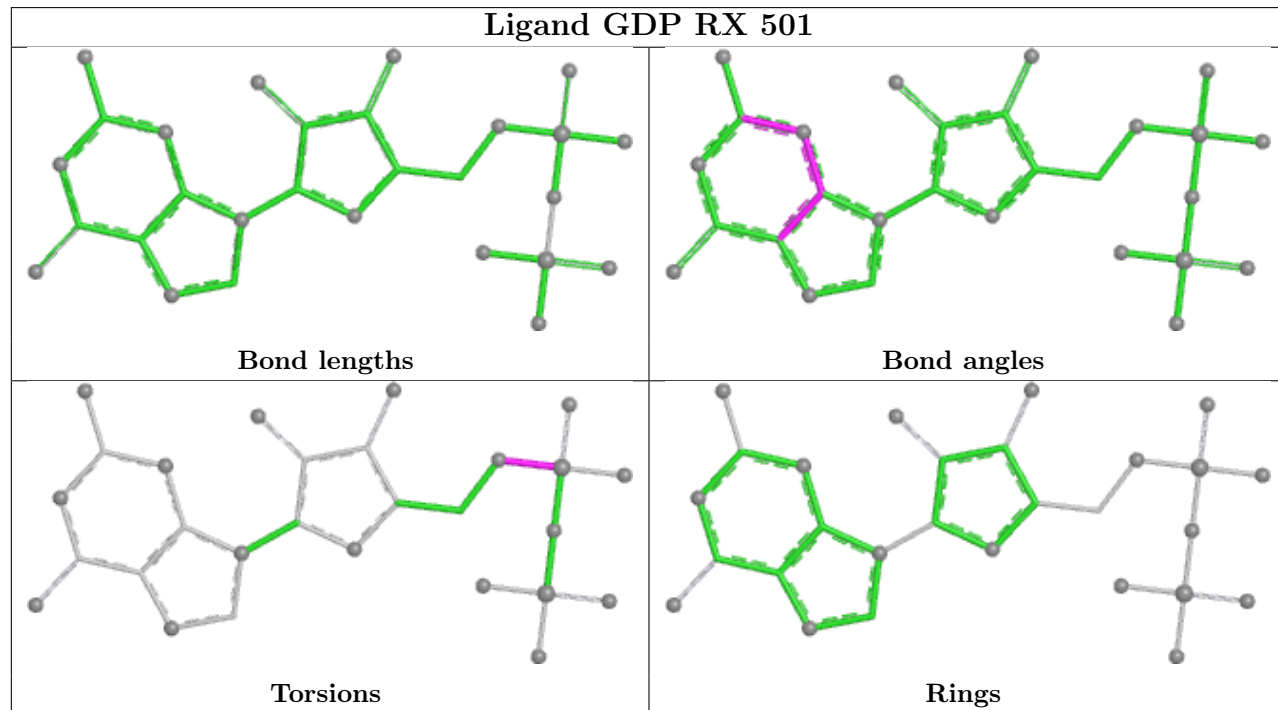




## Ligand GTP NT 602

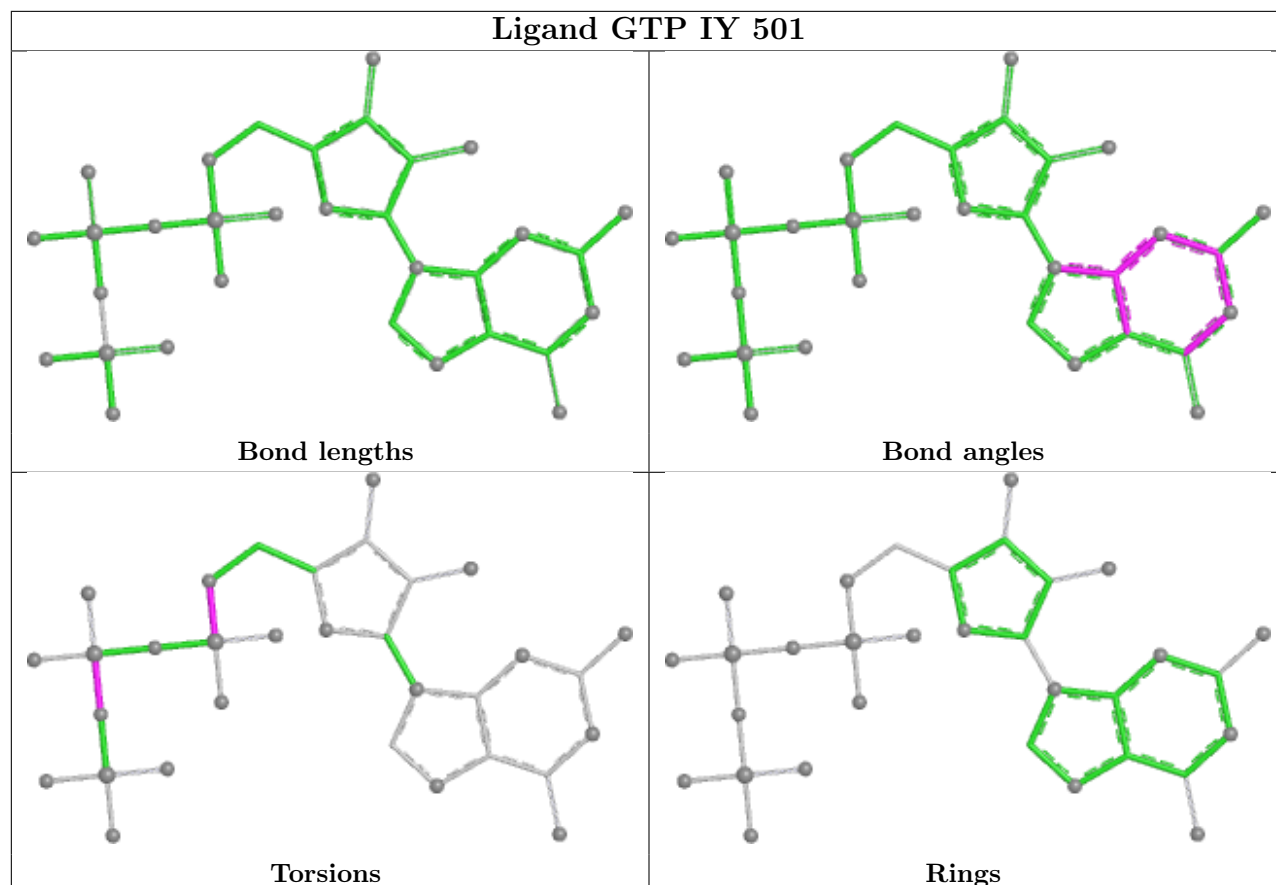


## Ligand GDP RX 501

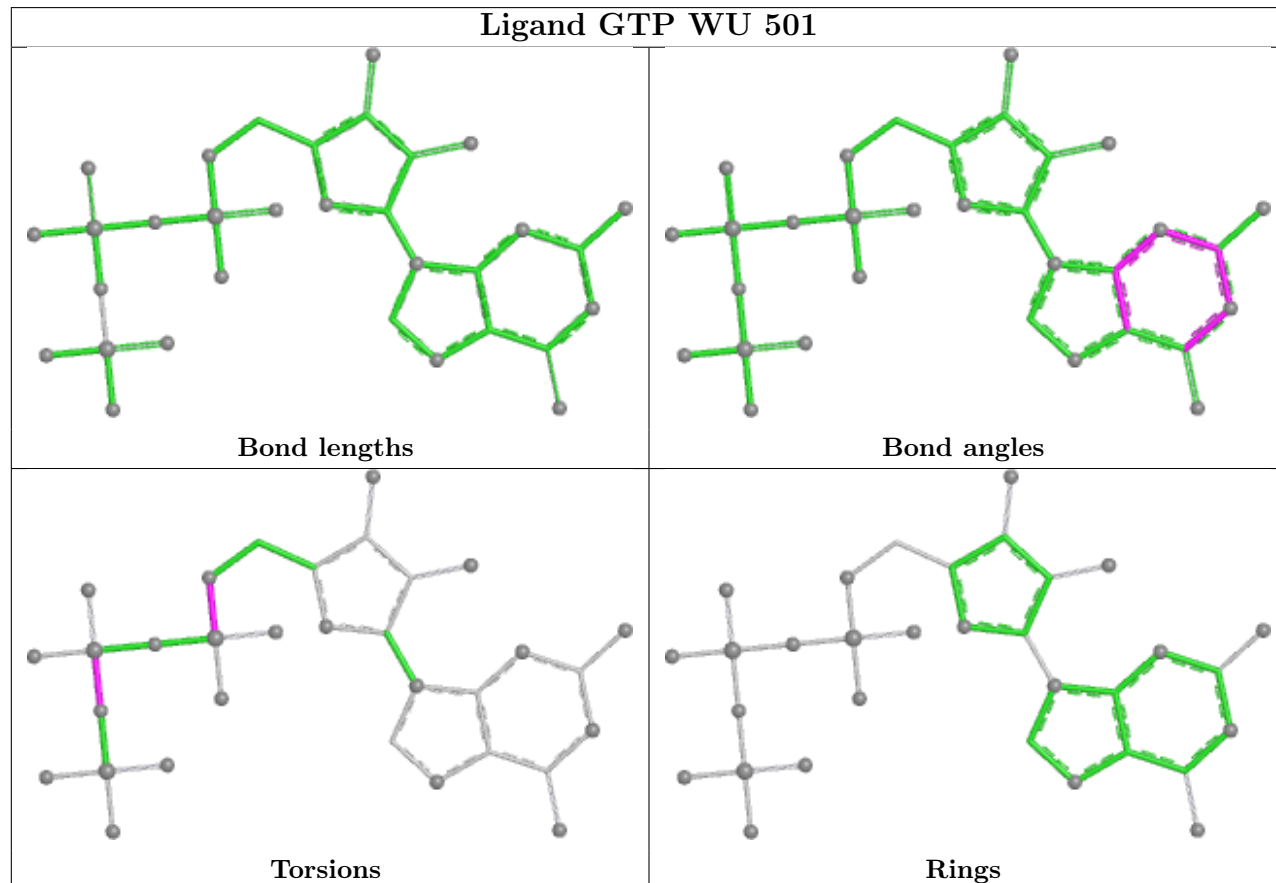


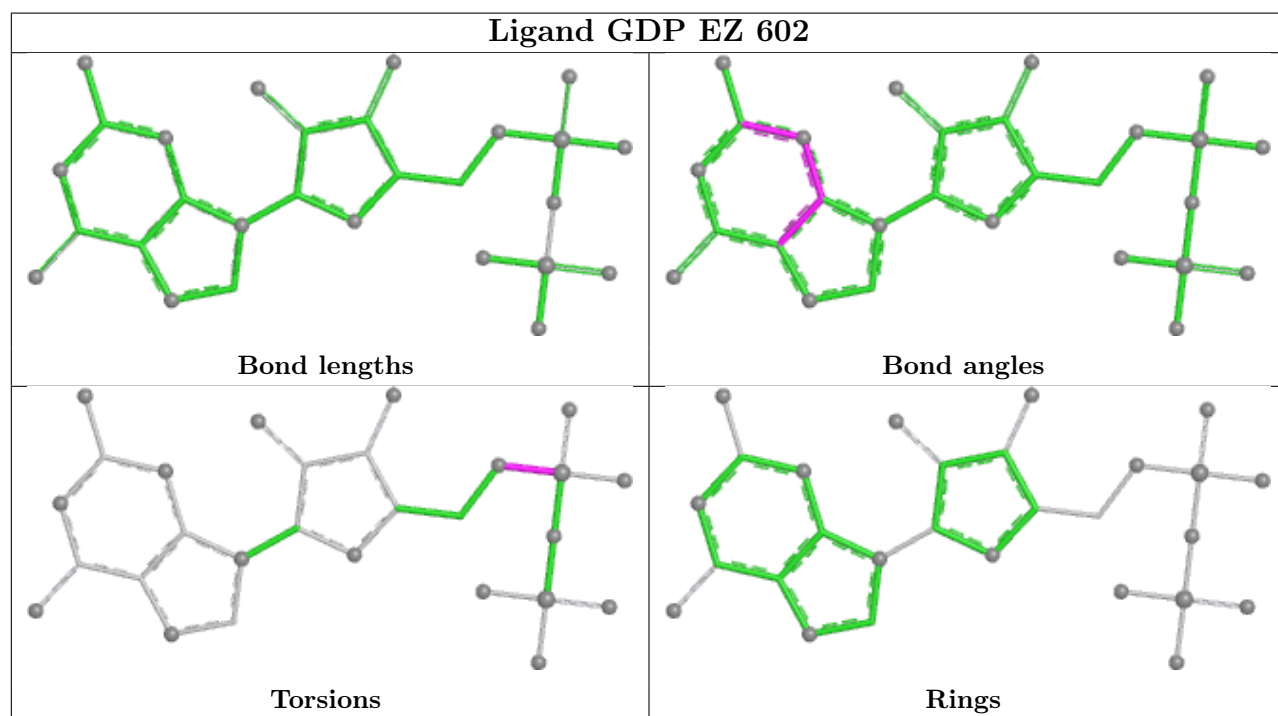
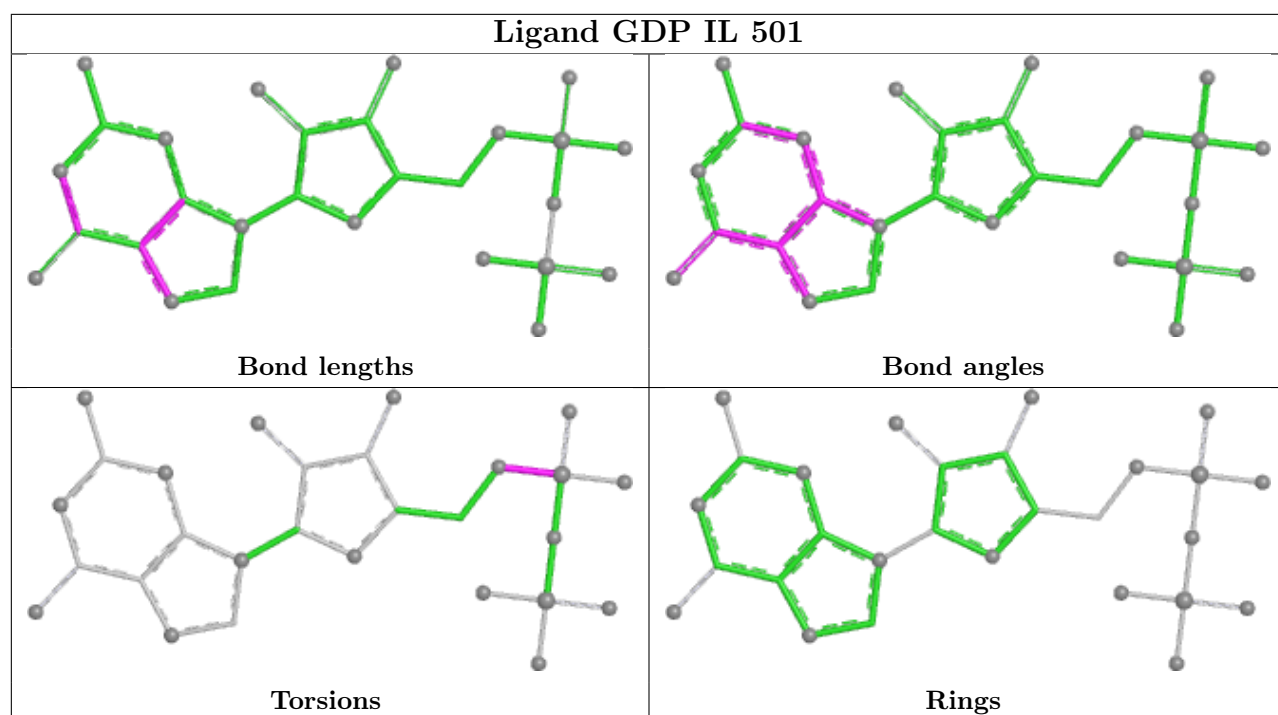


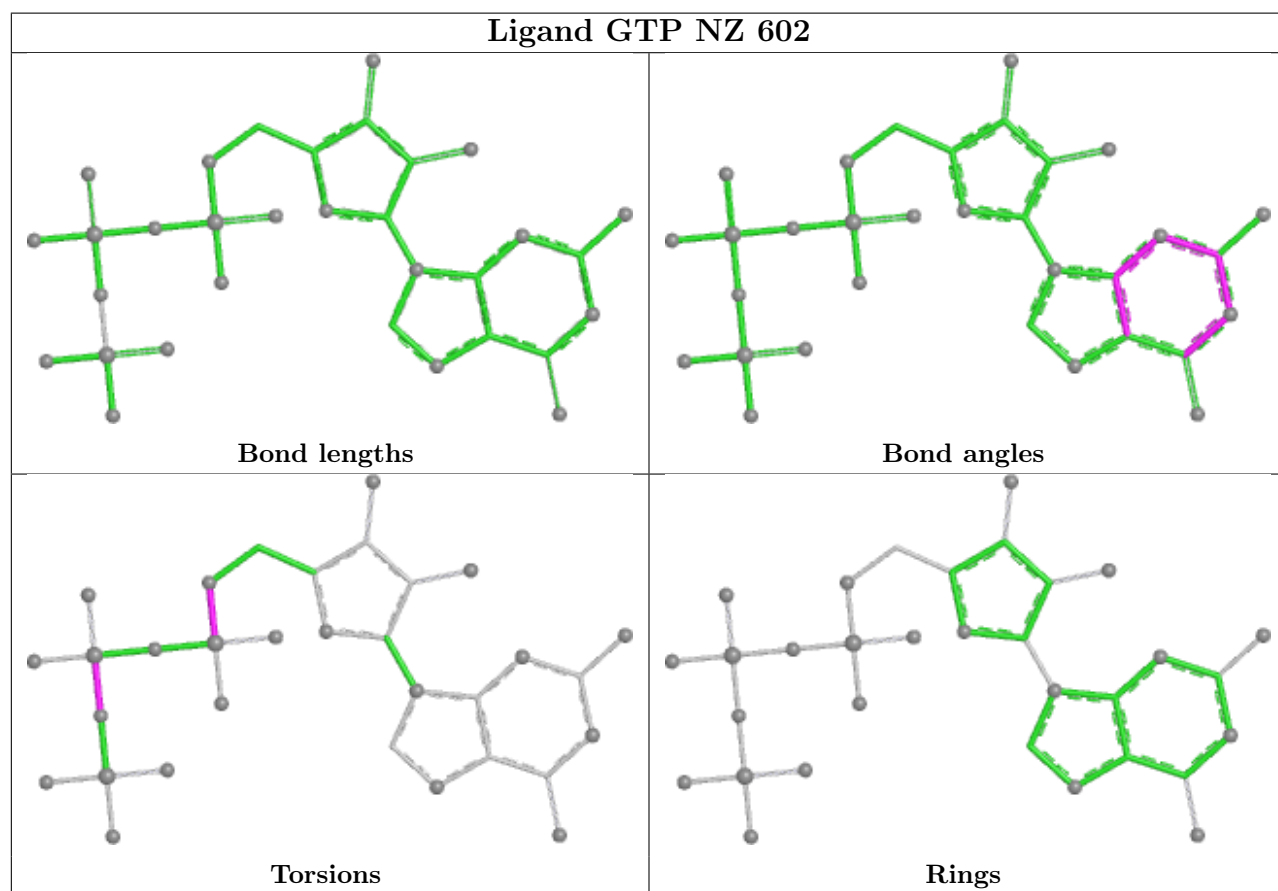
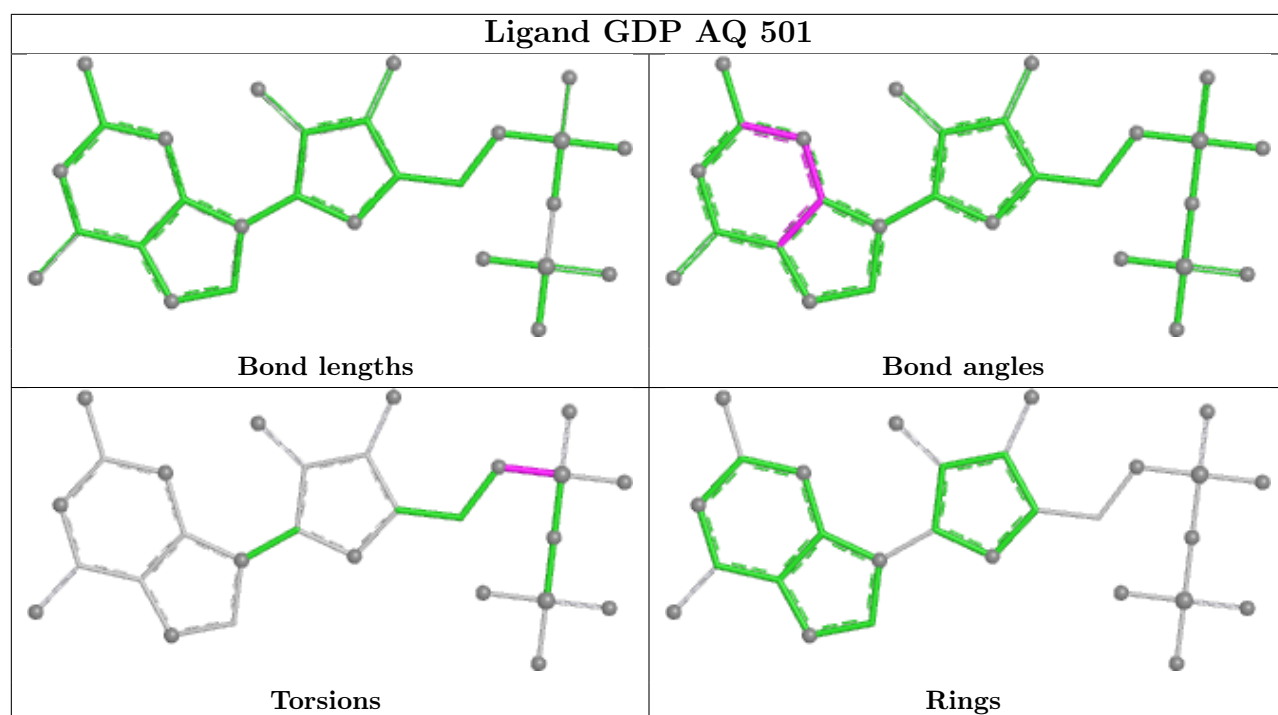
## Ligand GTP IY 501

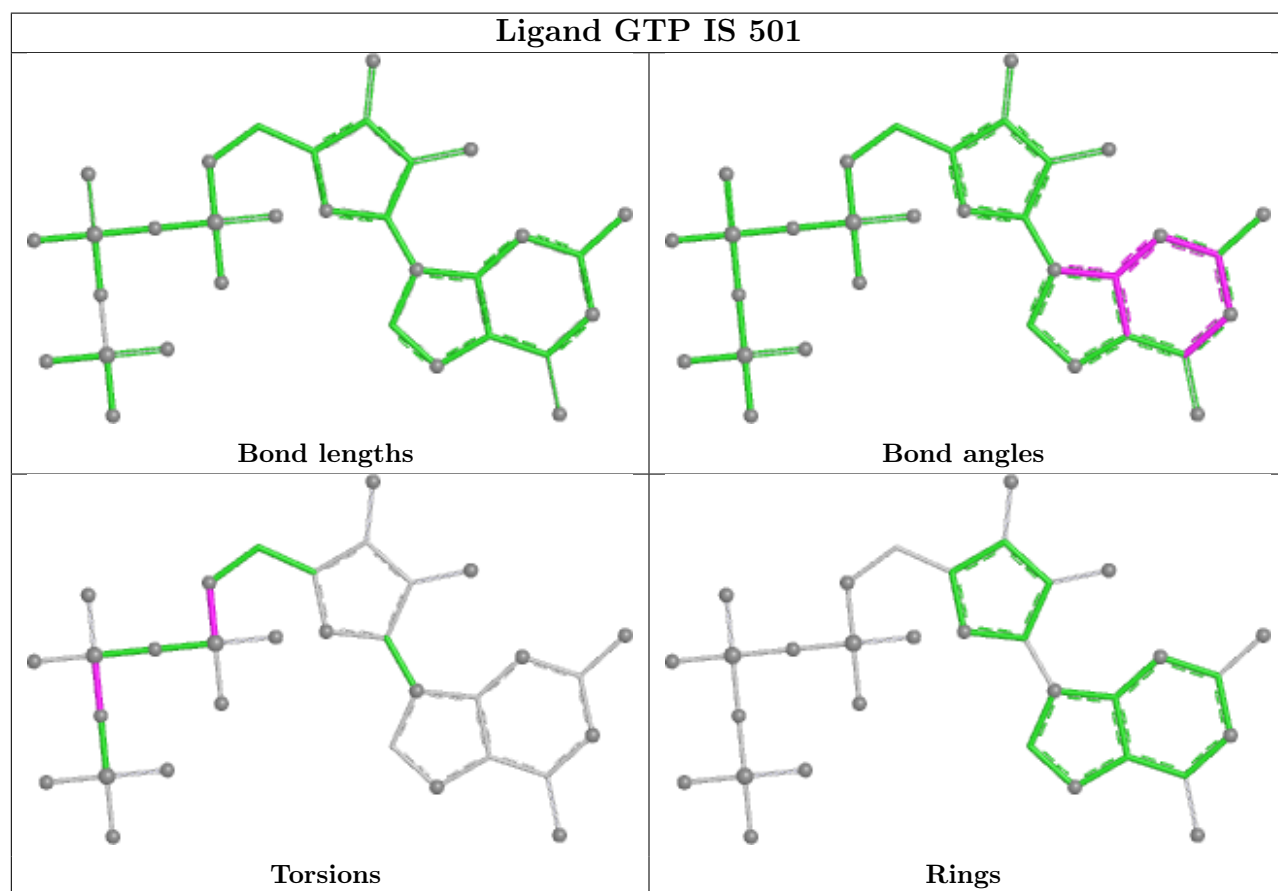
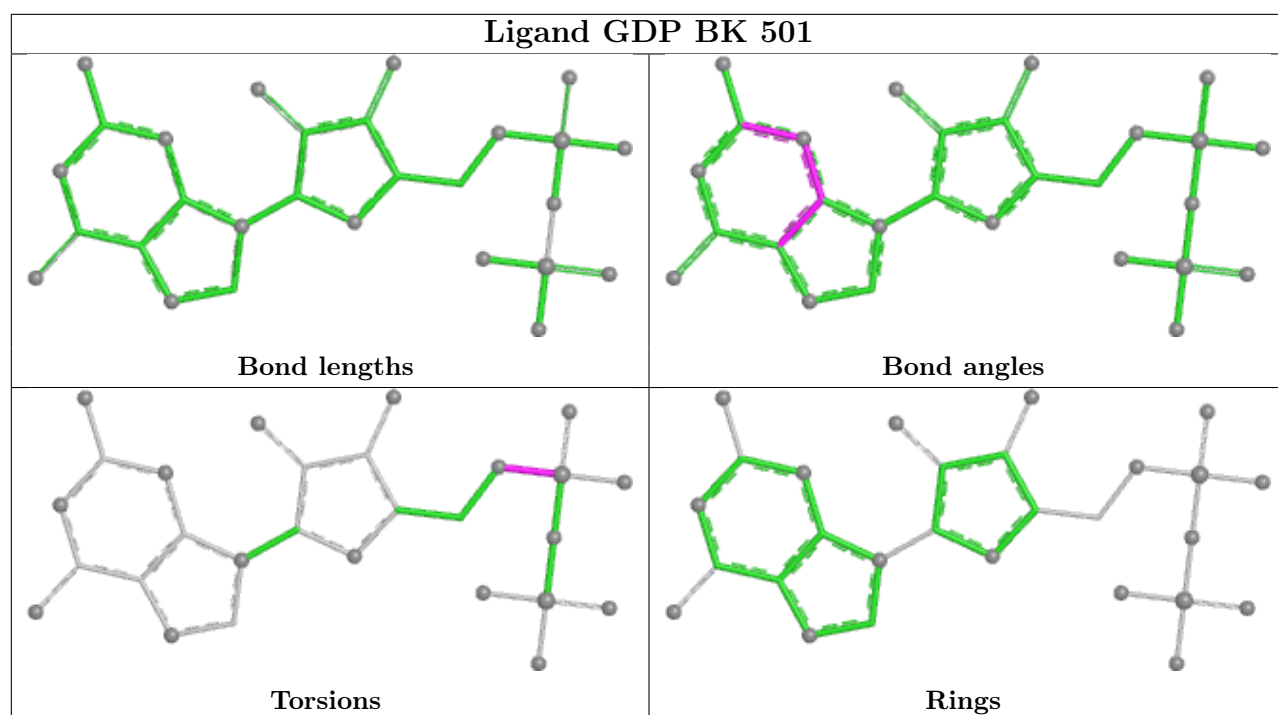


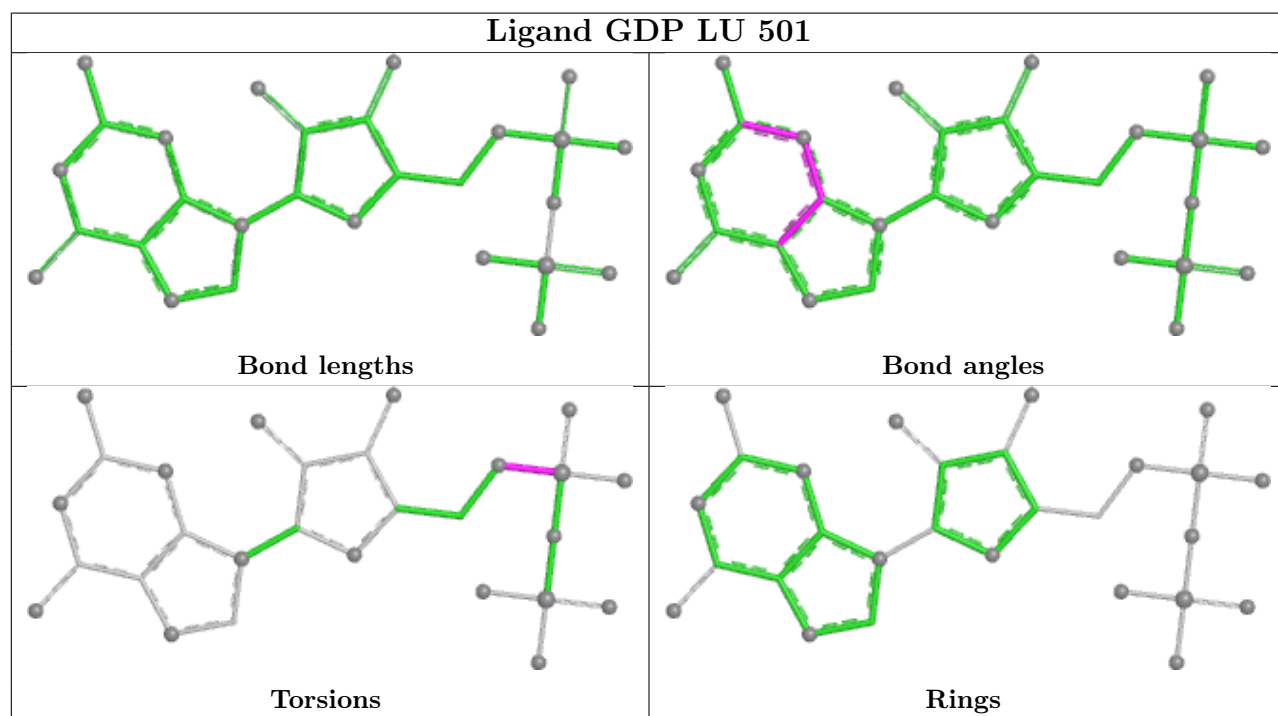
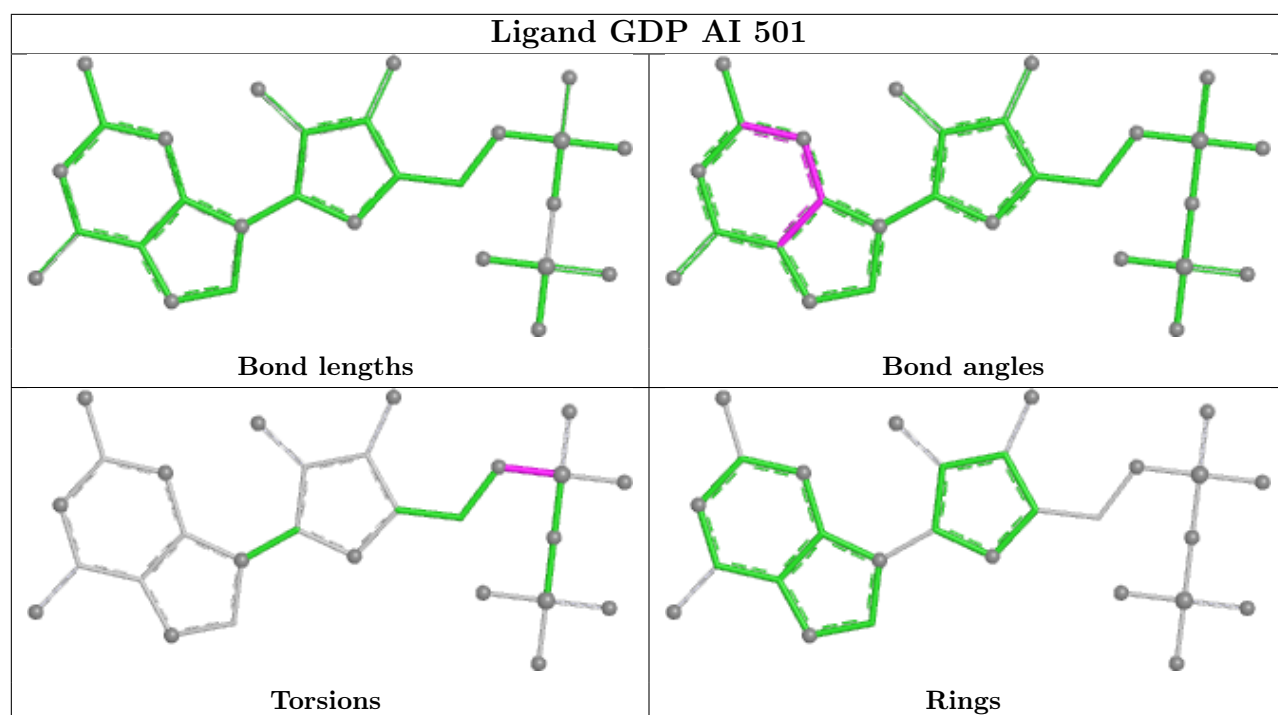
## Ligand GTP WU 501



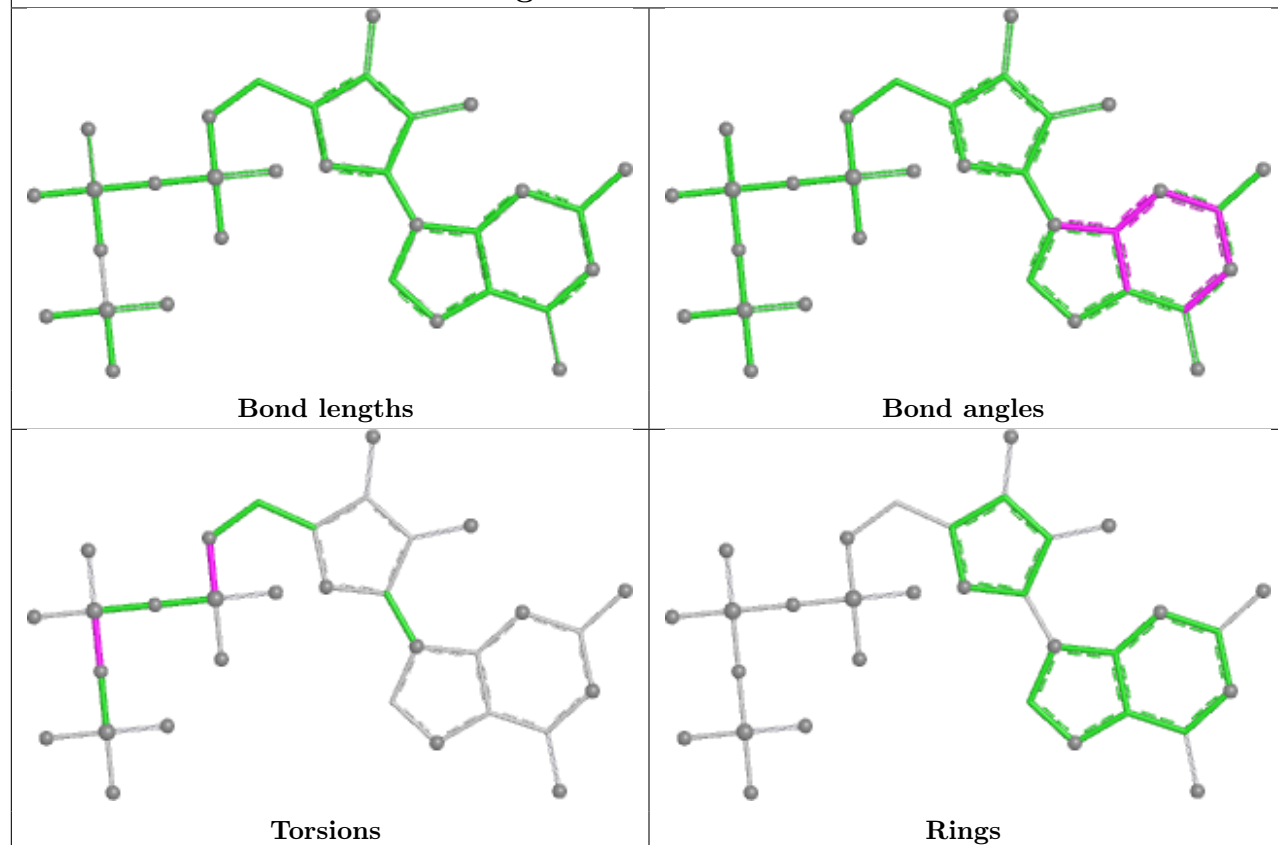




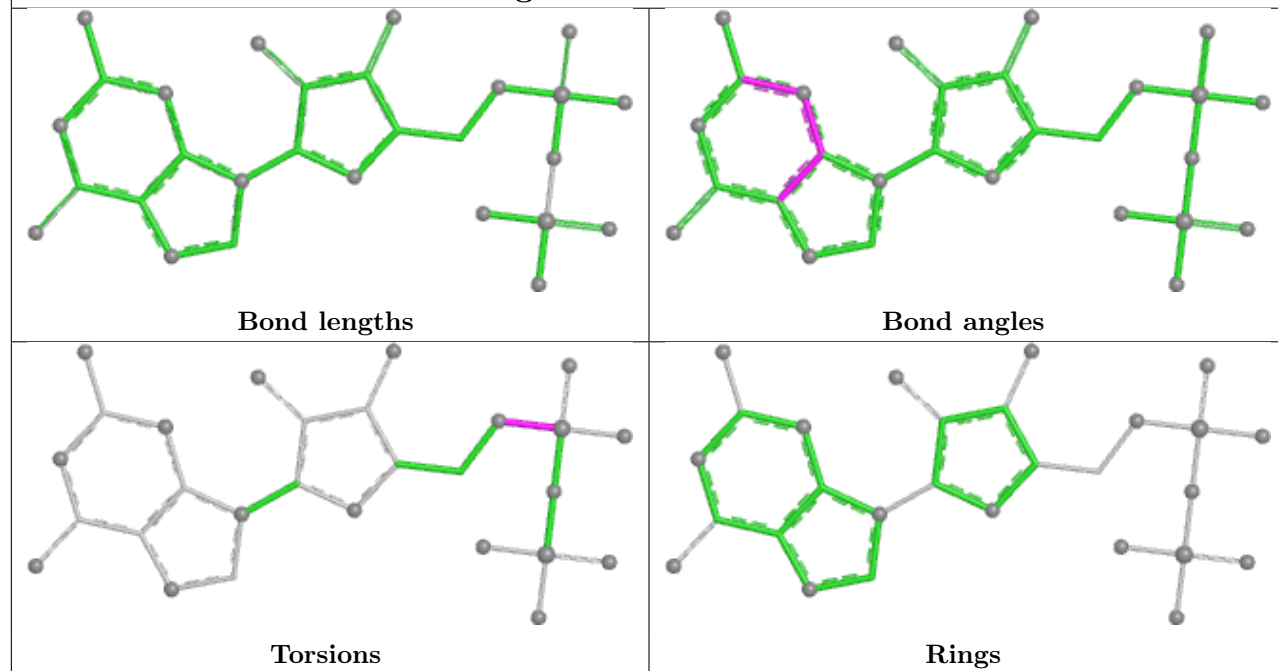


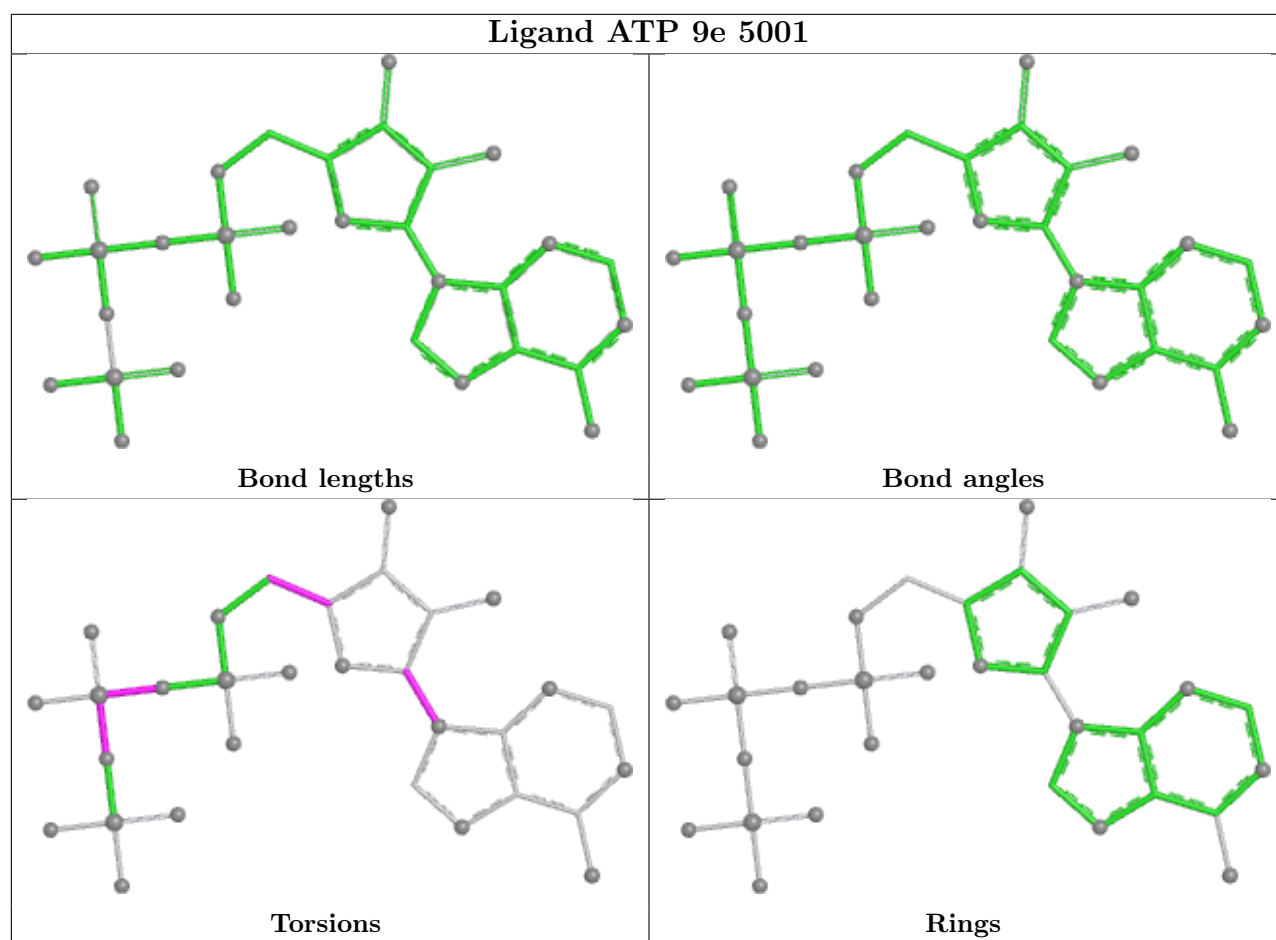


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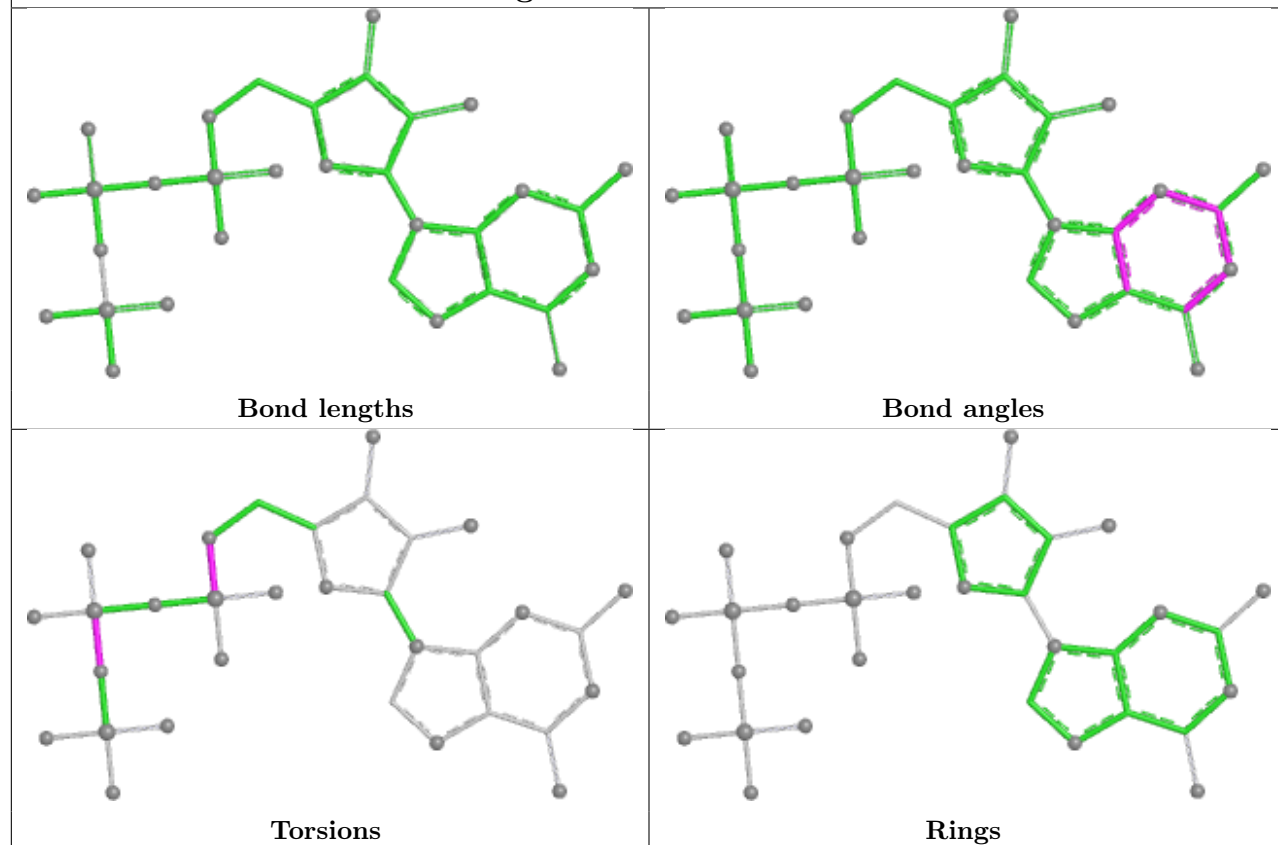


## Ligand GDP NC 501

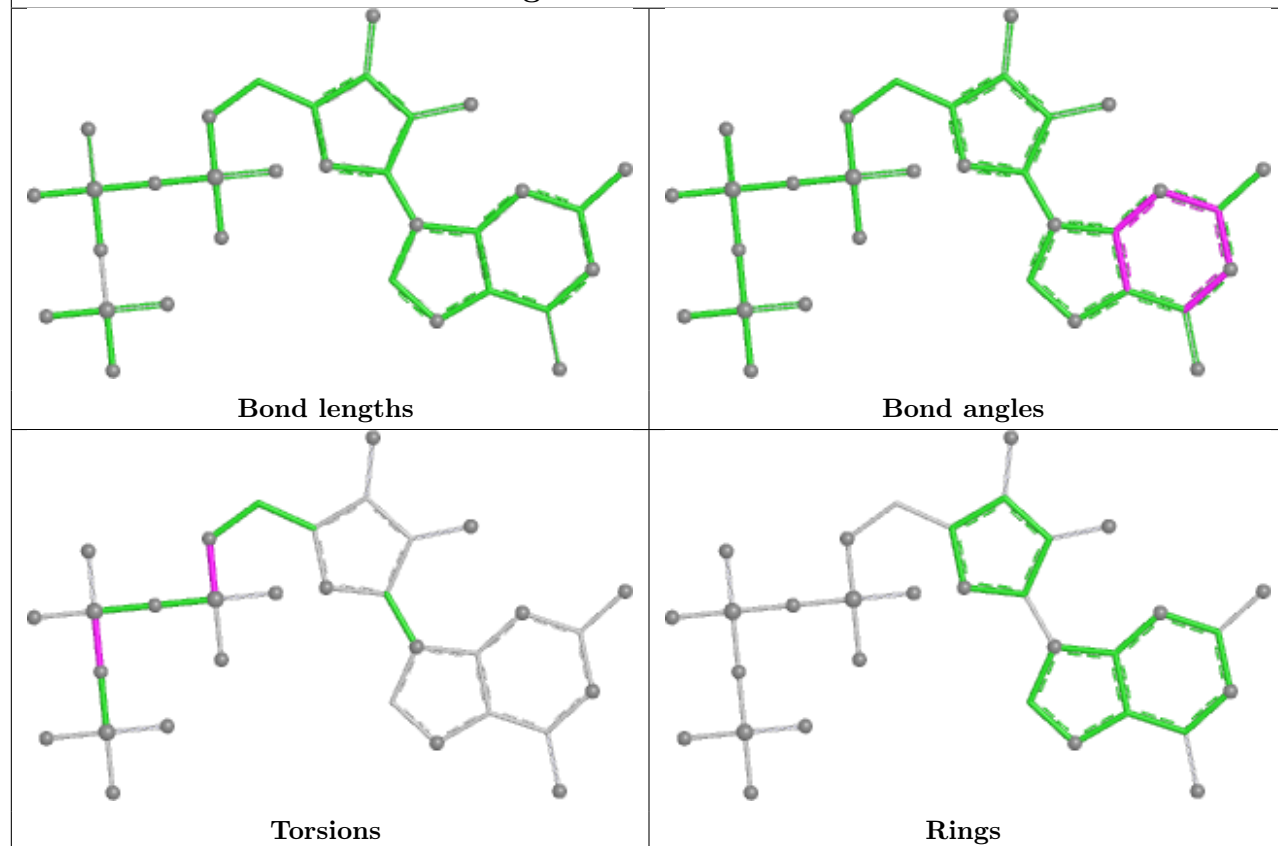




## Ligand GTP KV 602

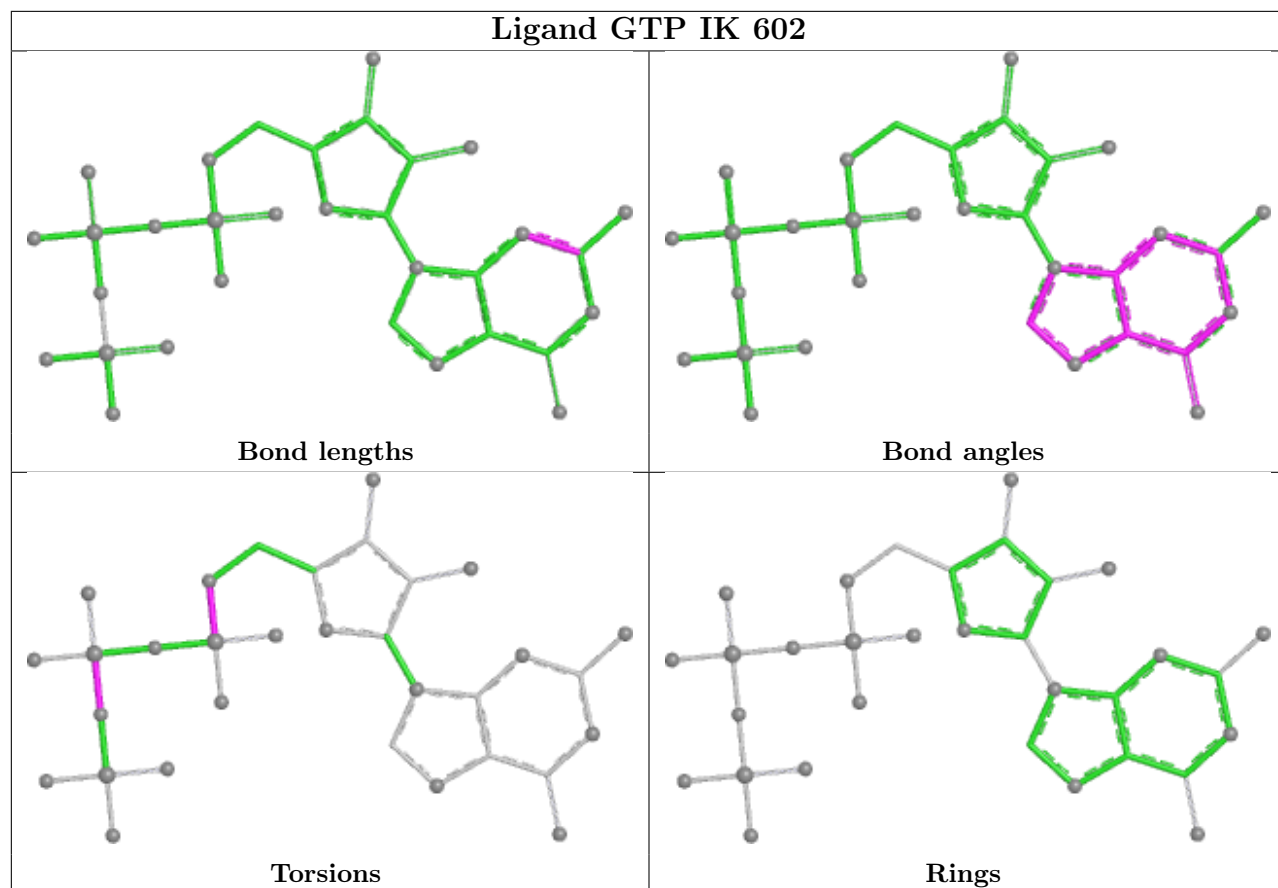


## Ligand GTP HI 602

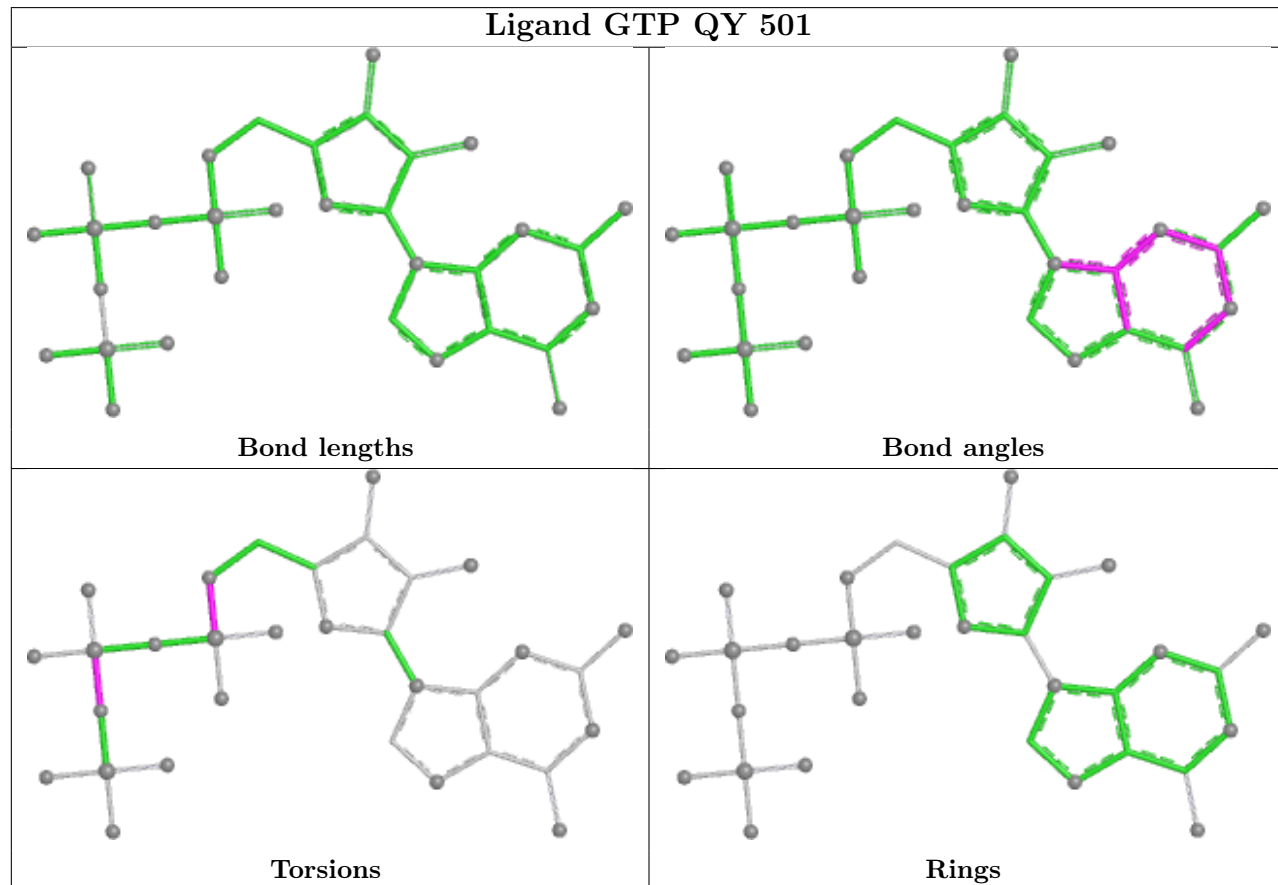


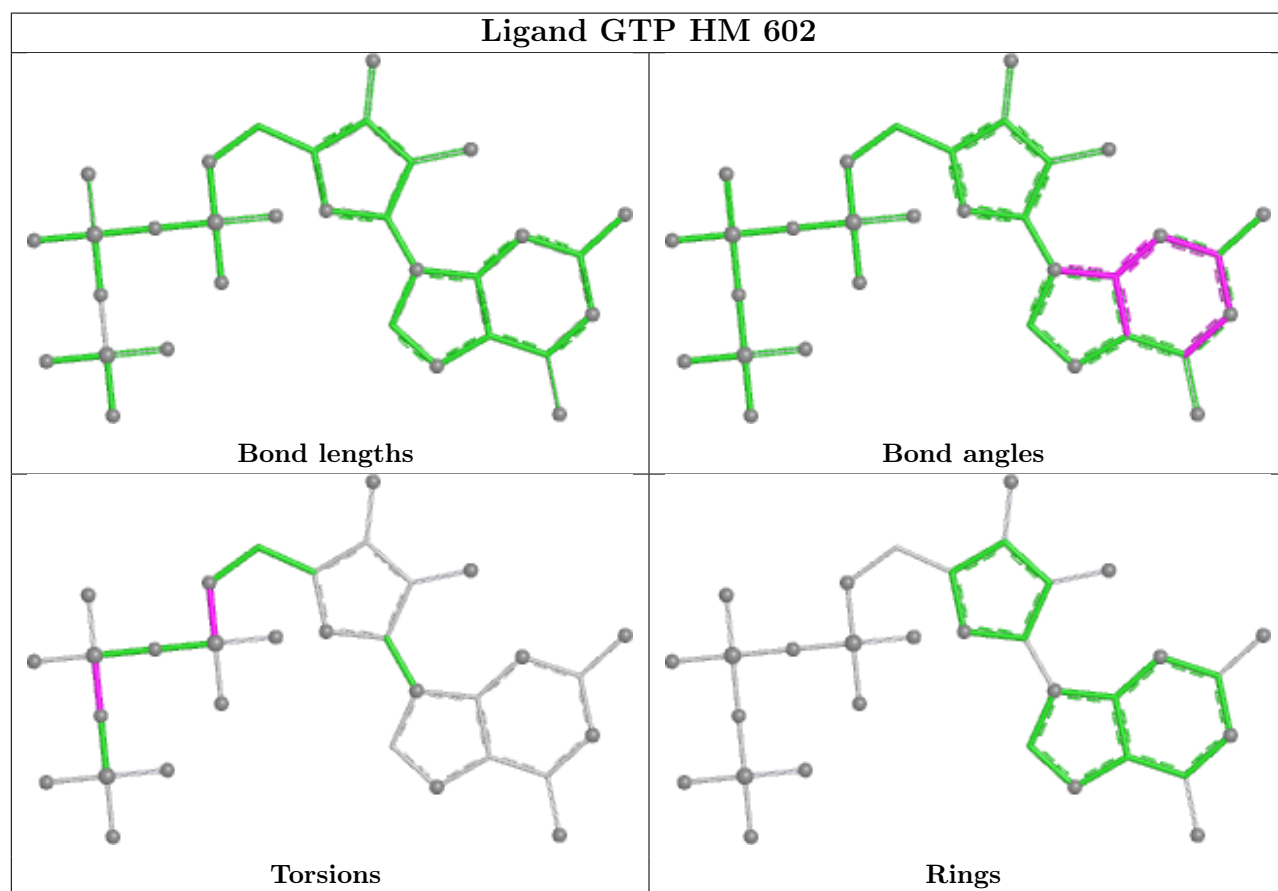
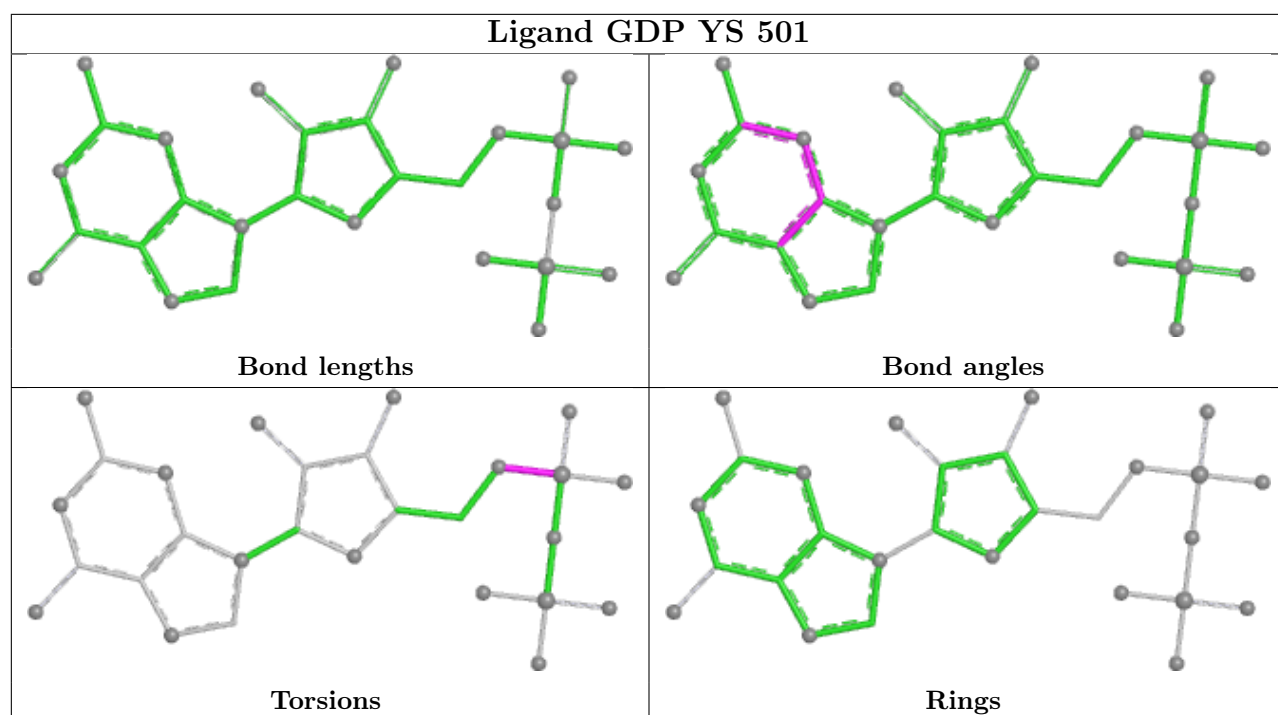


## Ligand GTP IK 602

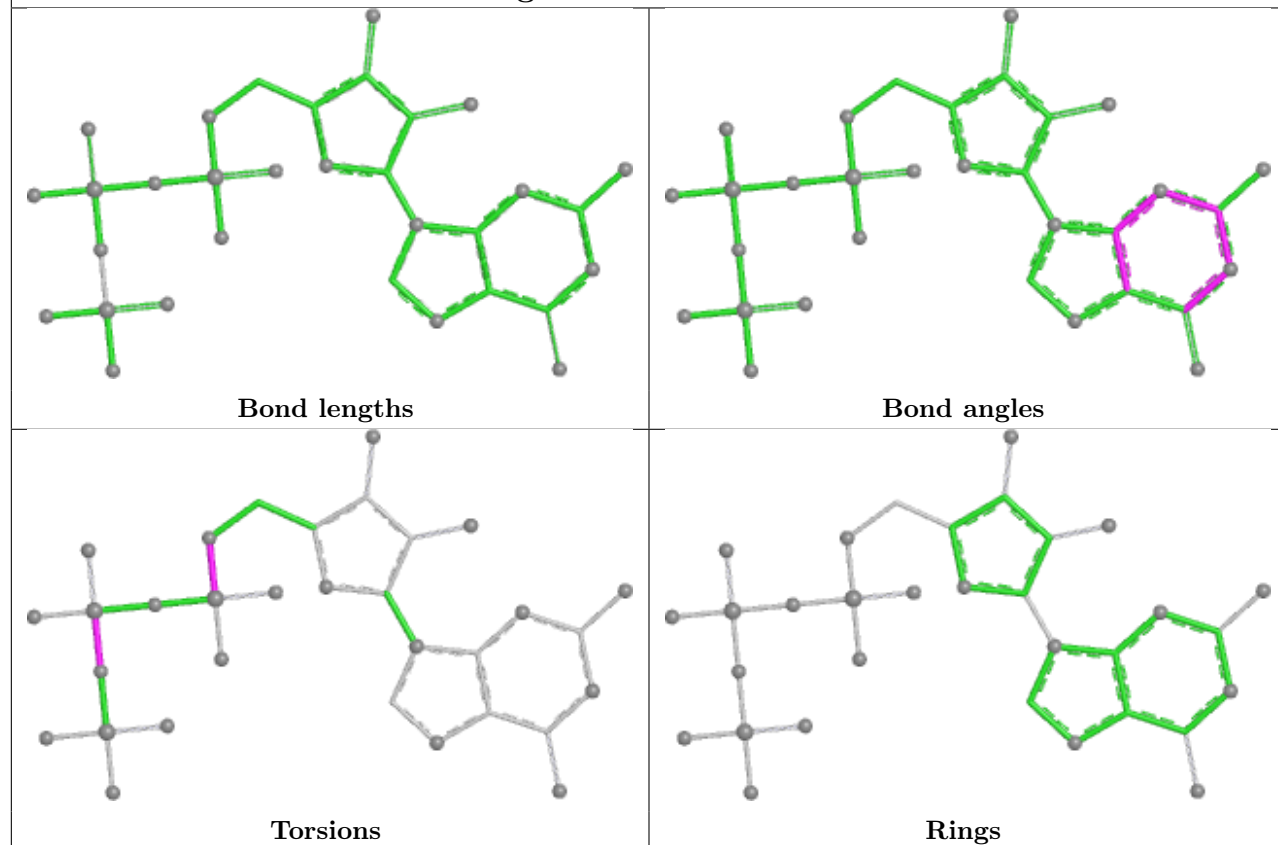


## Ligand GTP QY 501

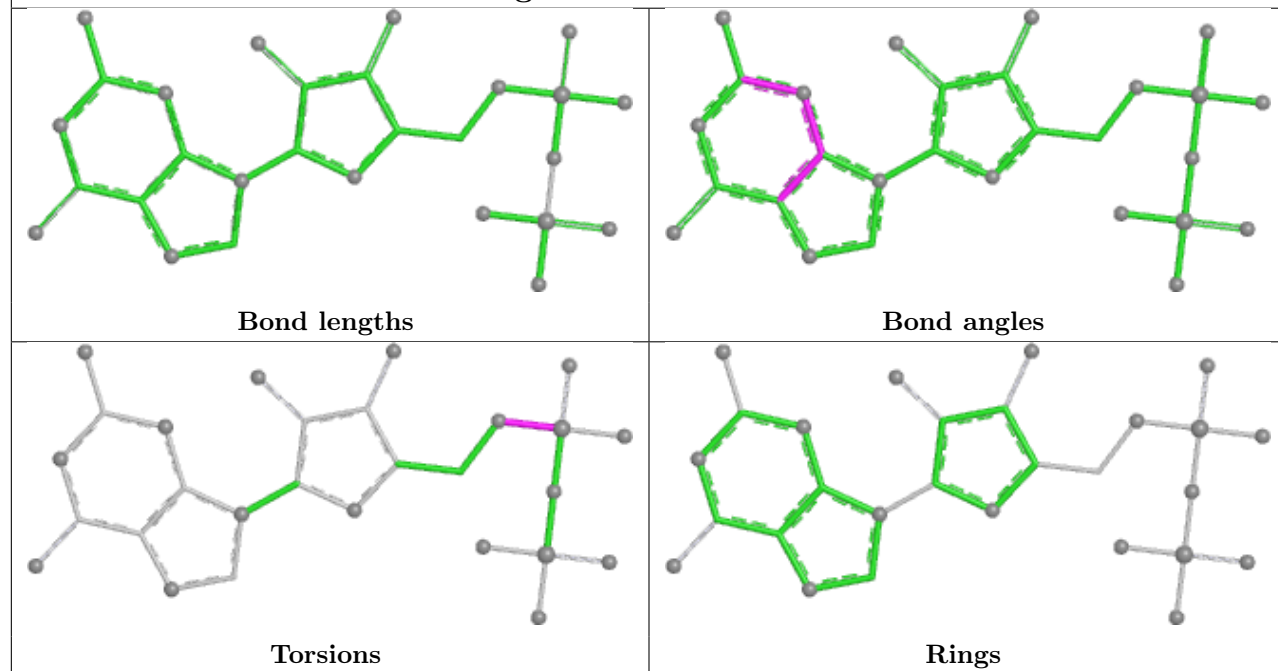




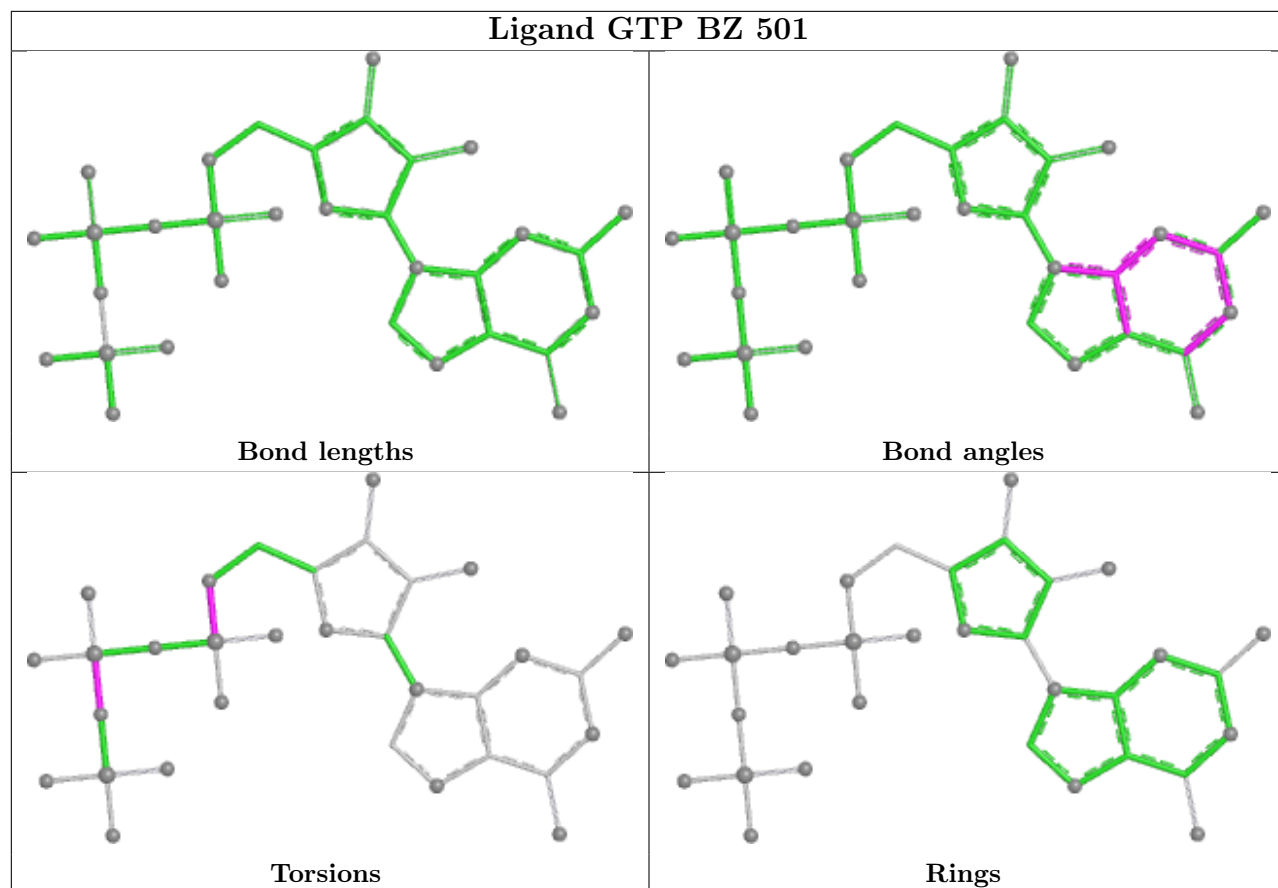
## Ligand GTP NB 501



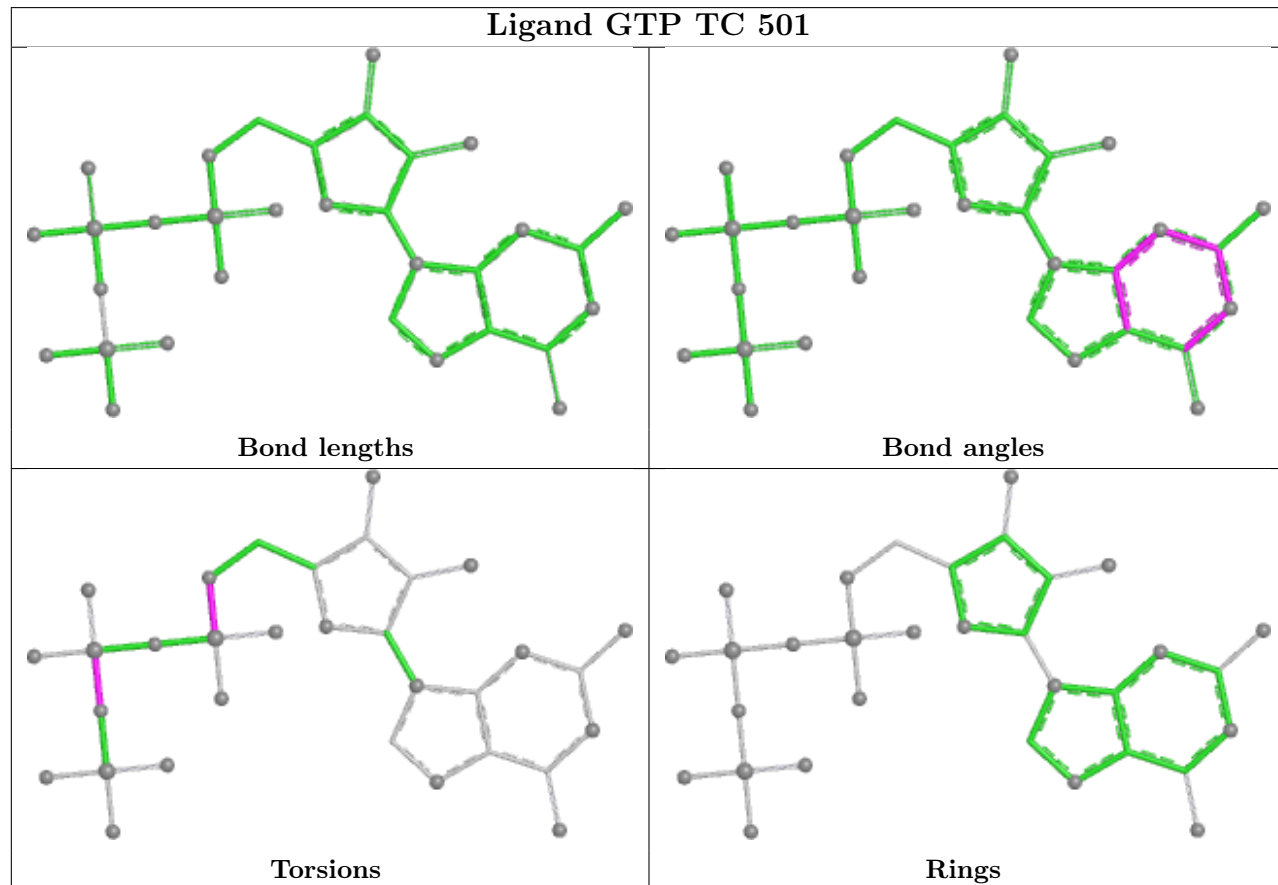
## Ligand GDP XD 501



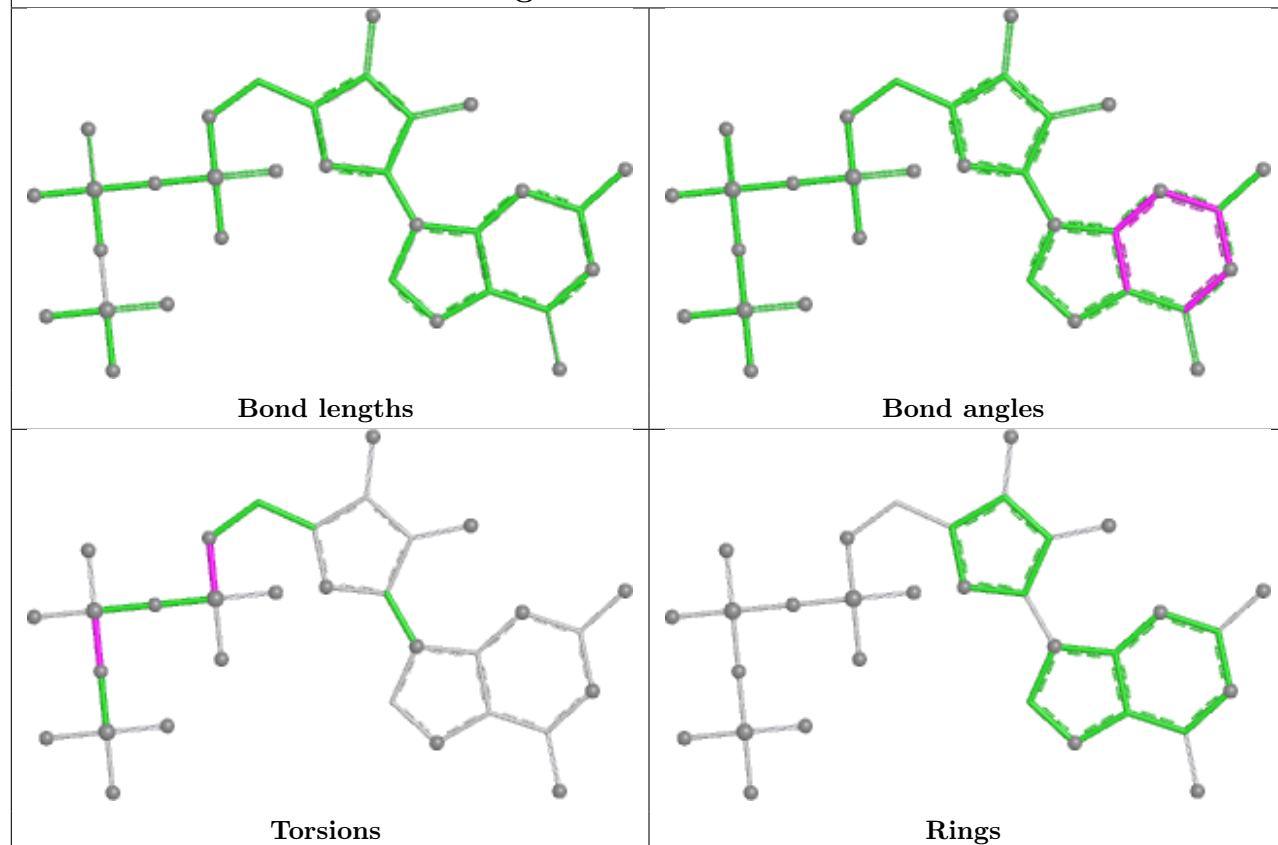
## Ligand GTP BZ 501



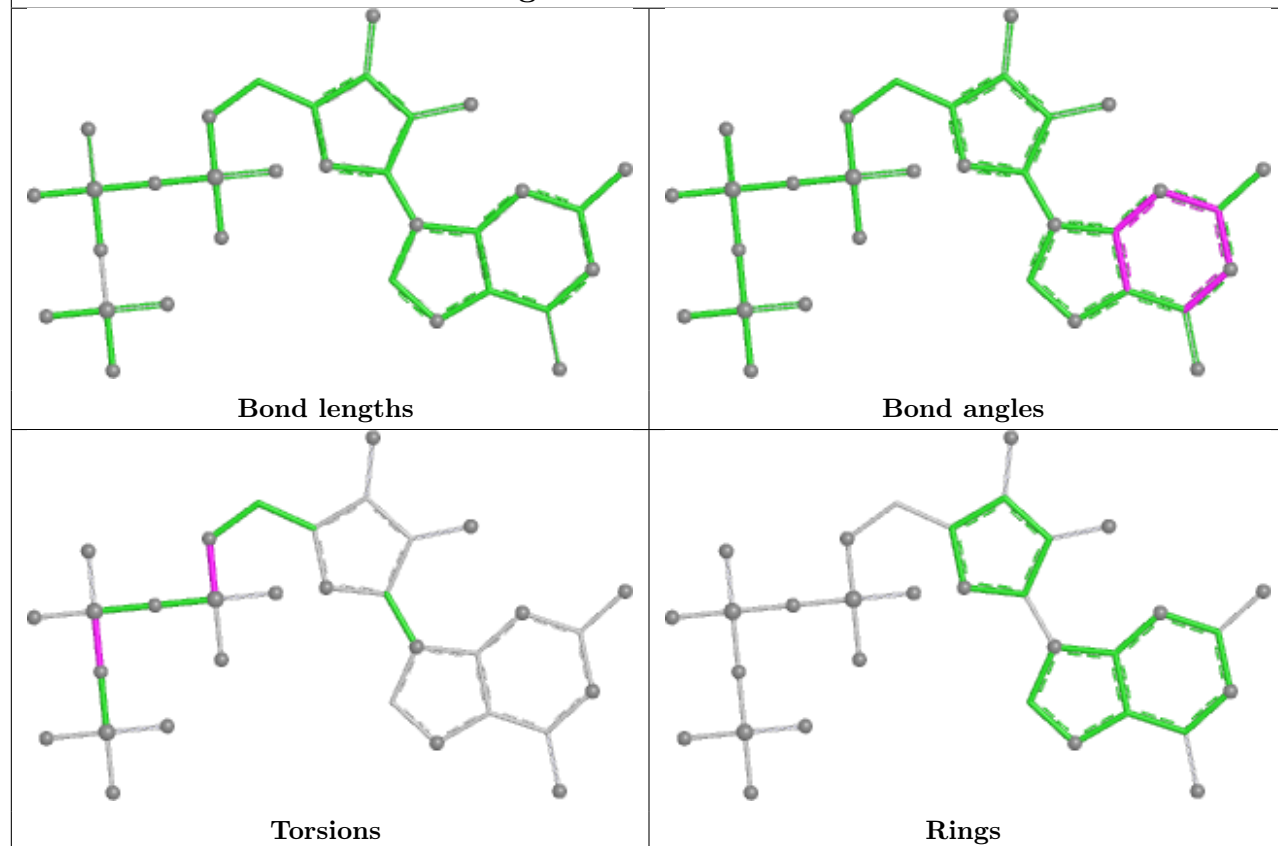
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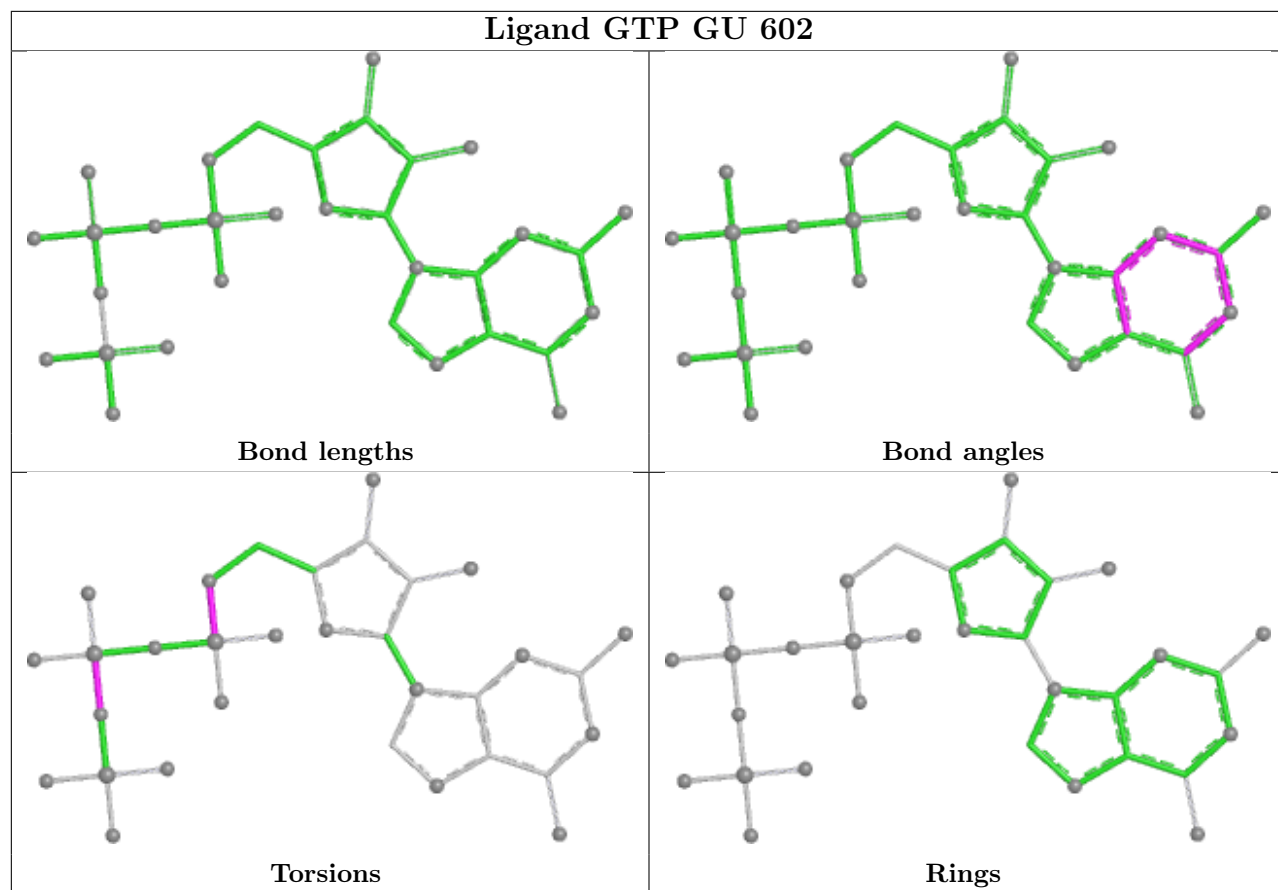


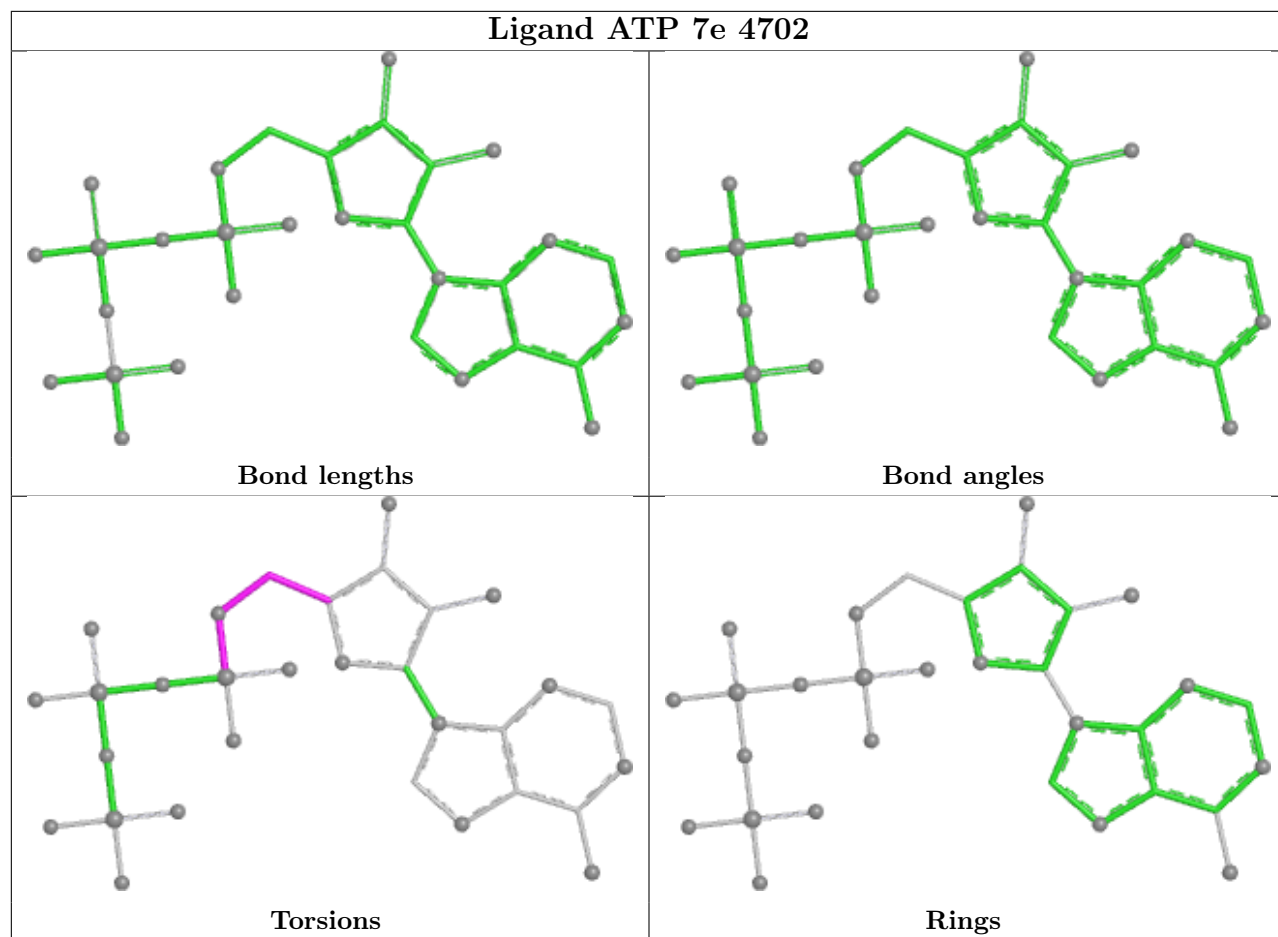
## Ligand GTP HG 501



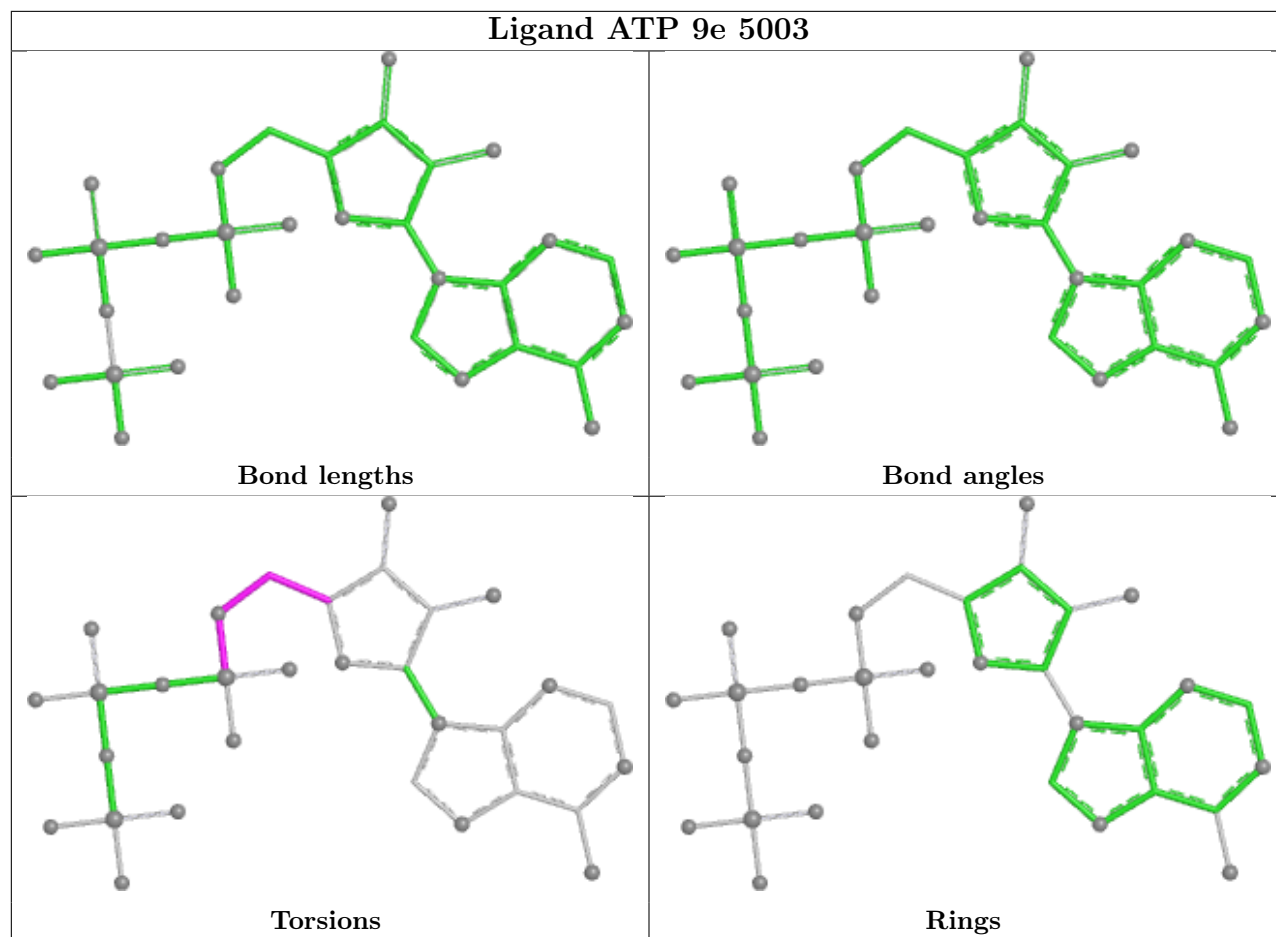
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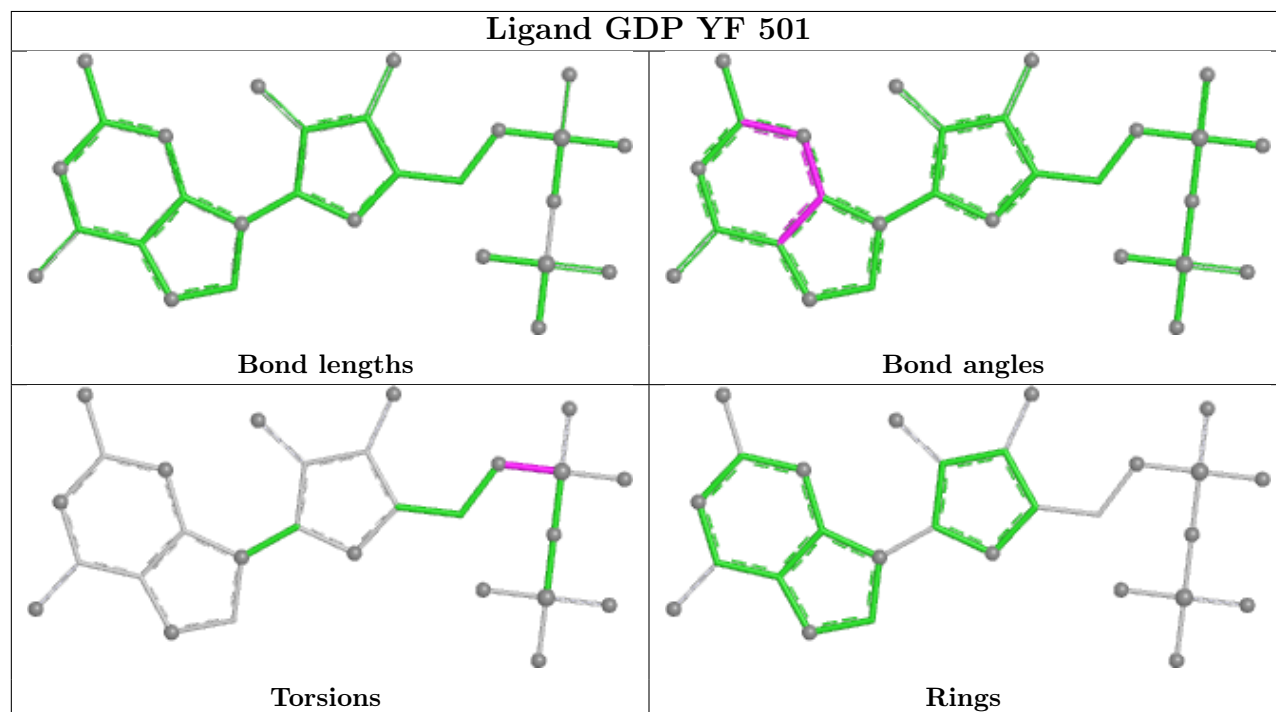




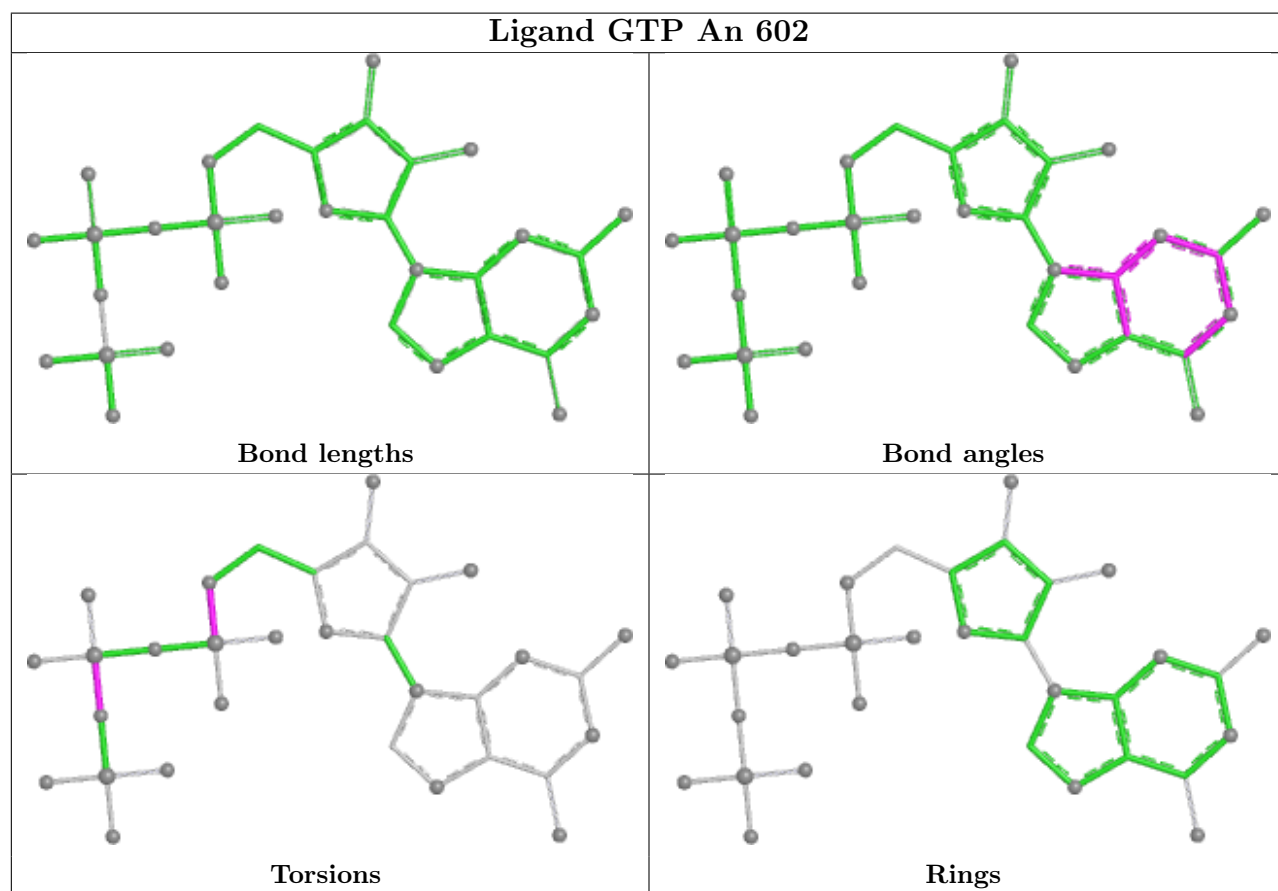
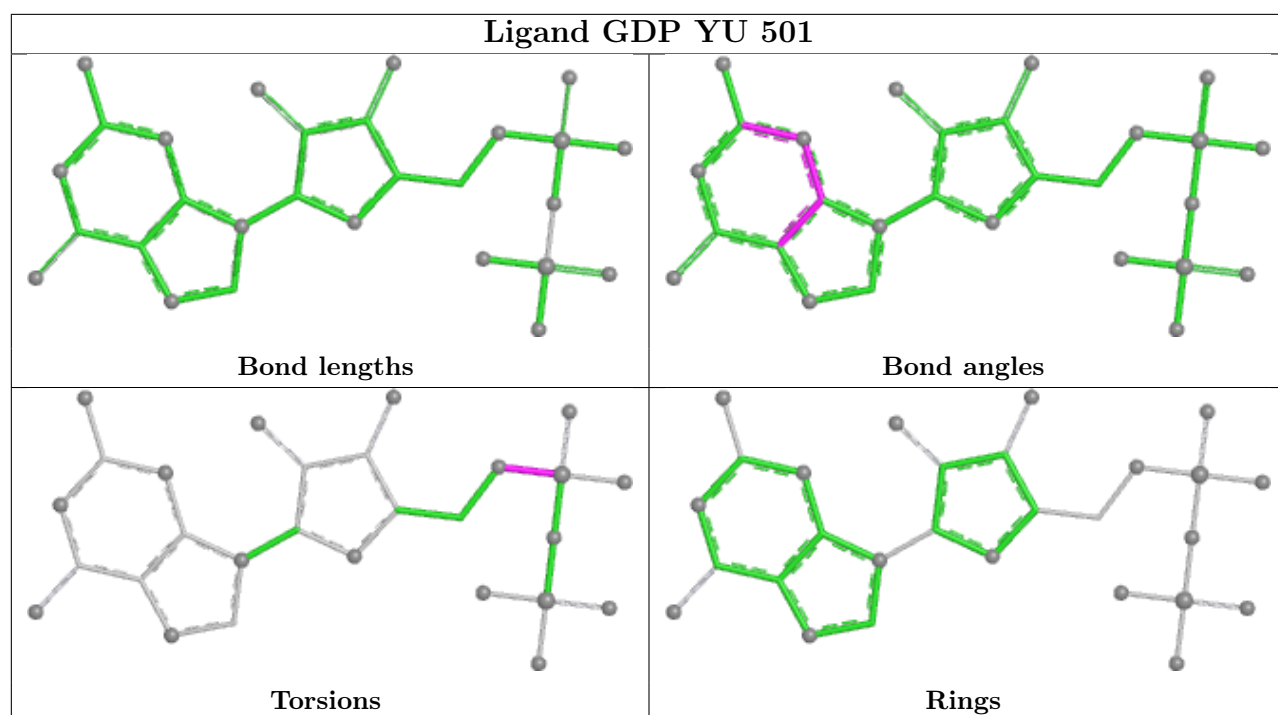
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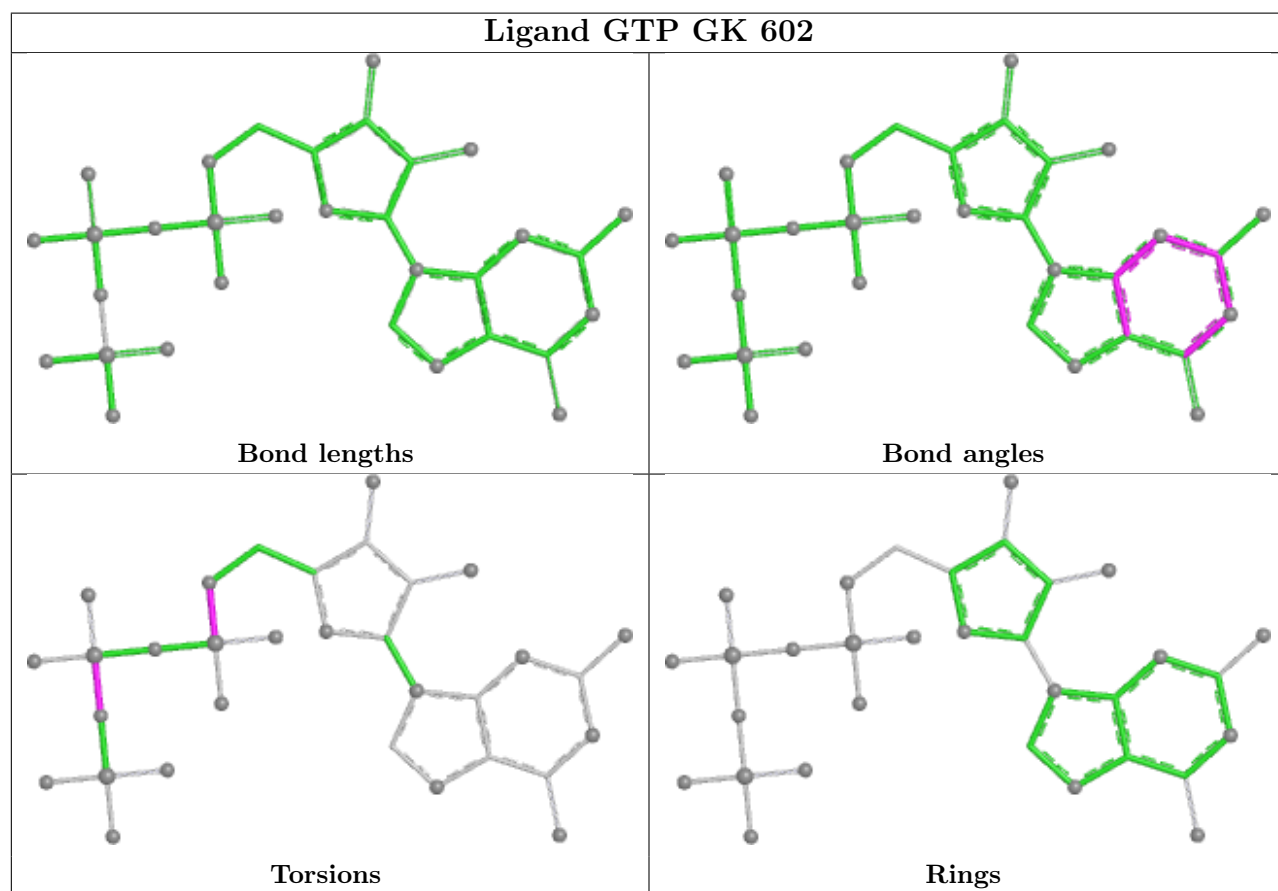
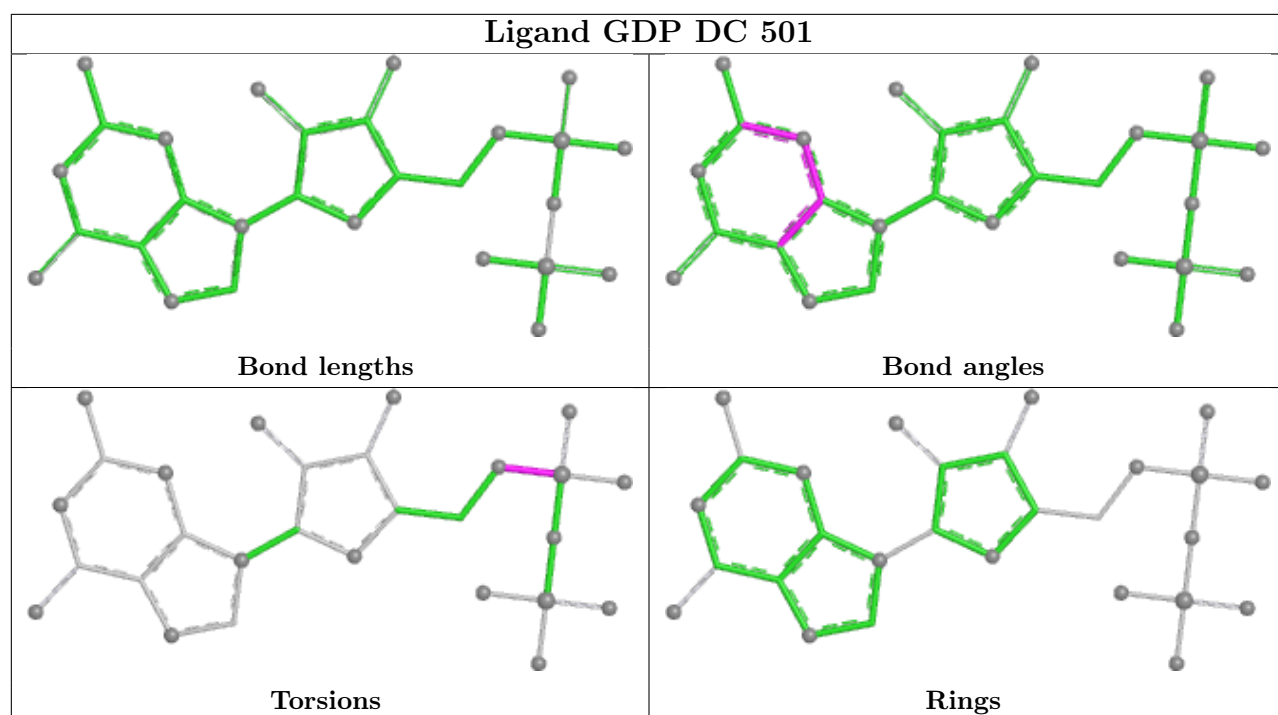


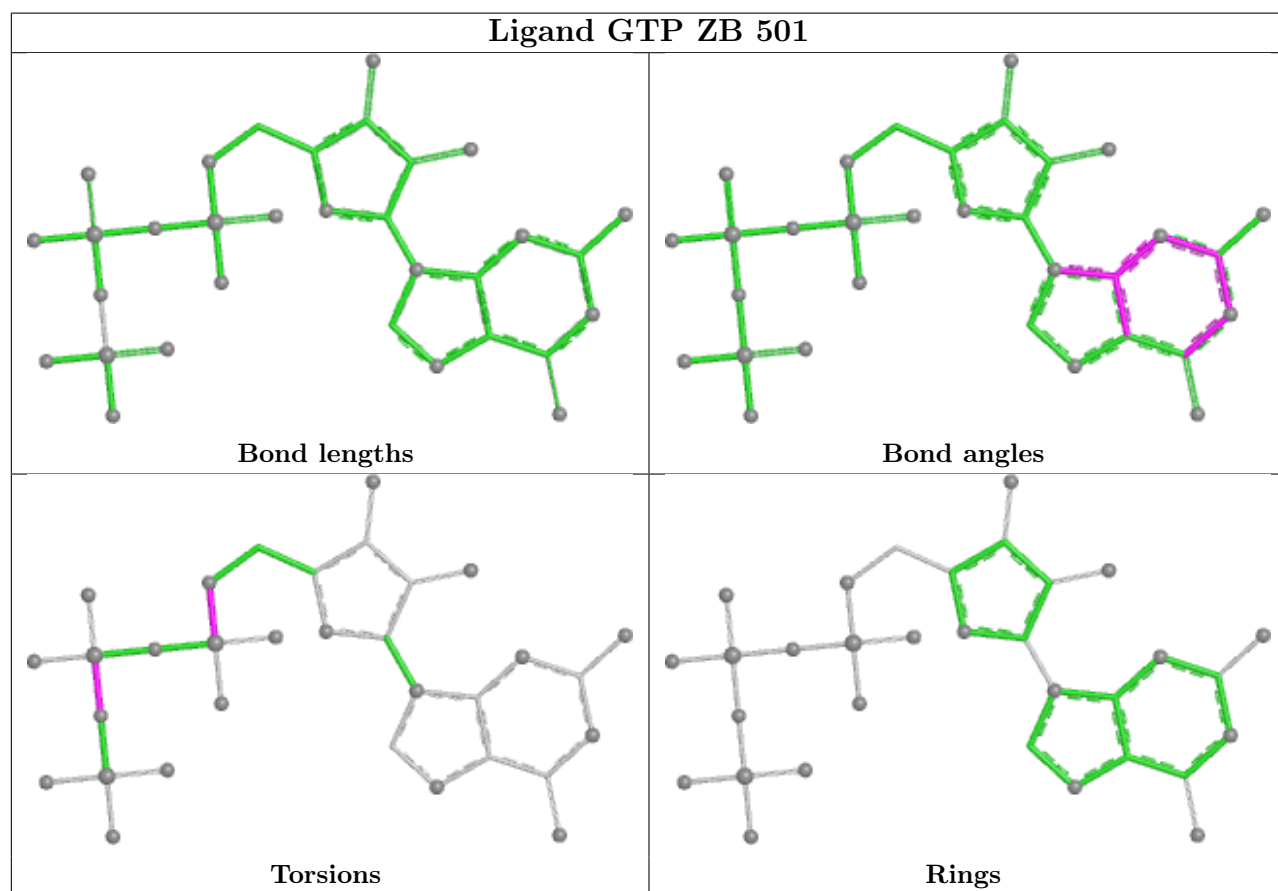
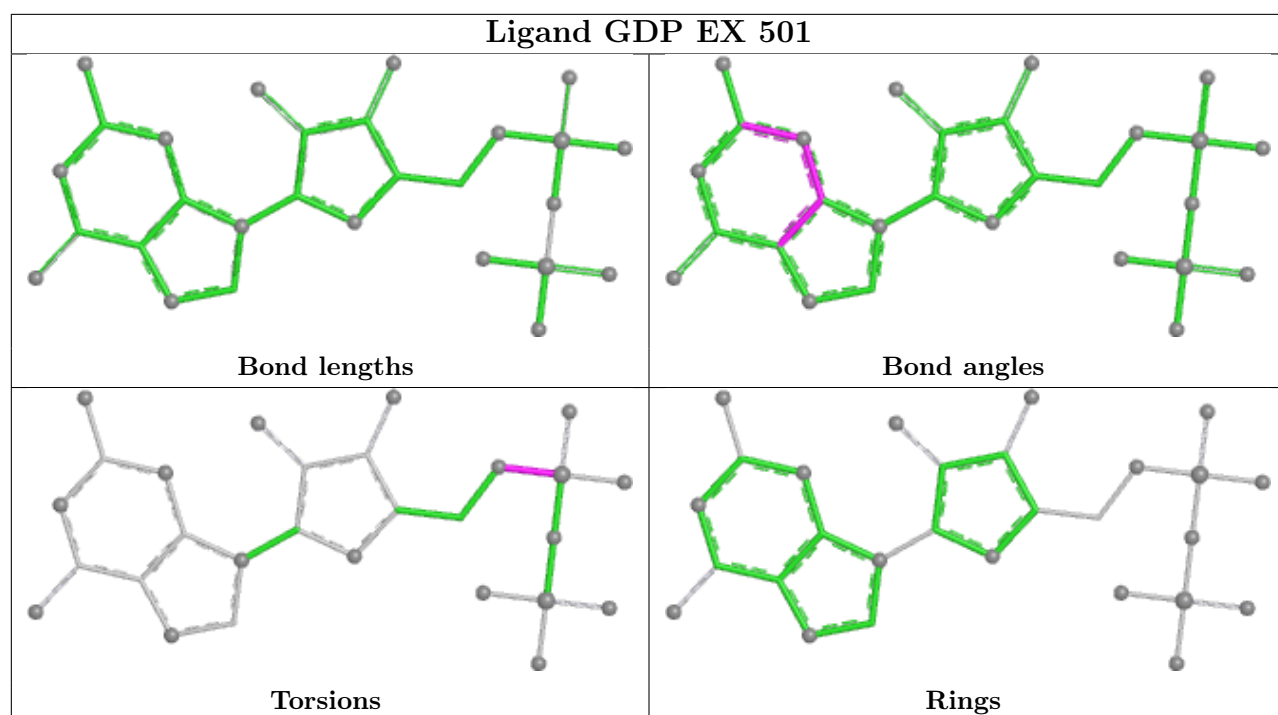
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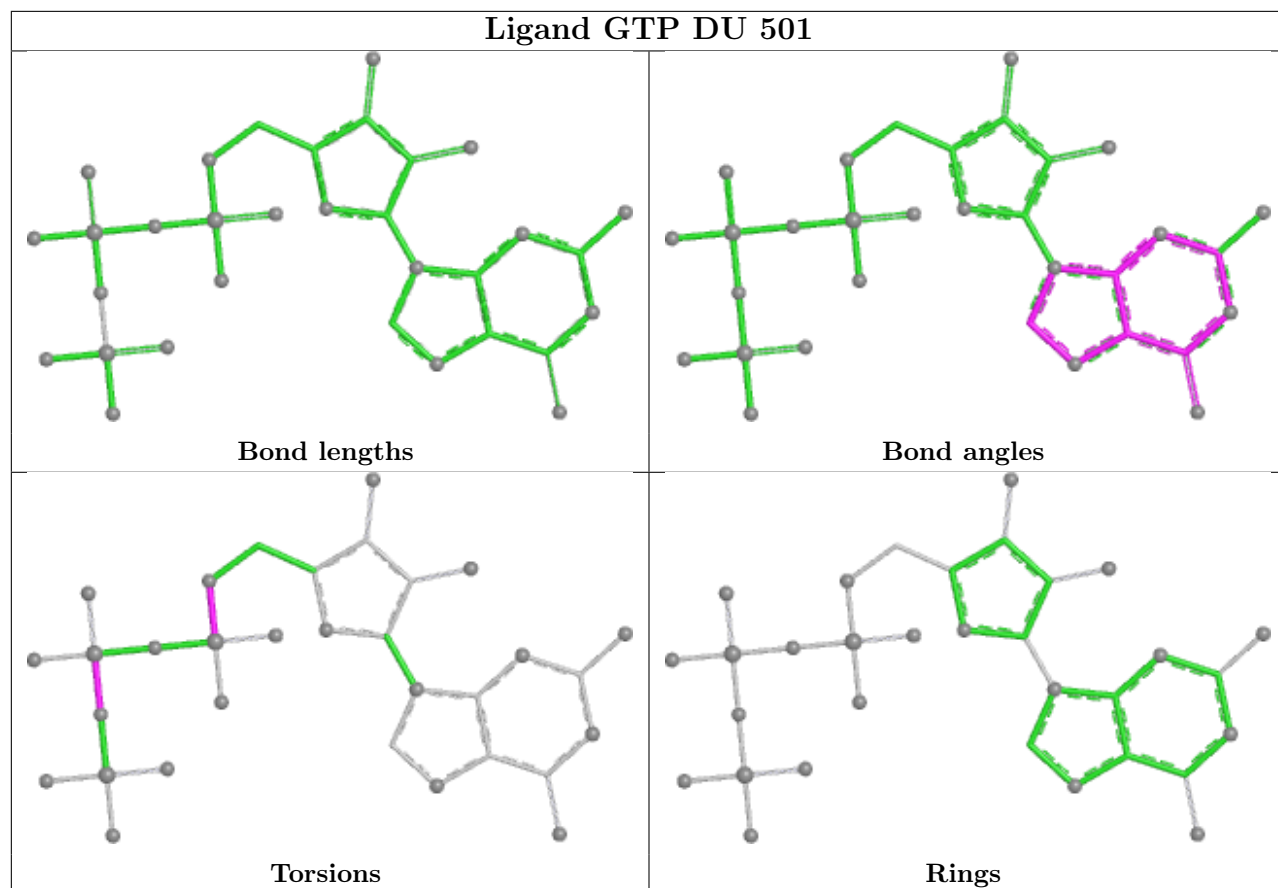




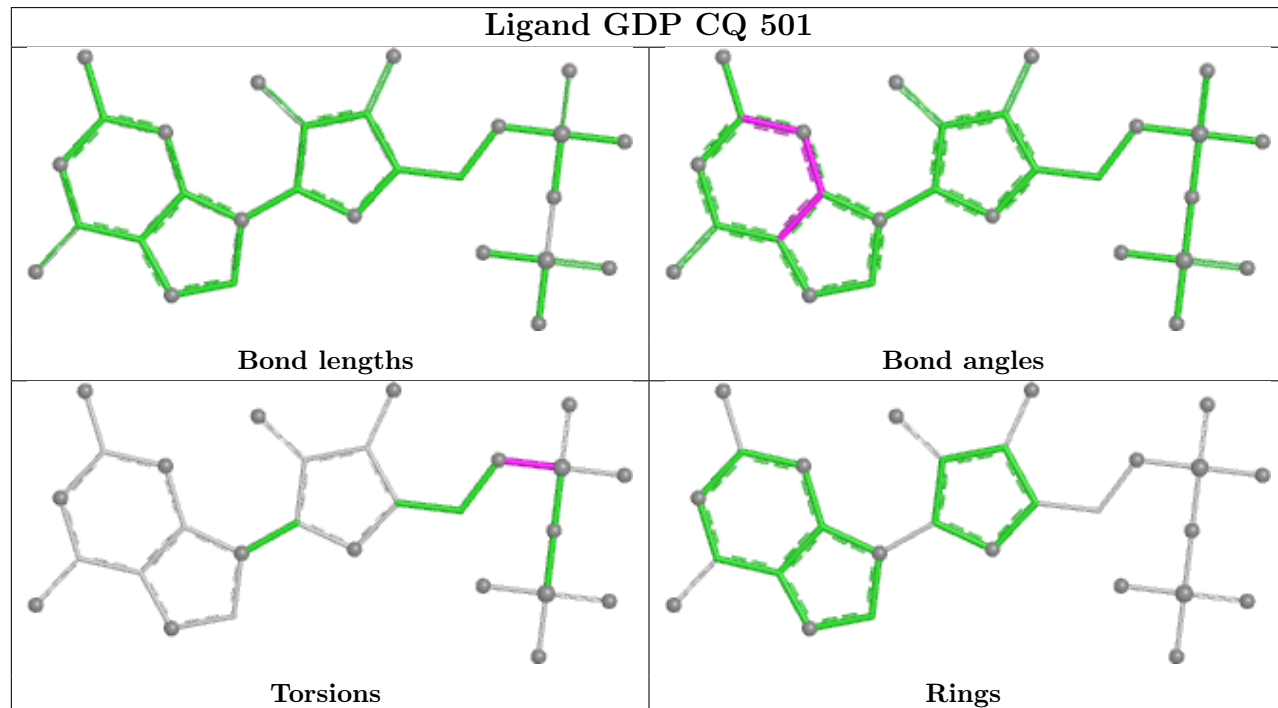




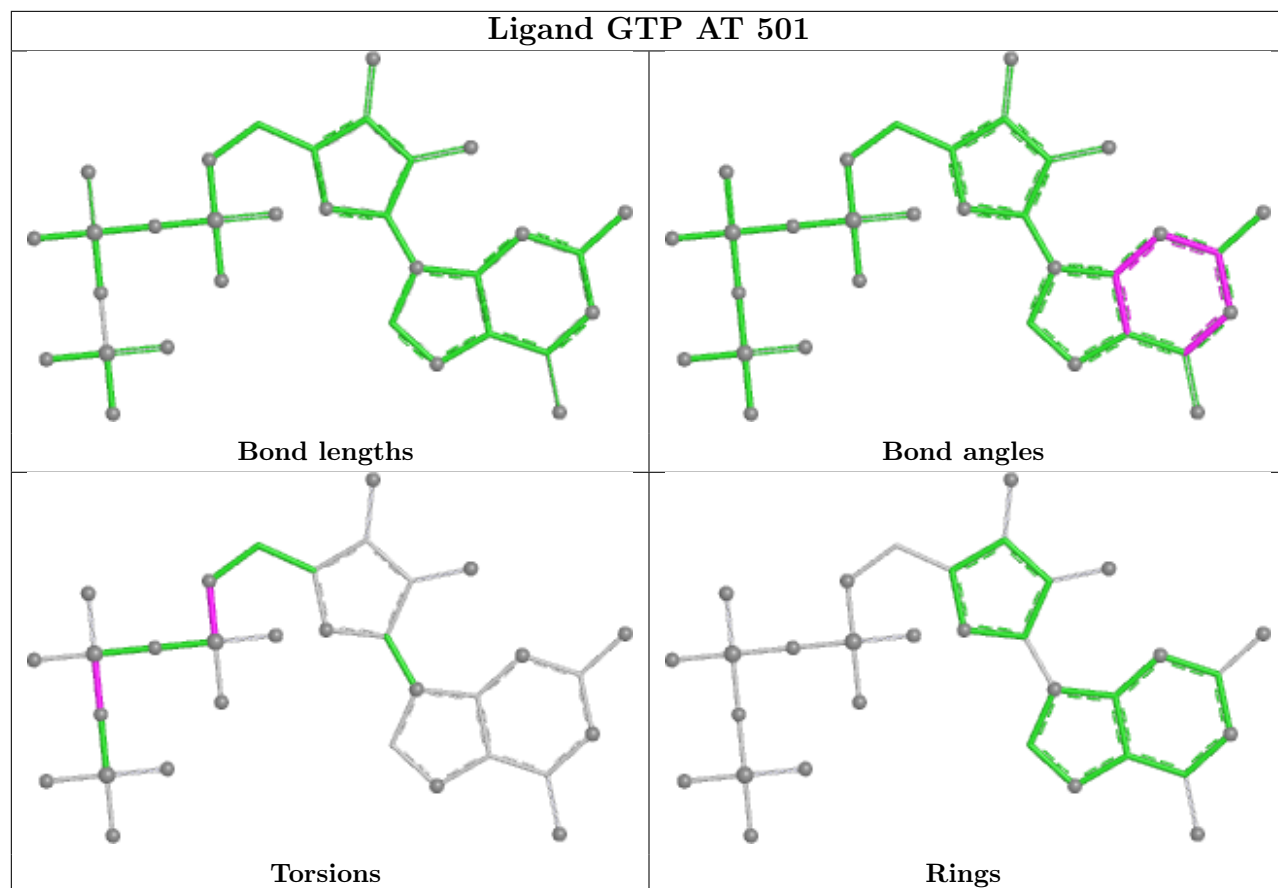
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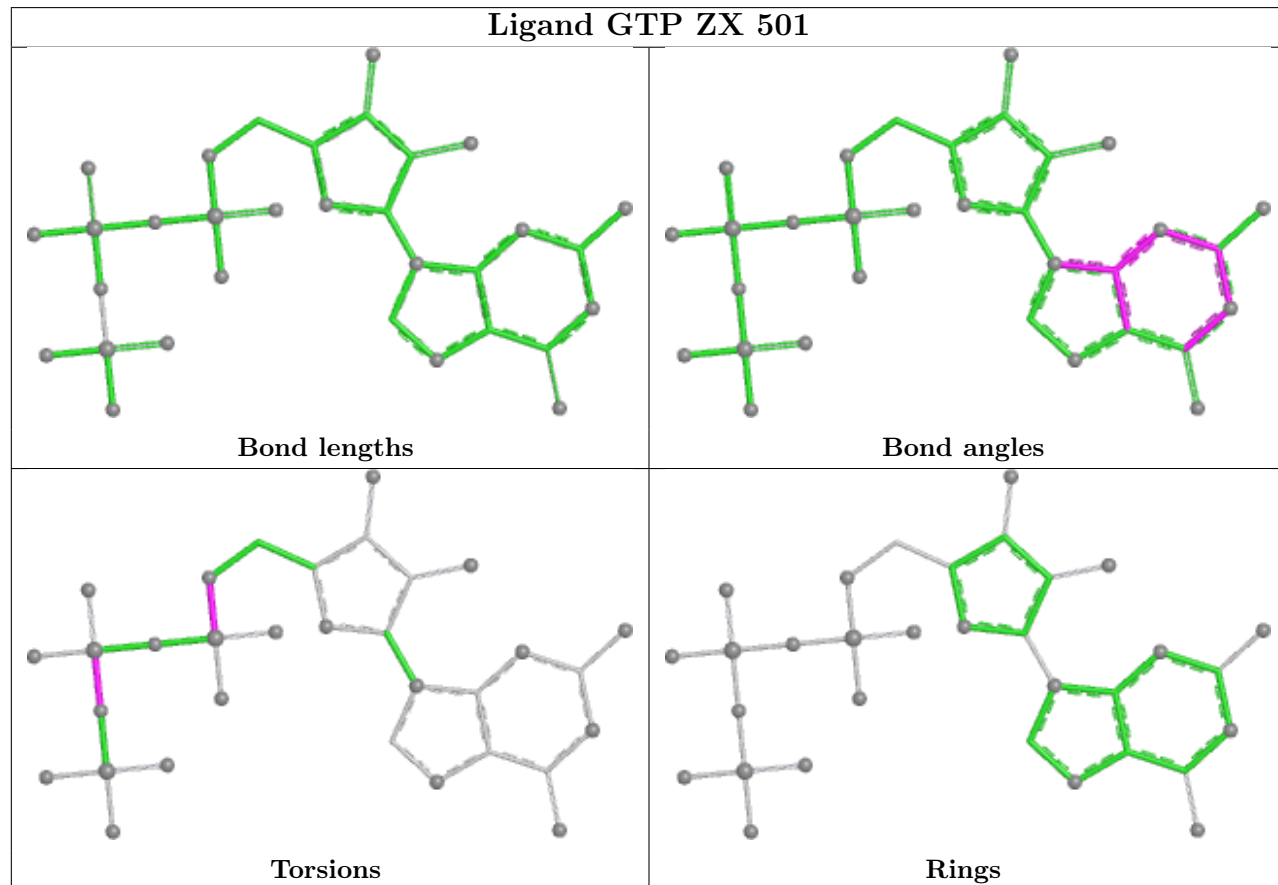
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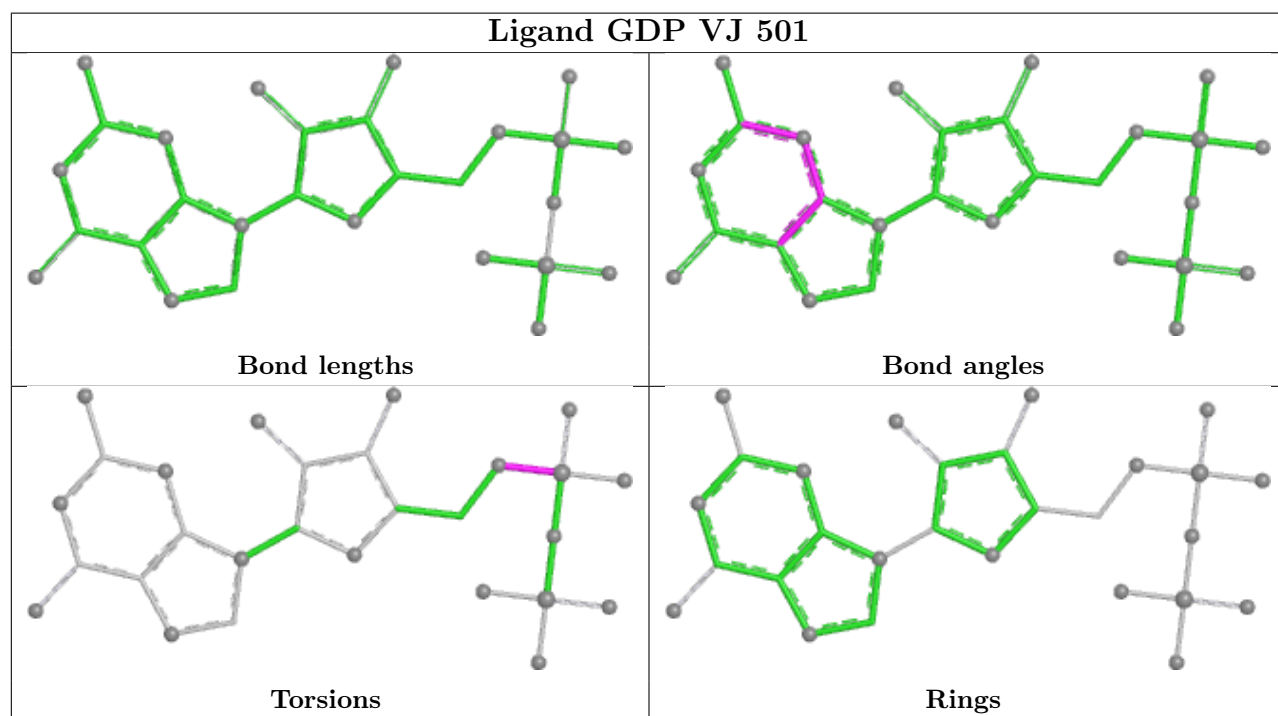
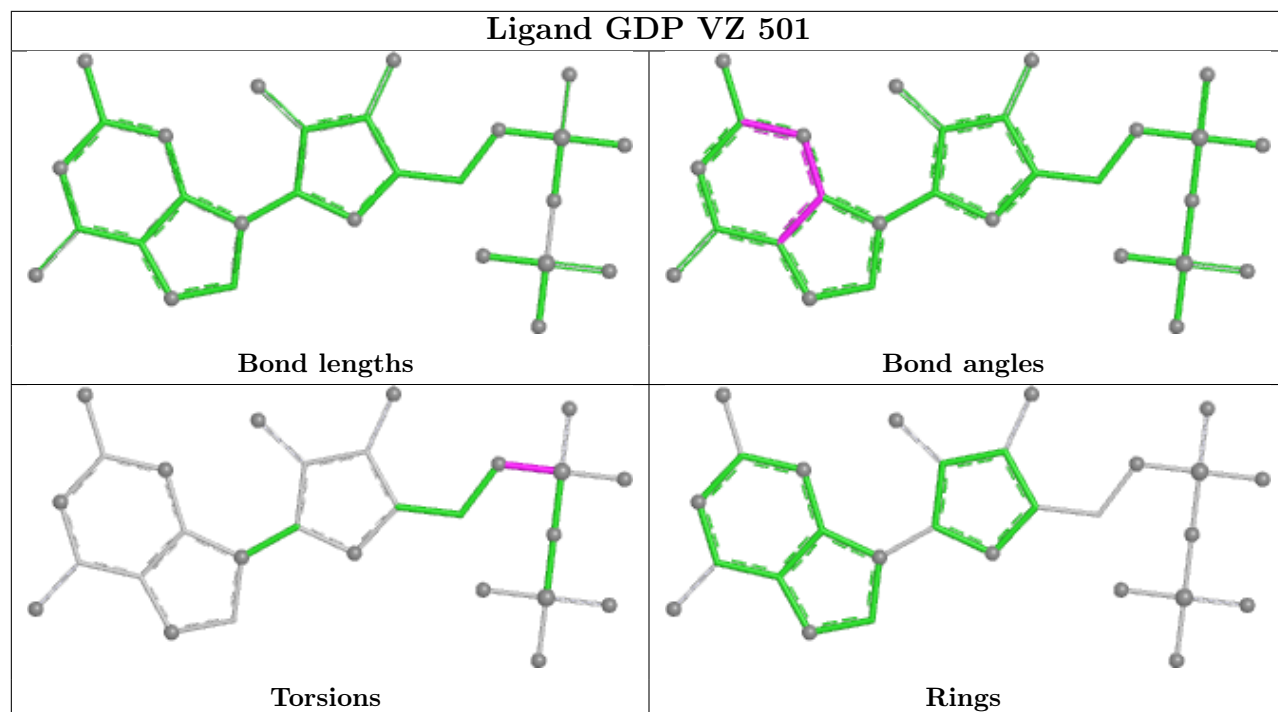


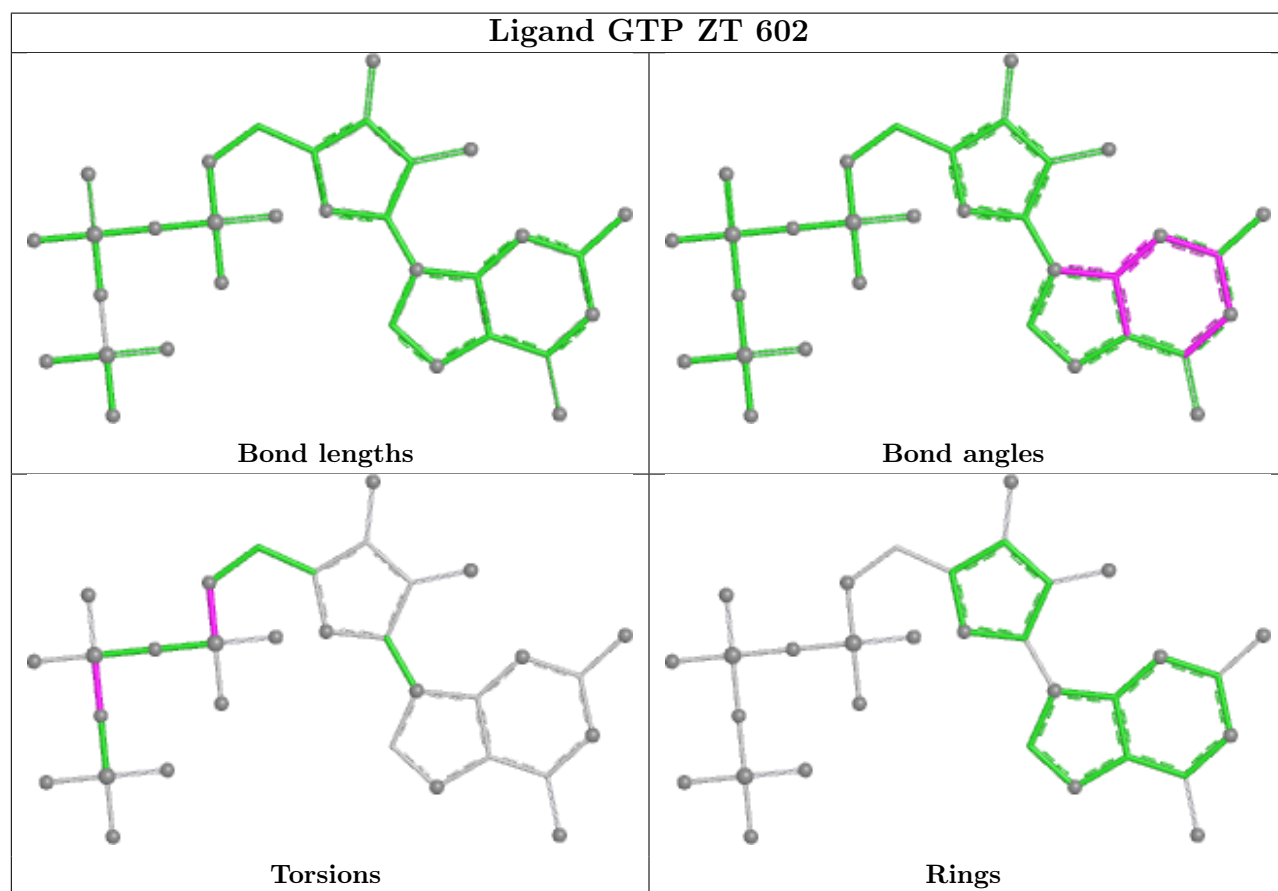
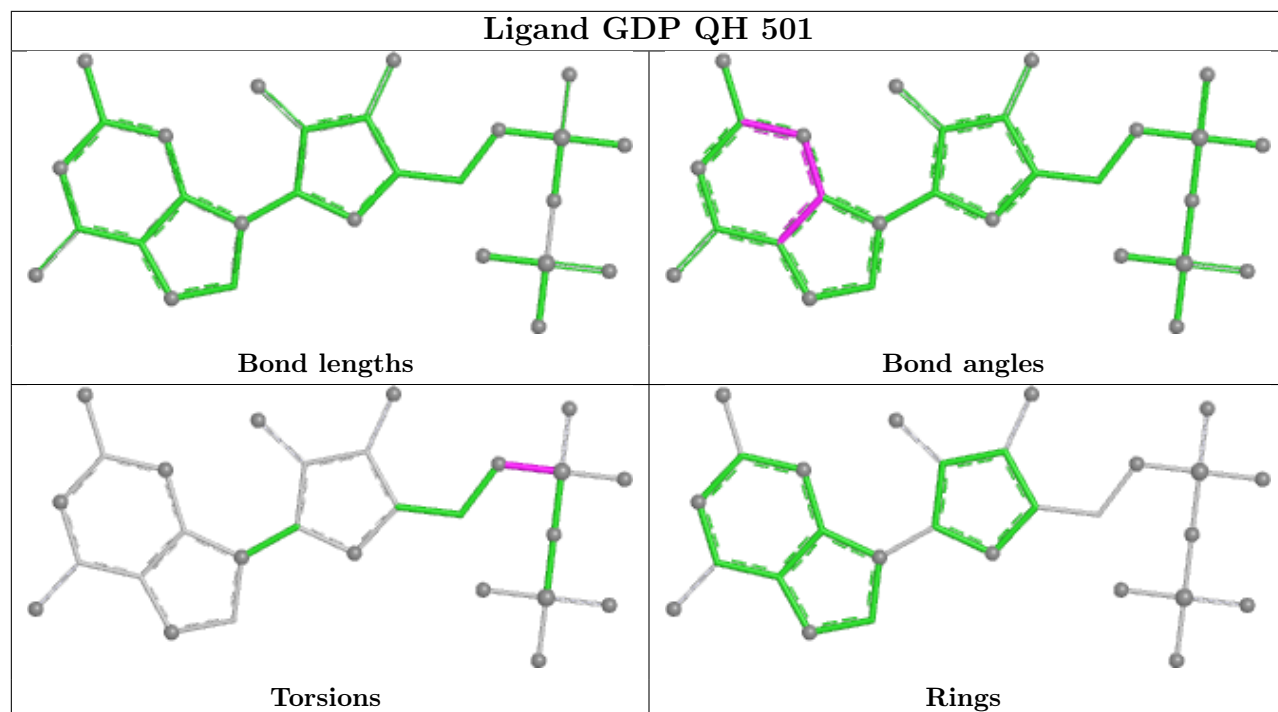
## Ligand GTP AT 501



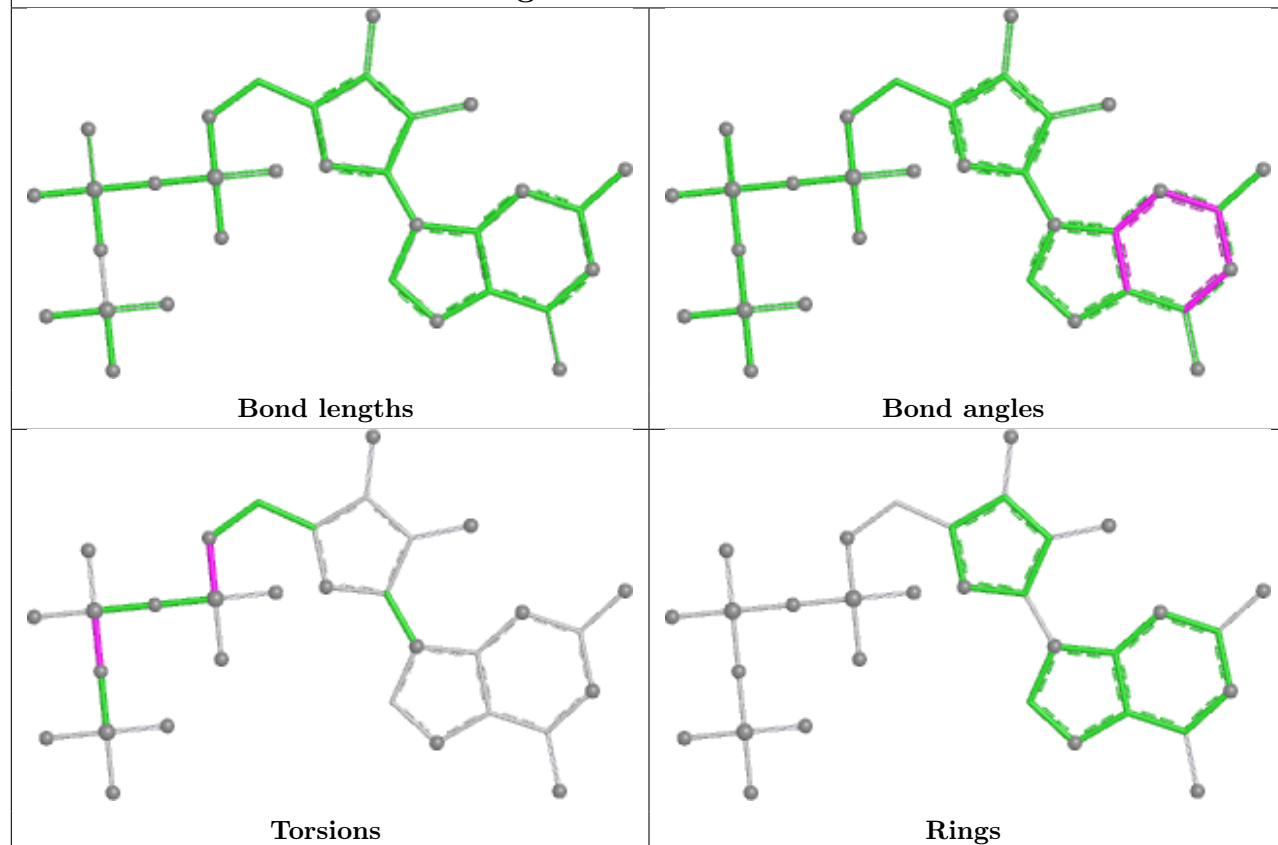
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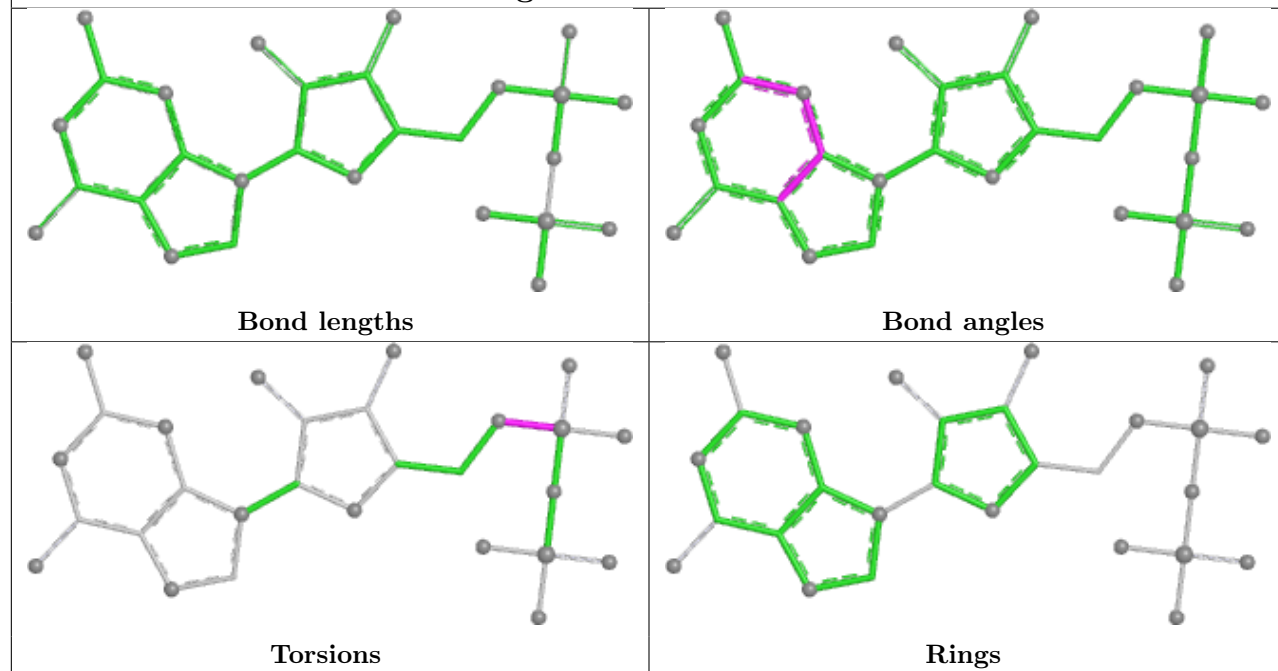




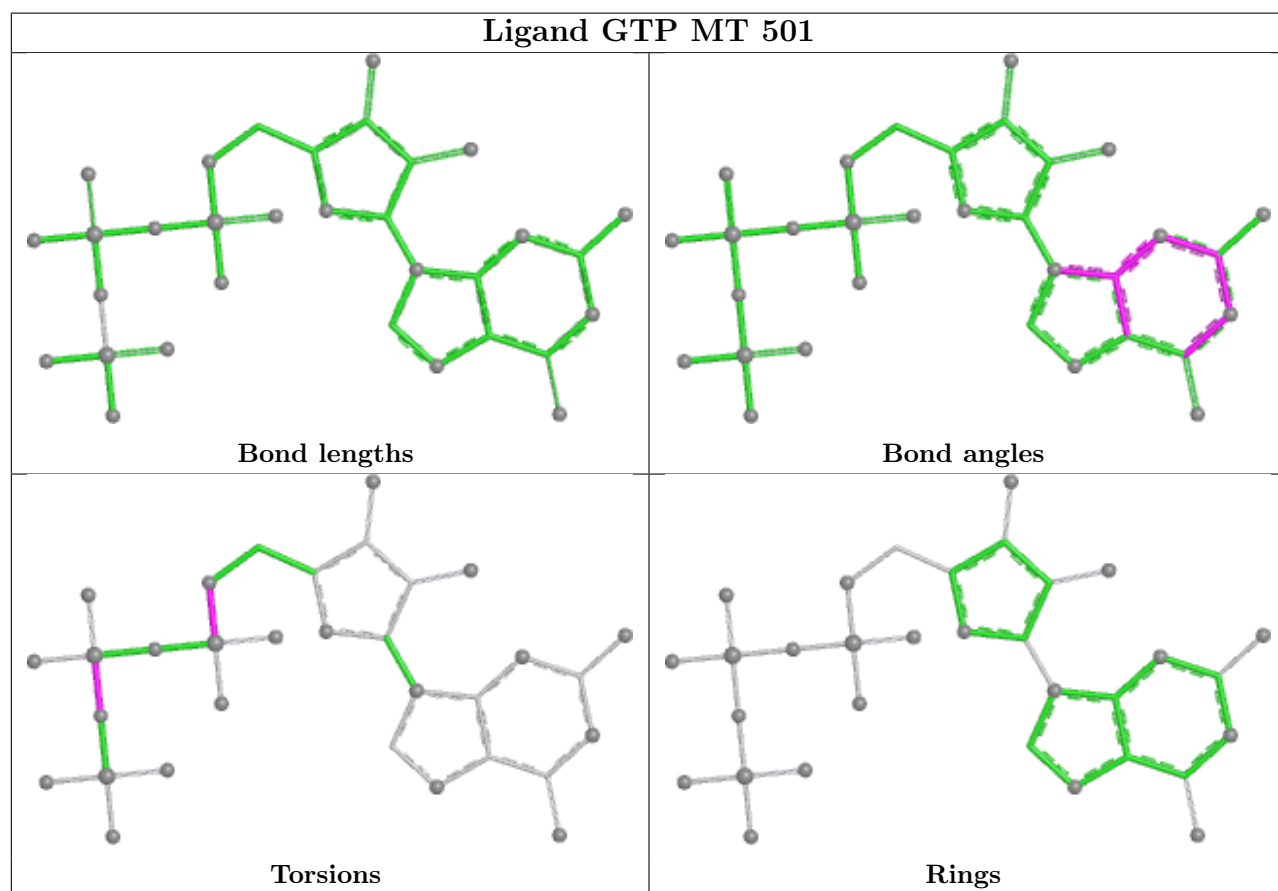
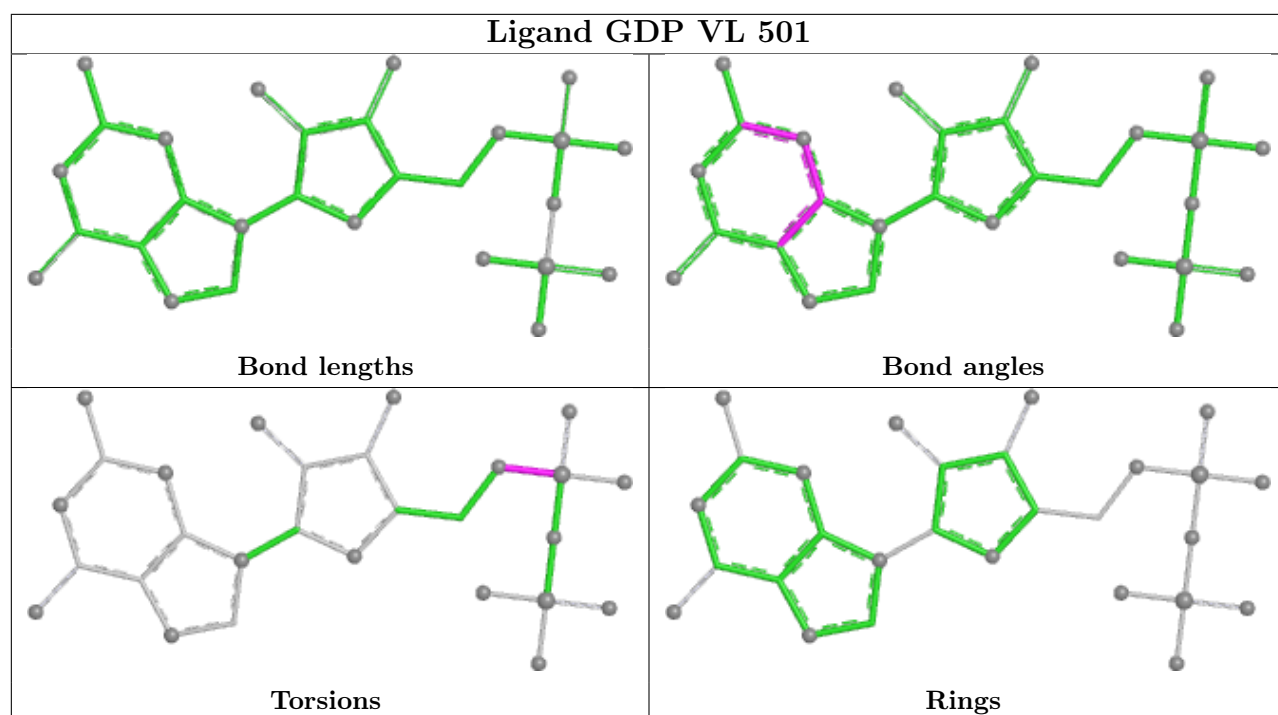
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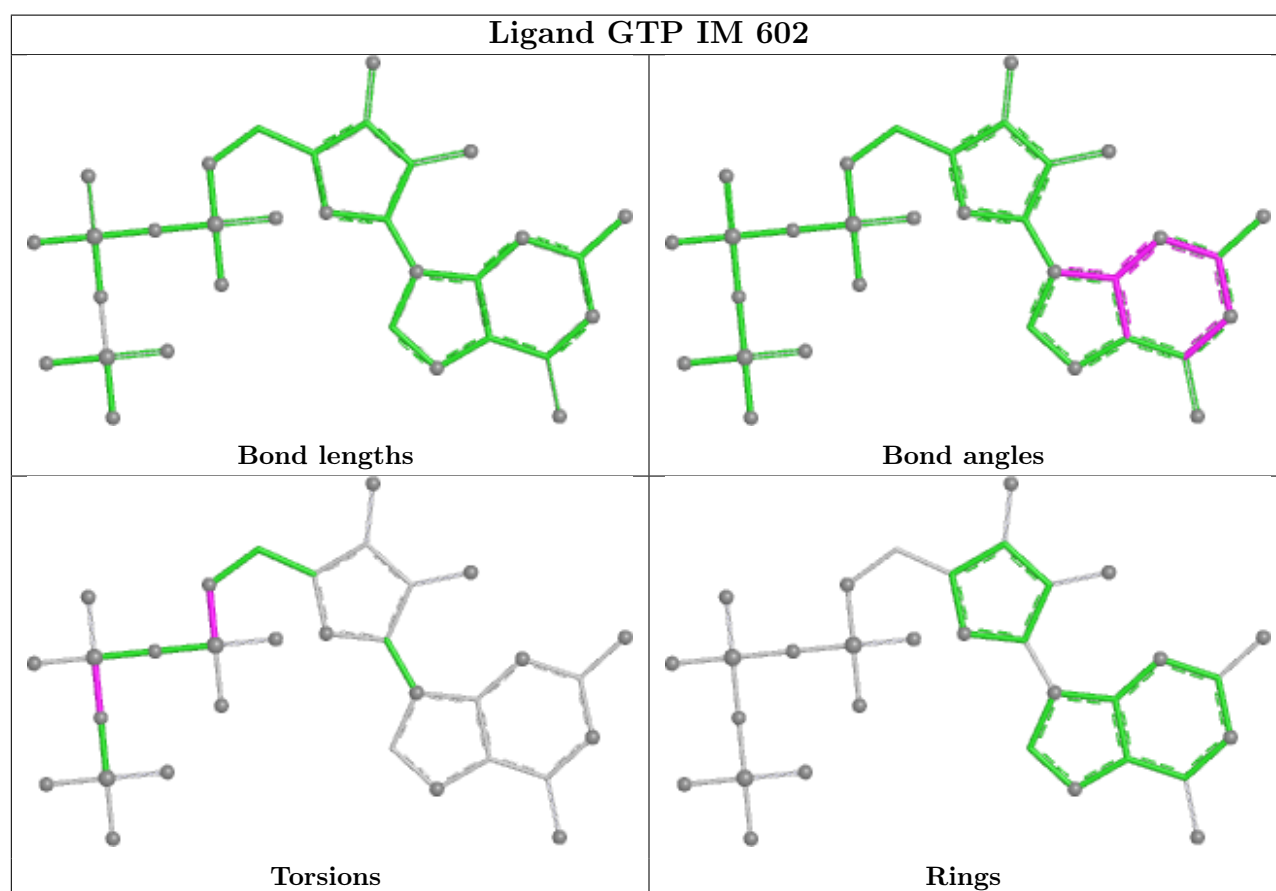
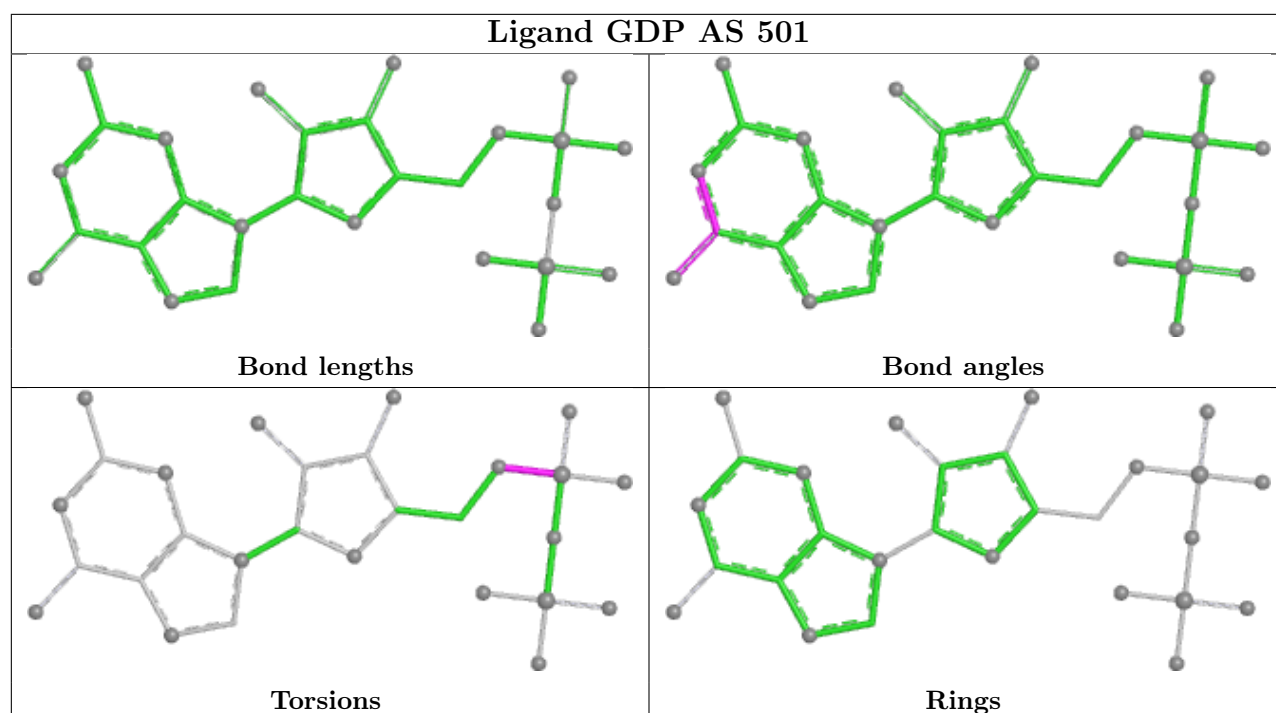


## Ligand GDP XT 501

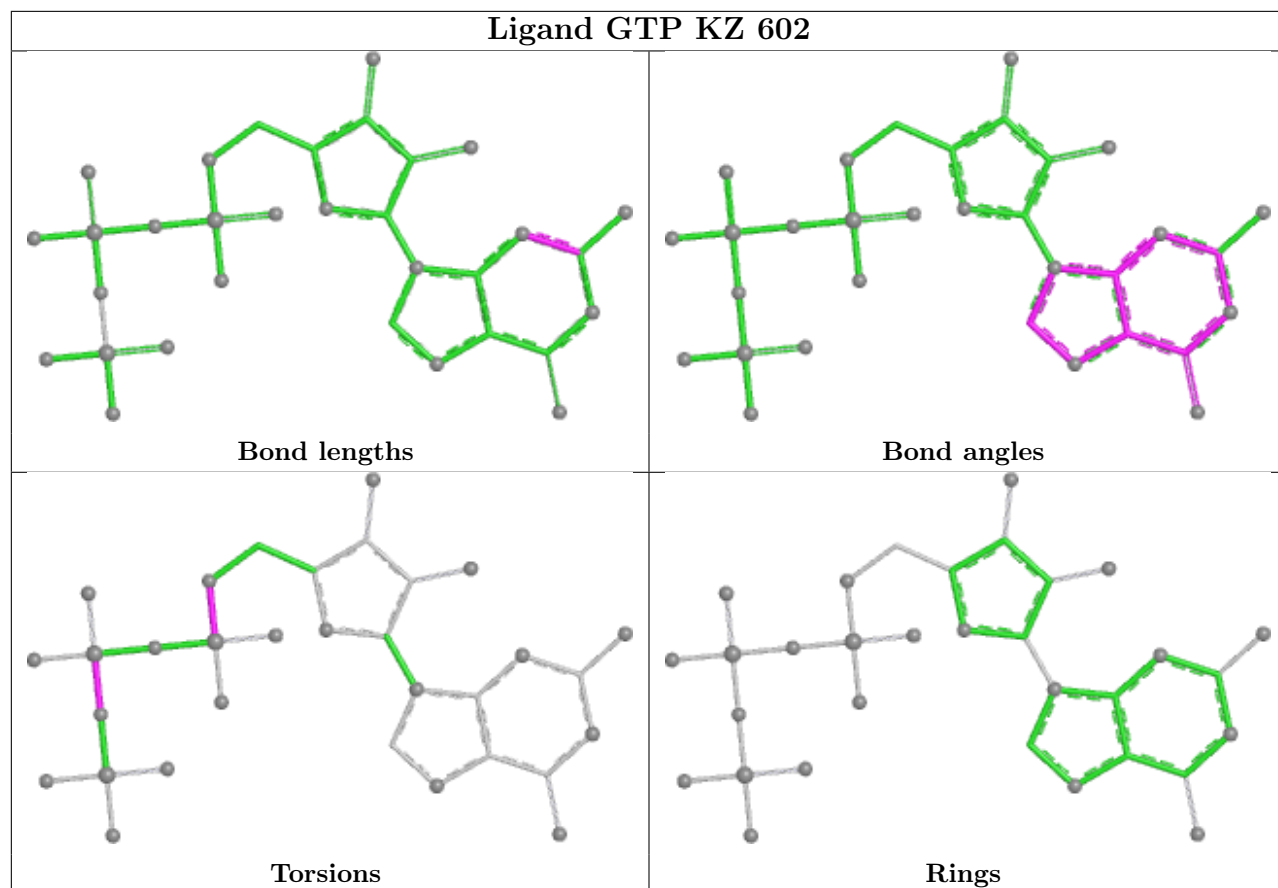




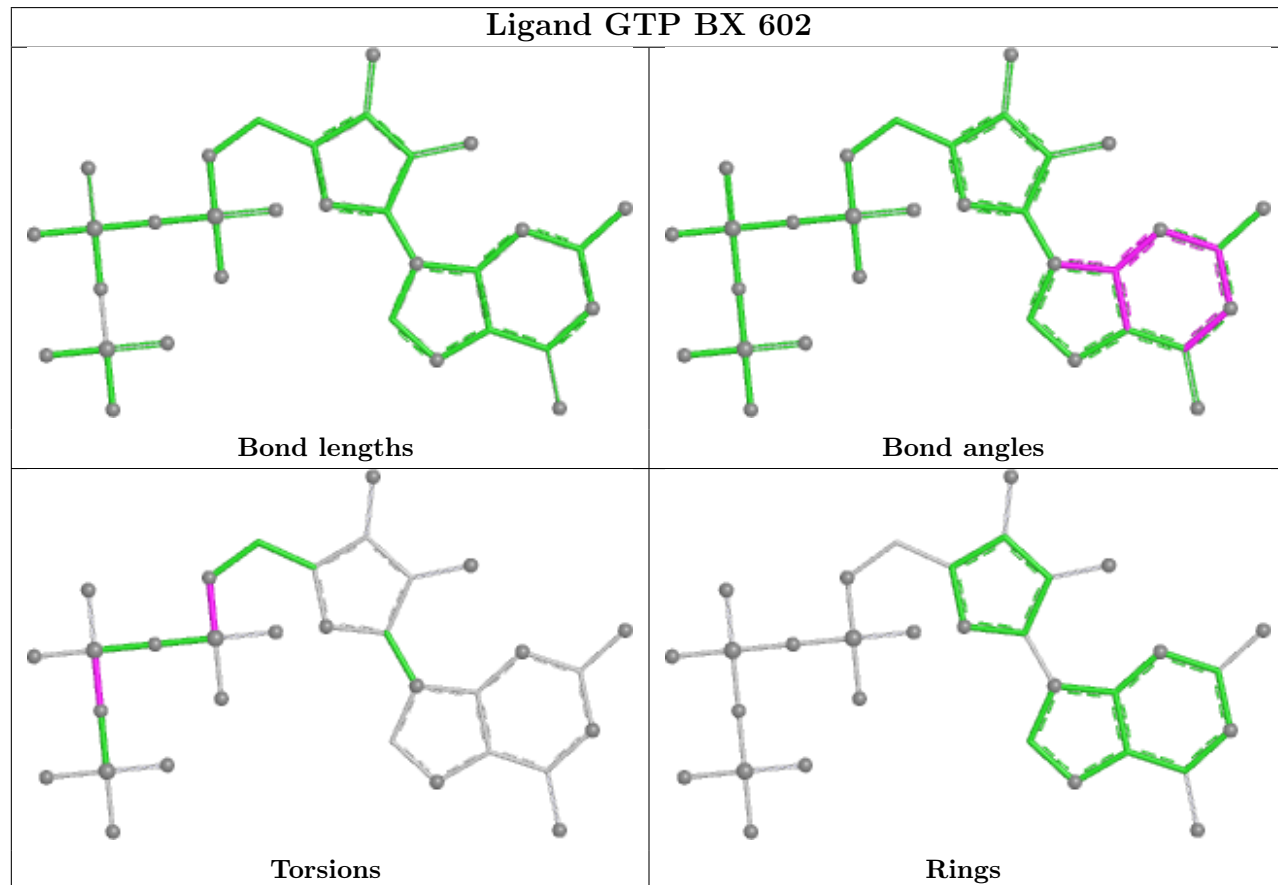


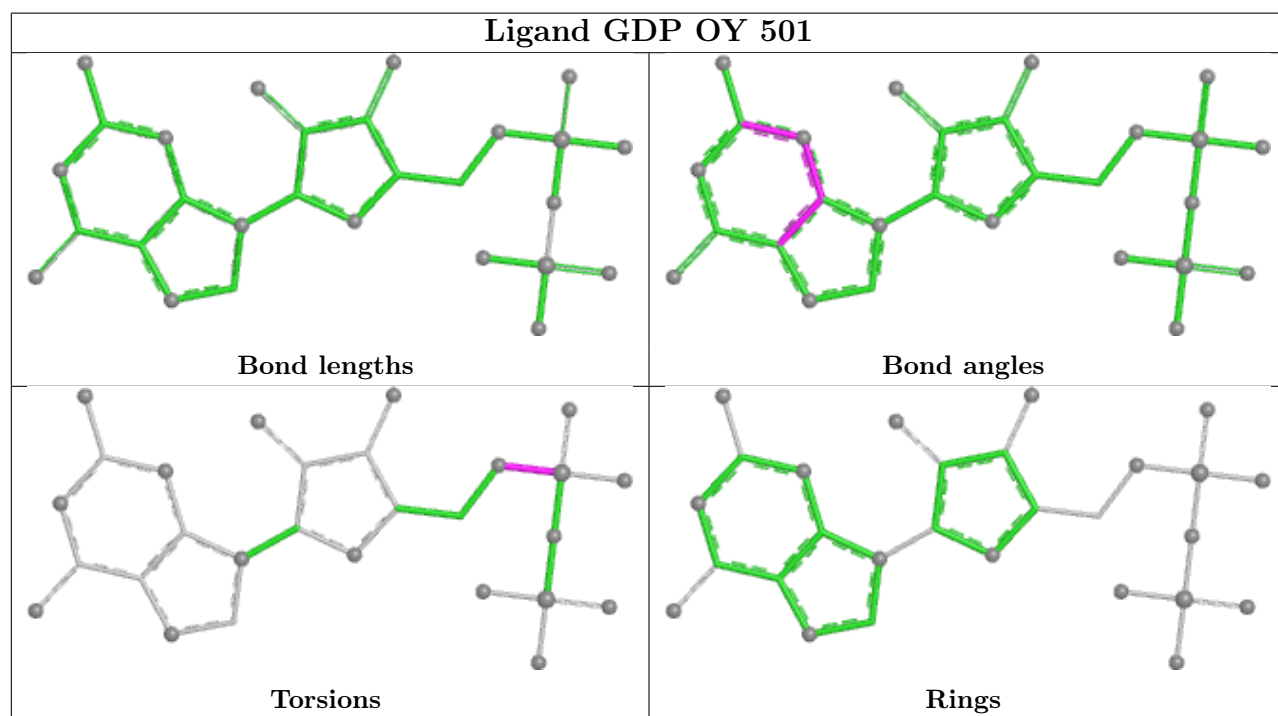
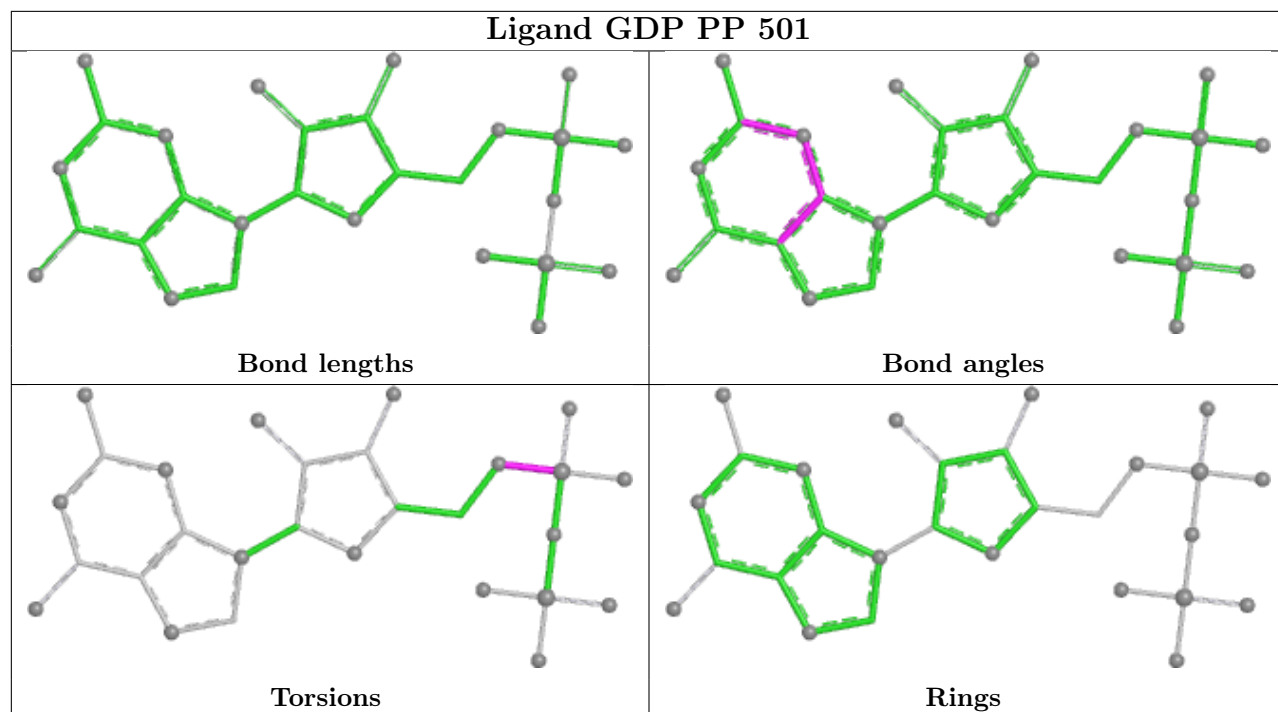


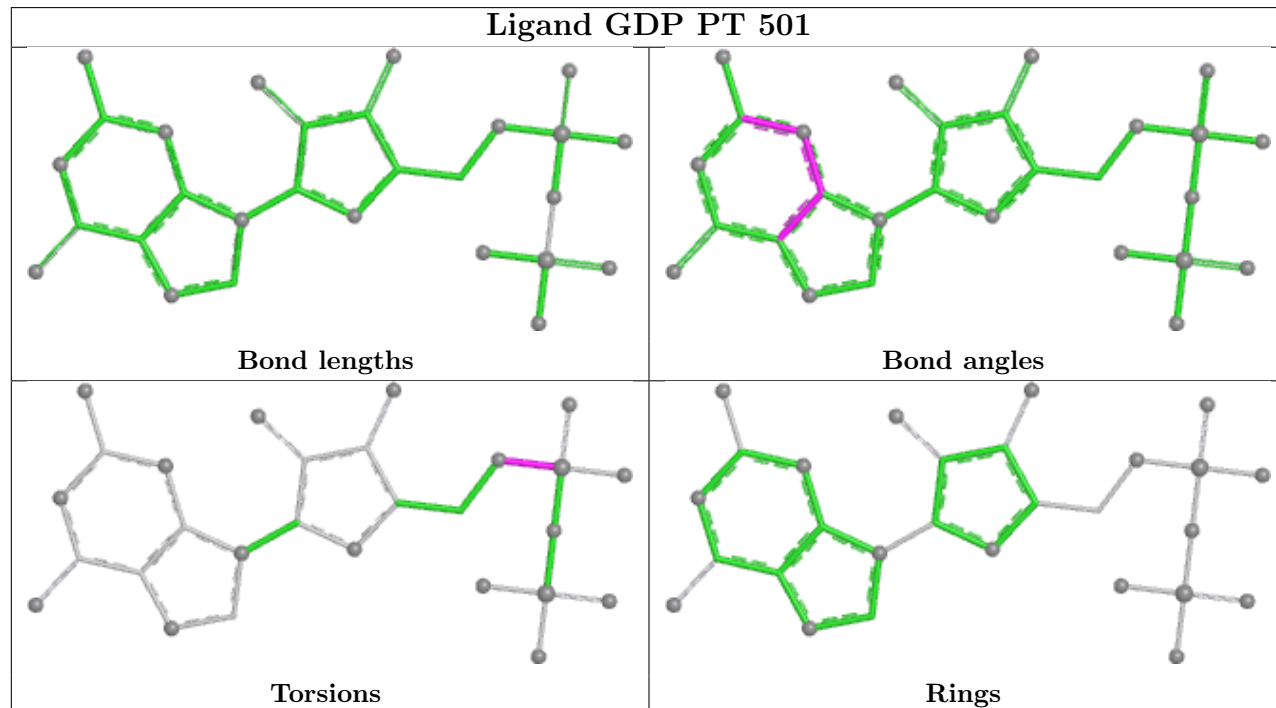
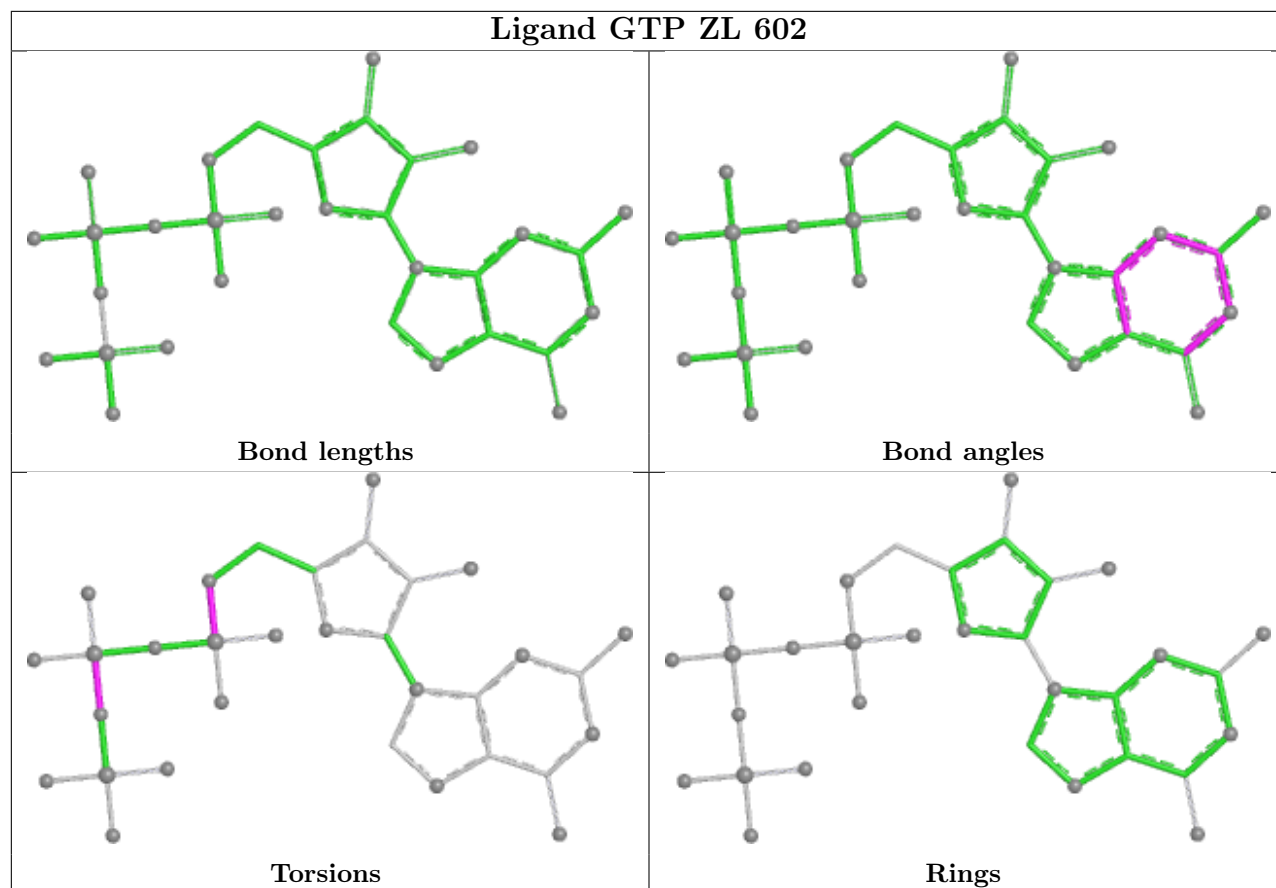
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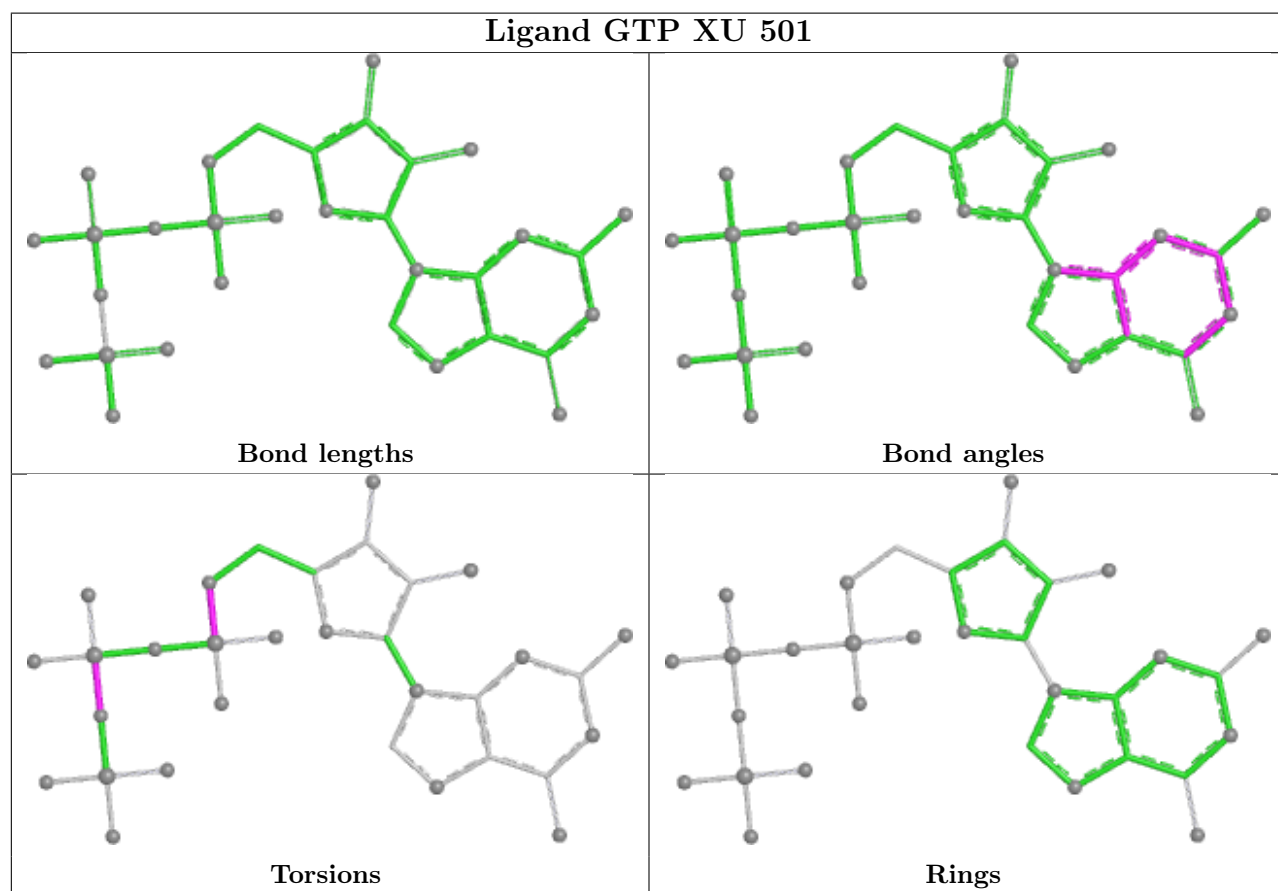
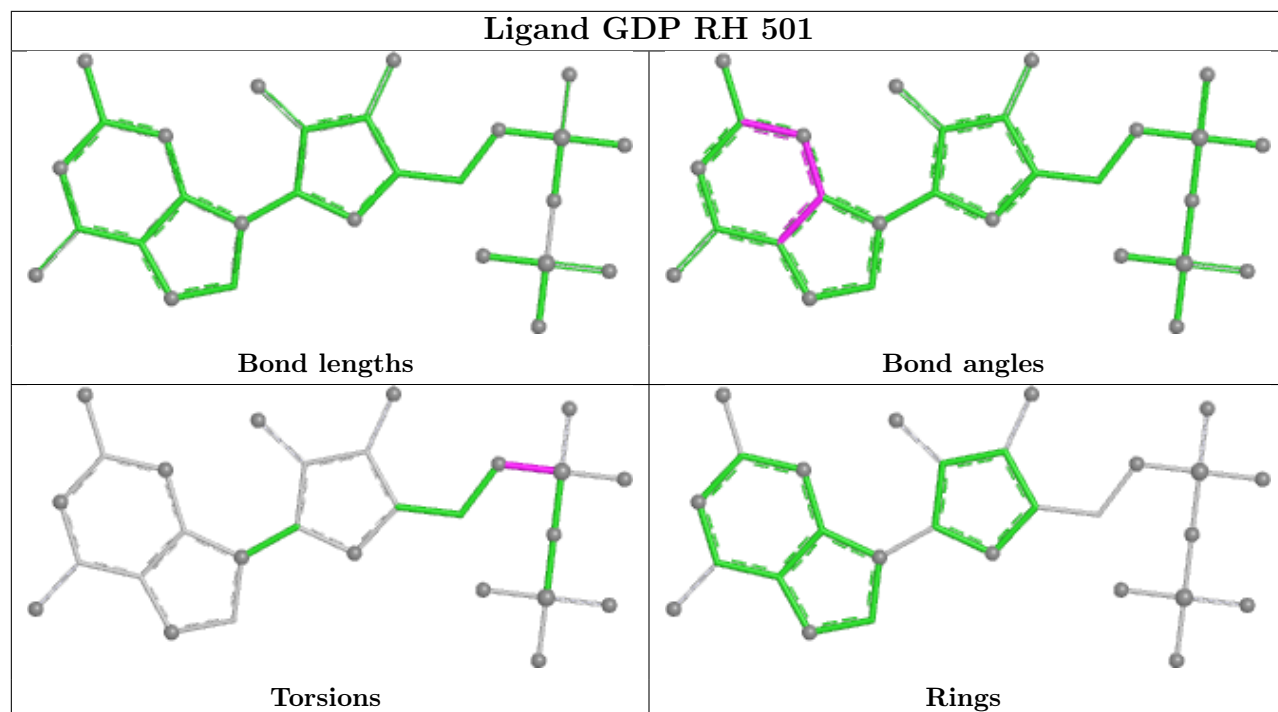


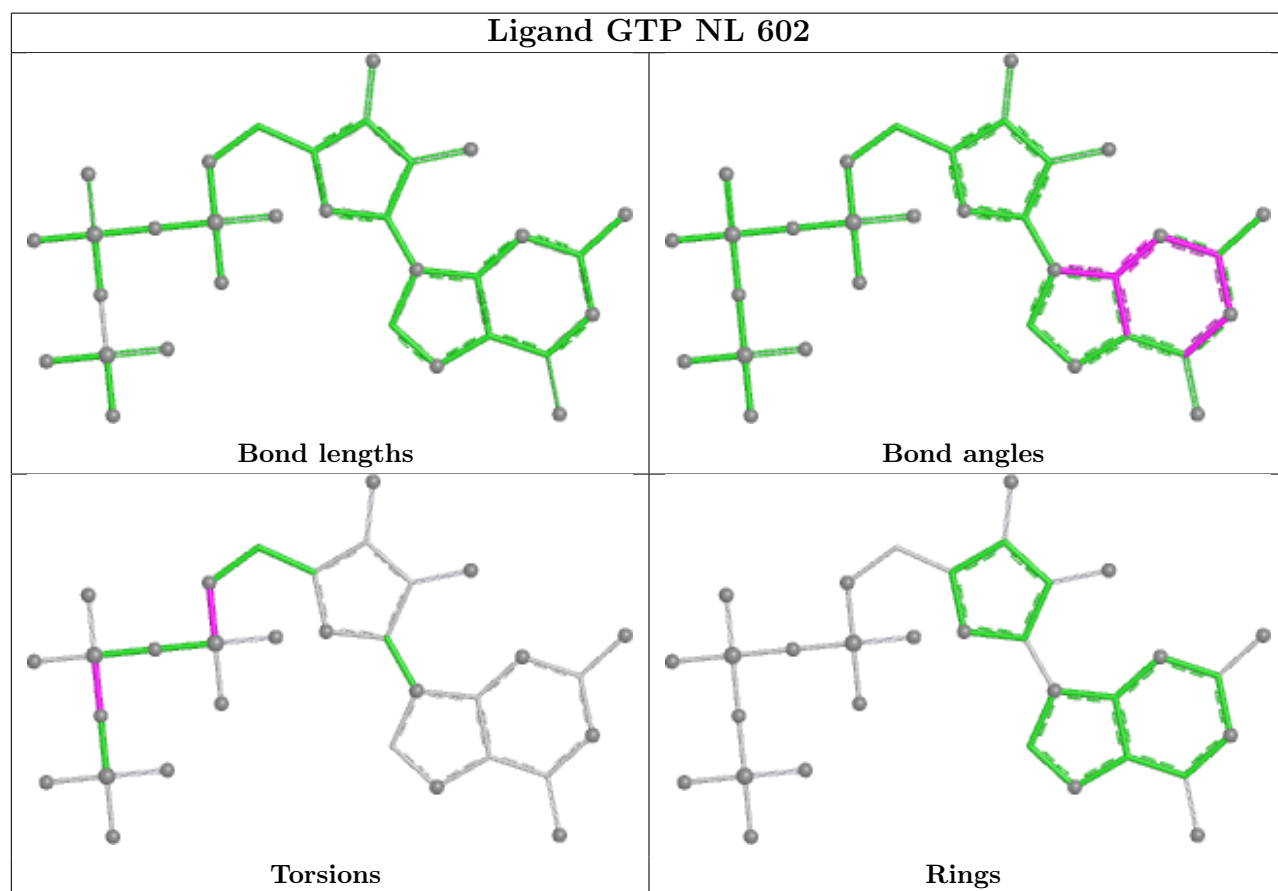
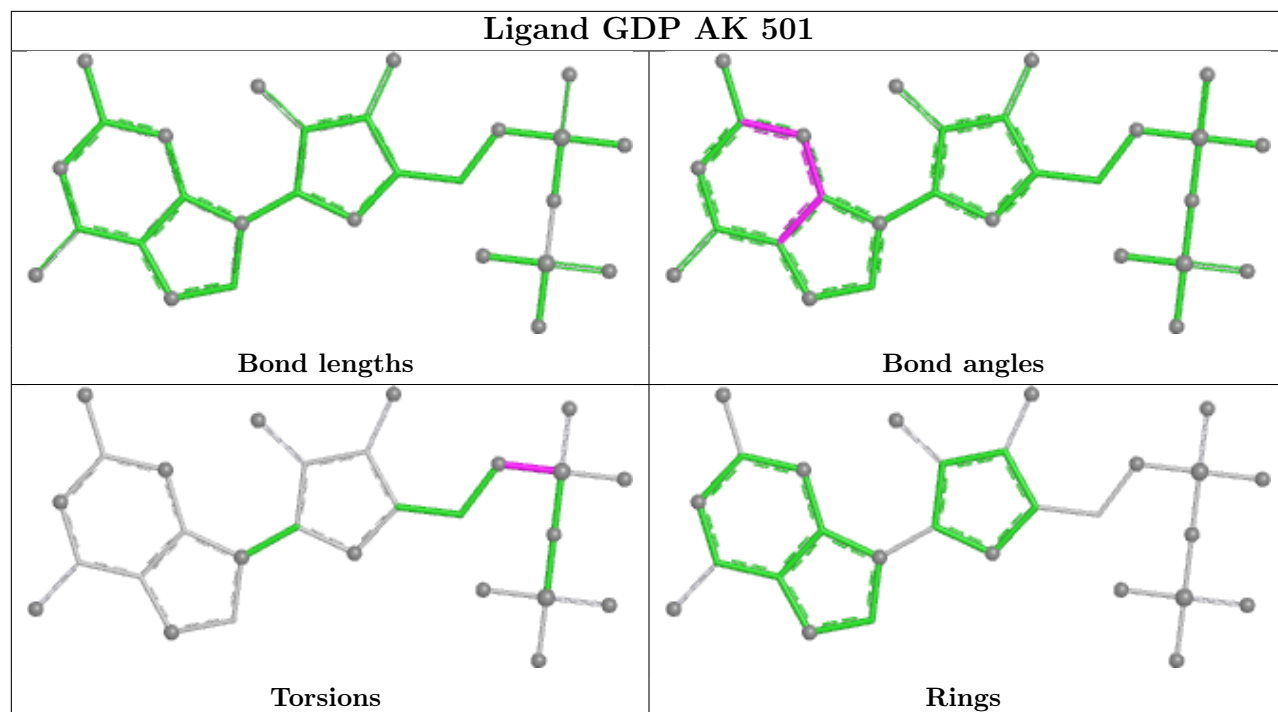
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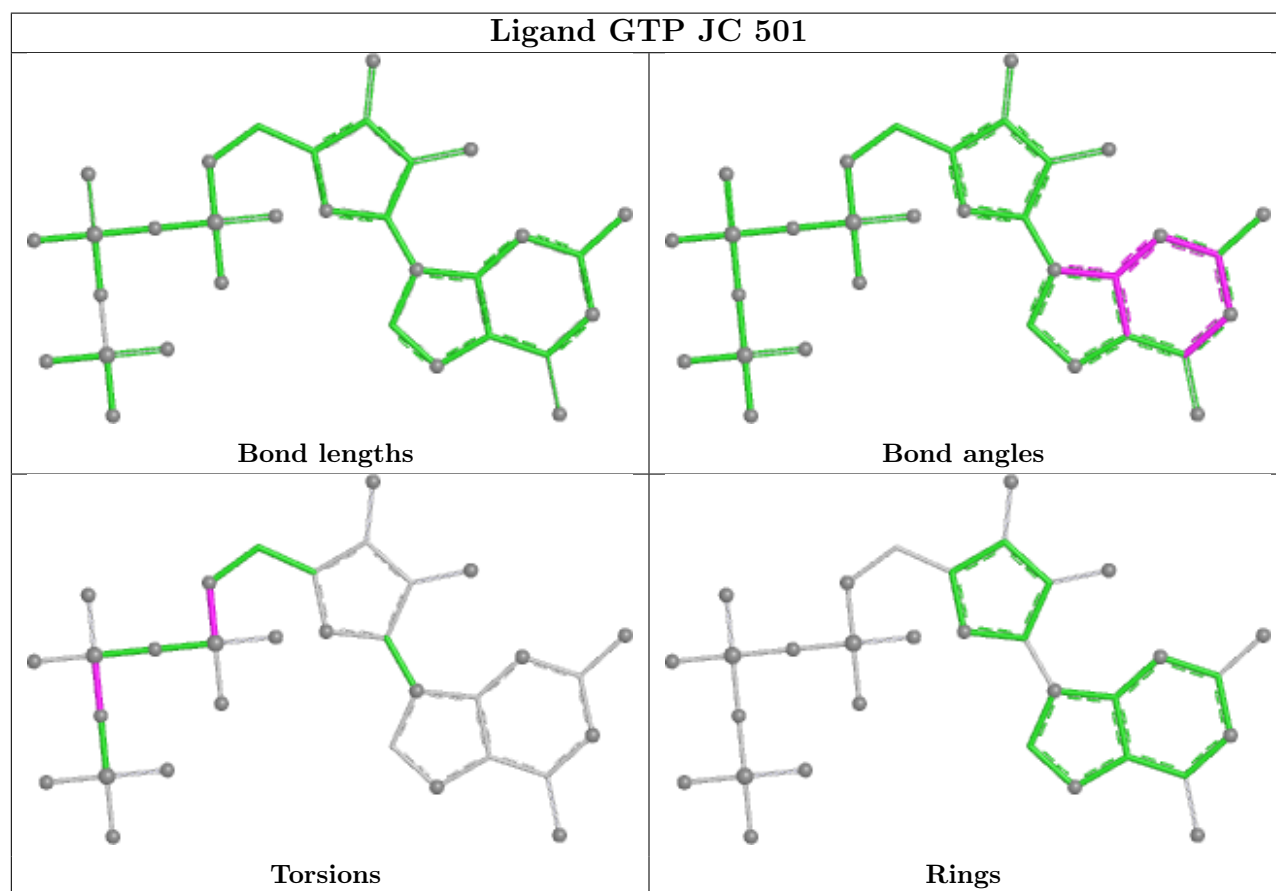
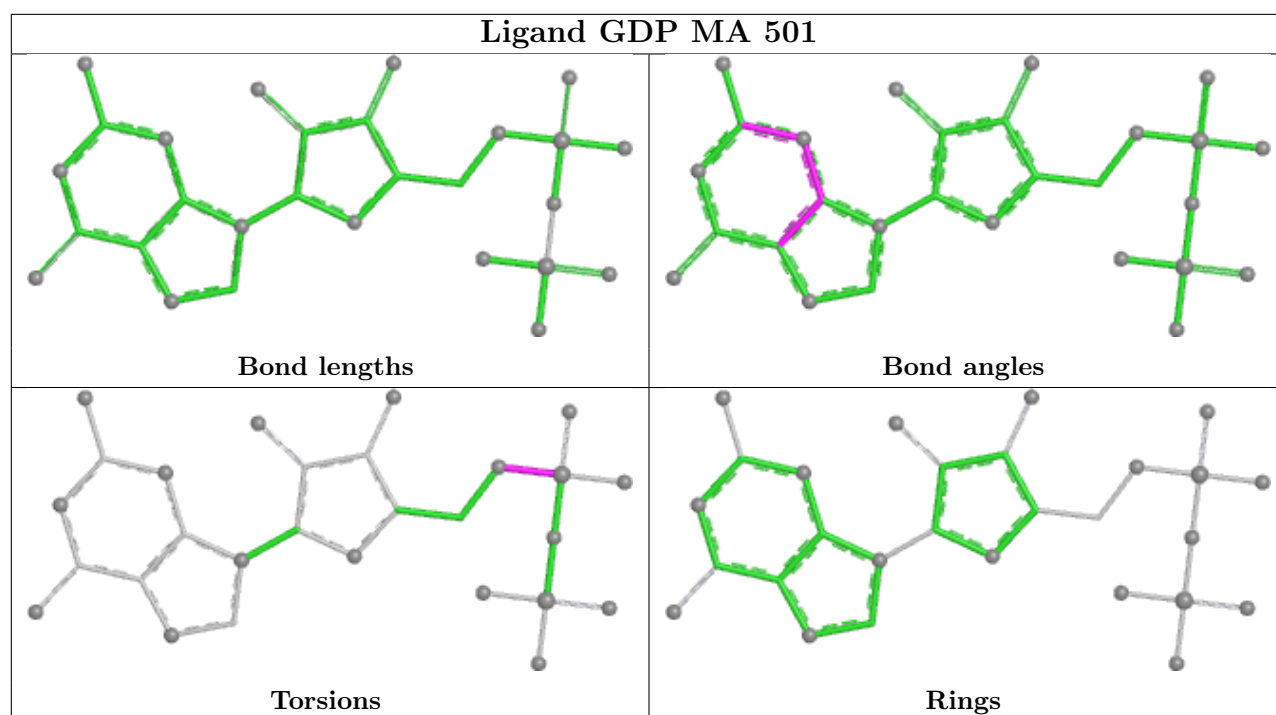




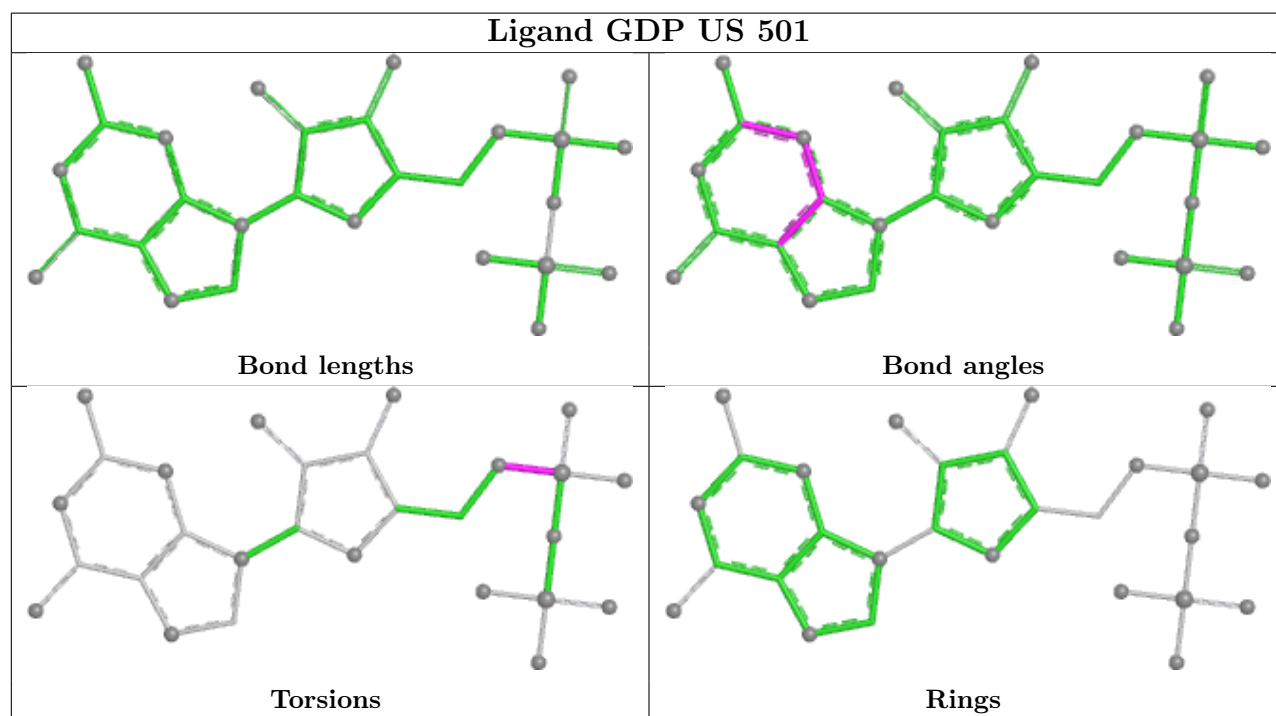
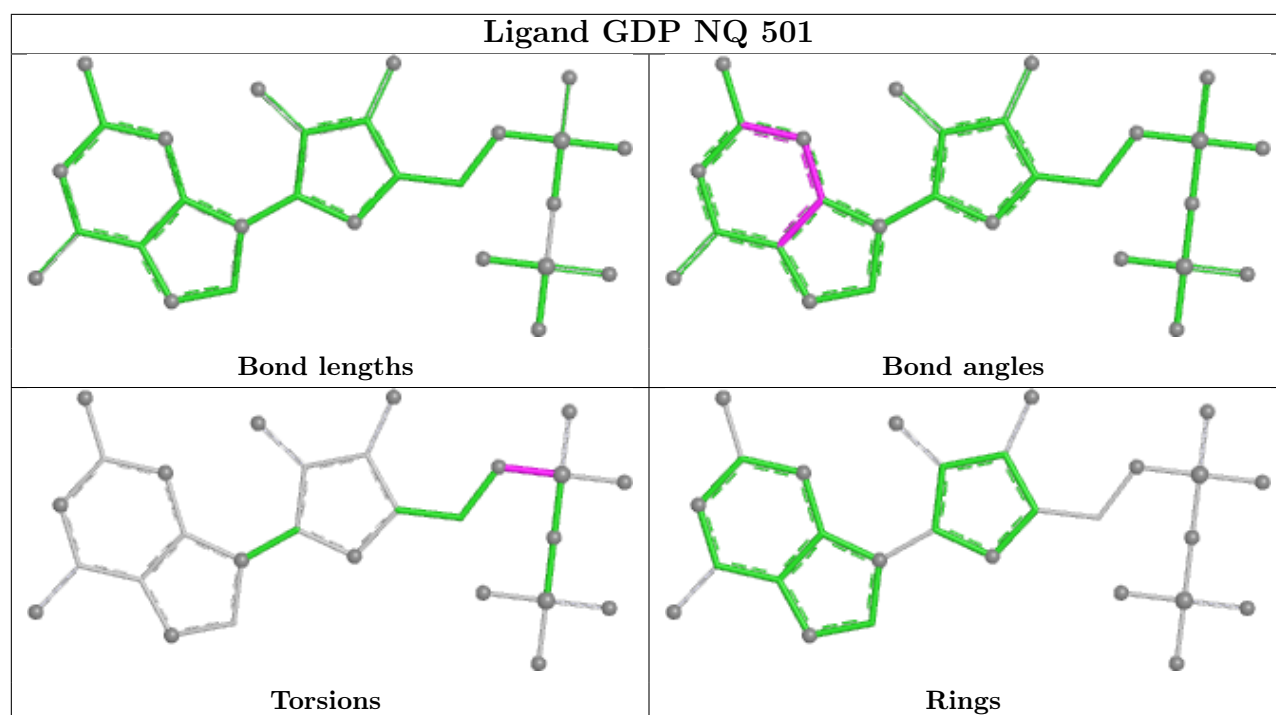


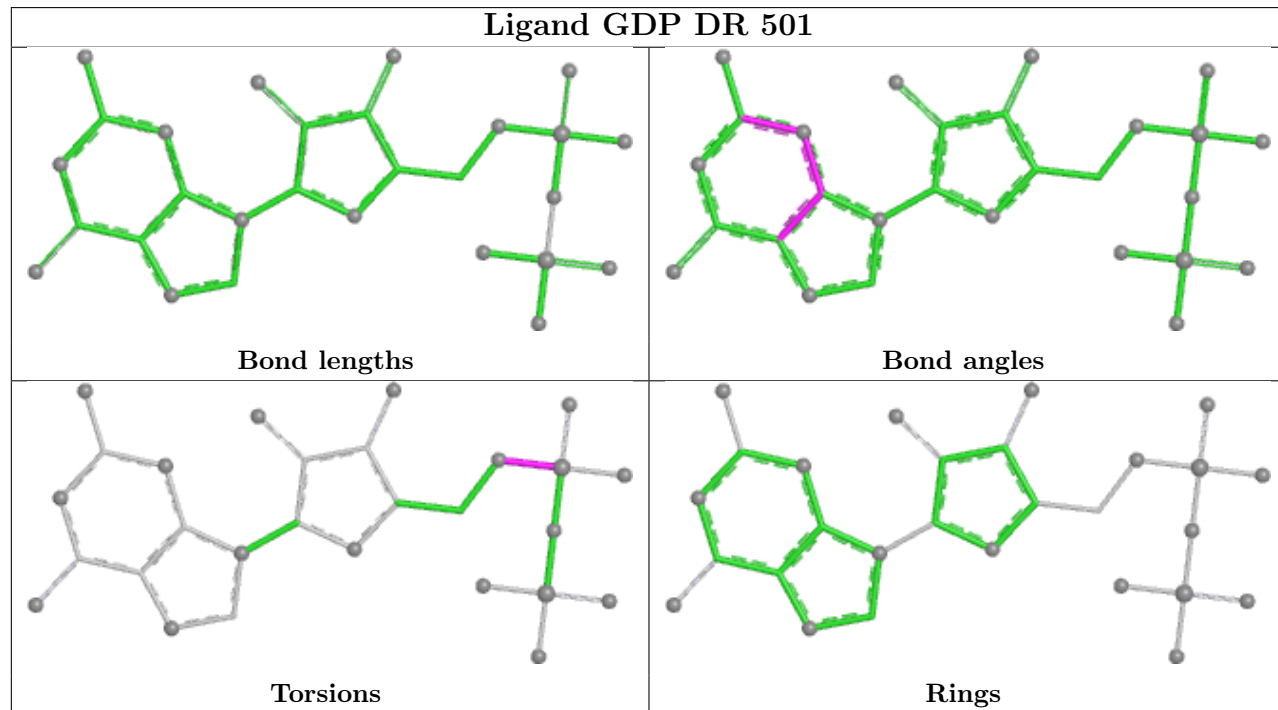
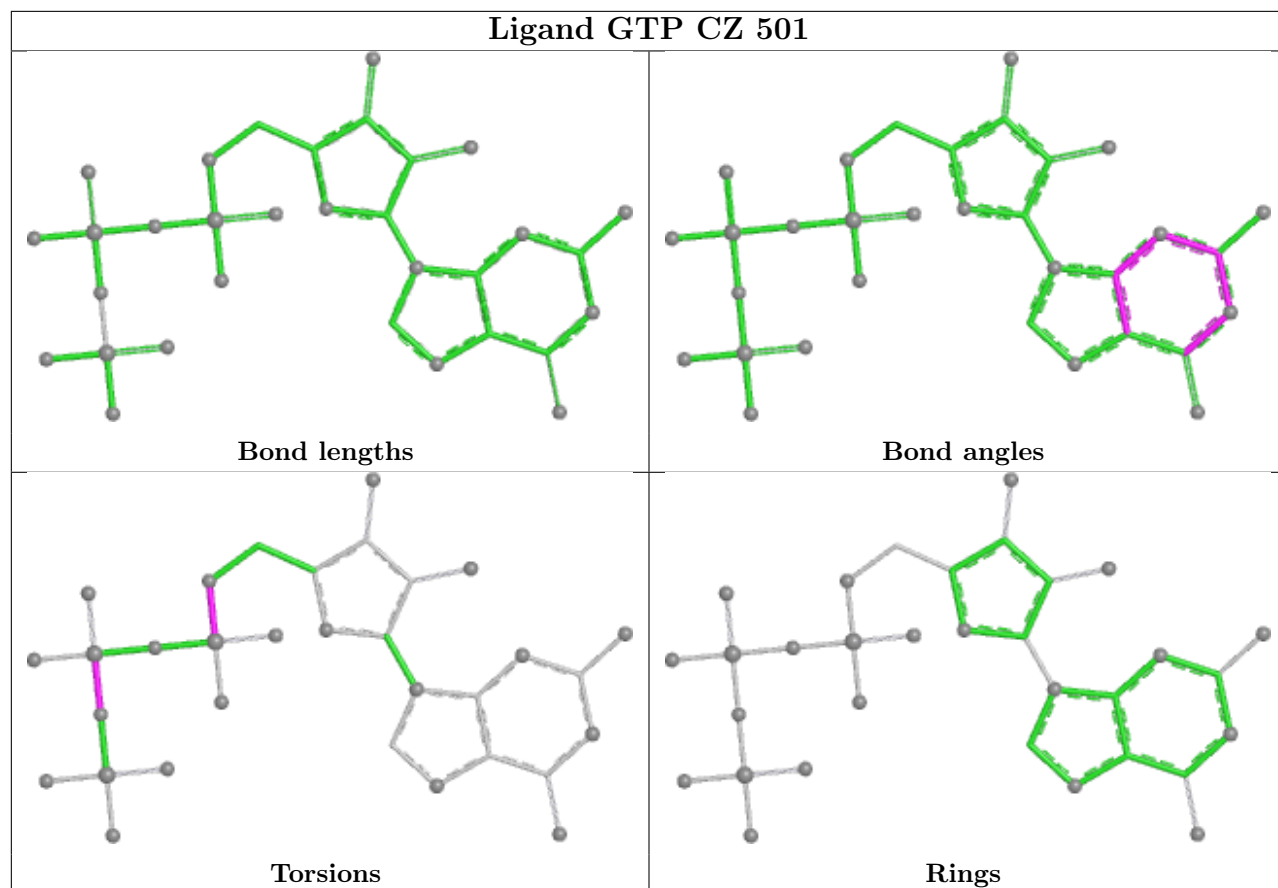


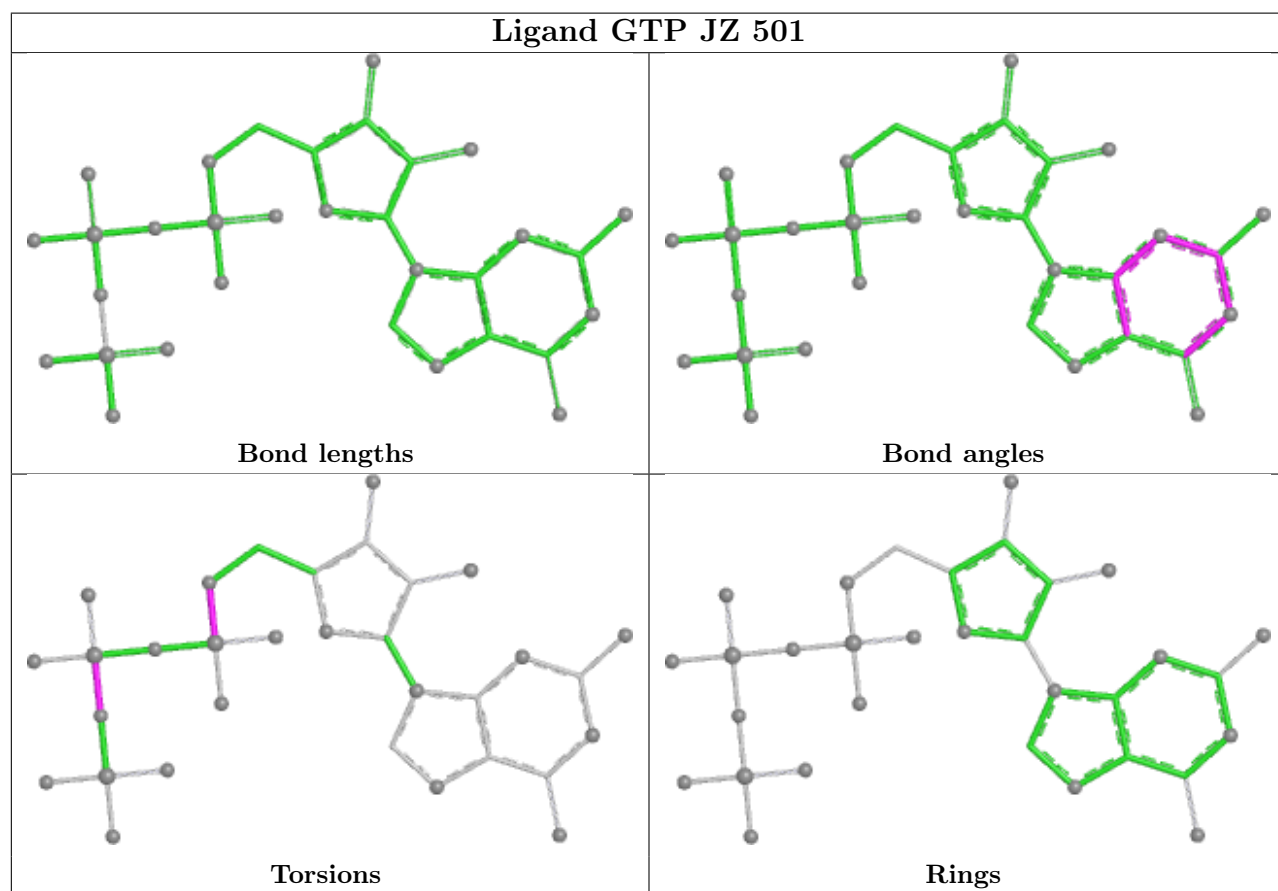
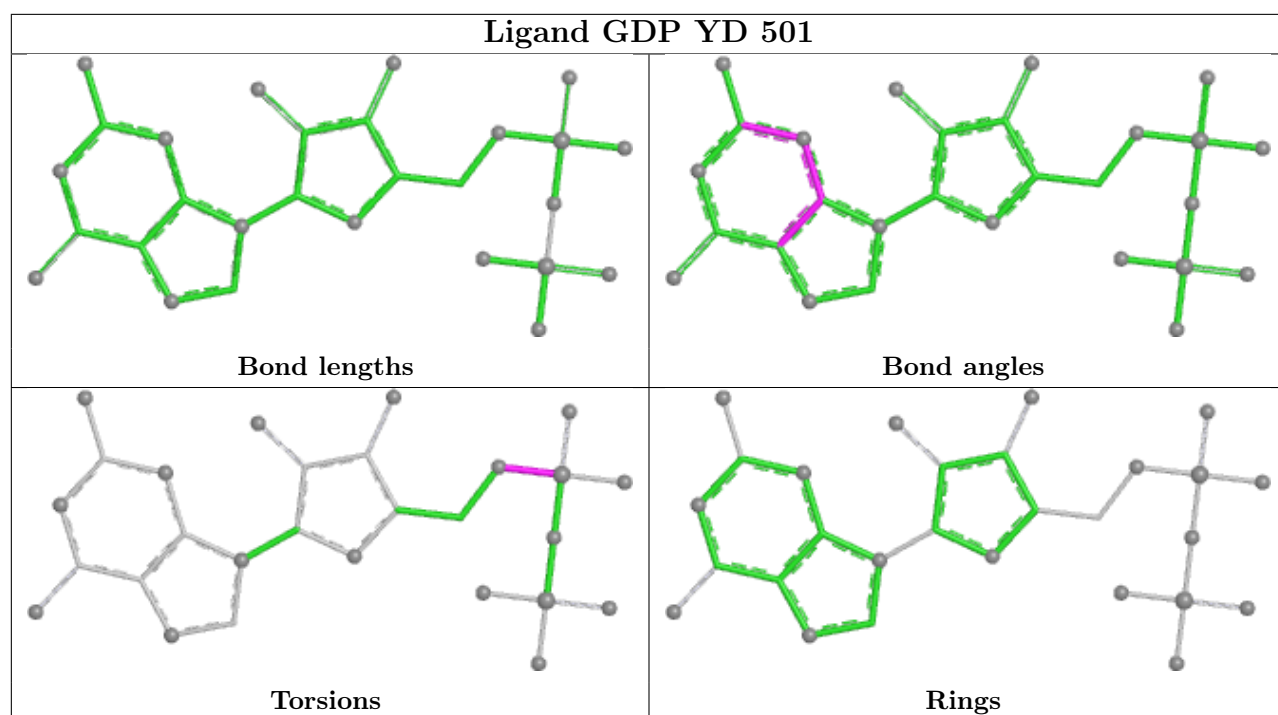




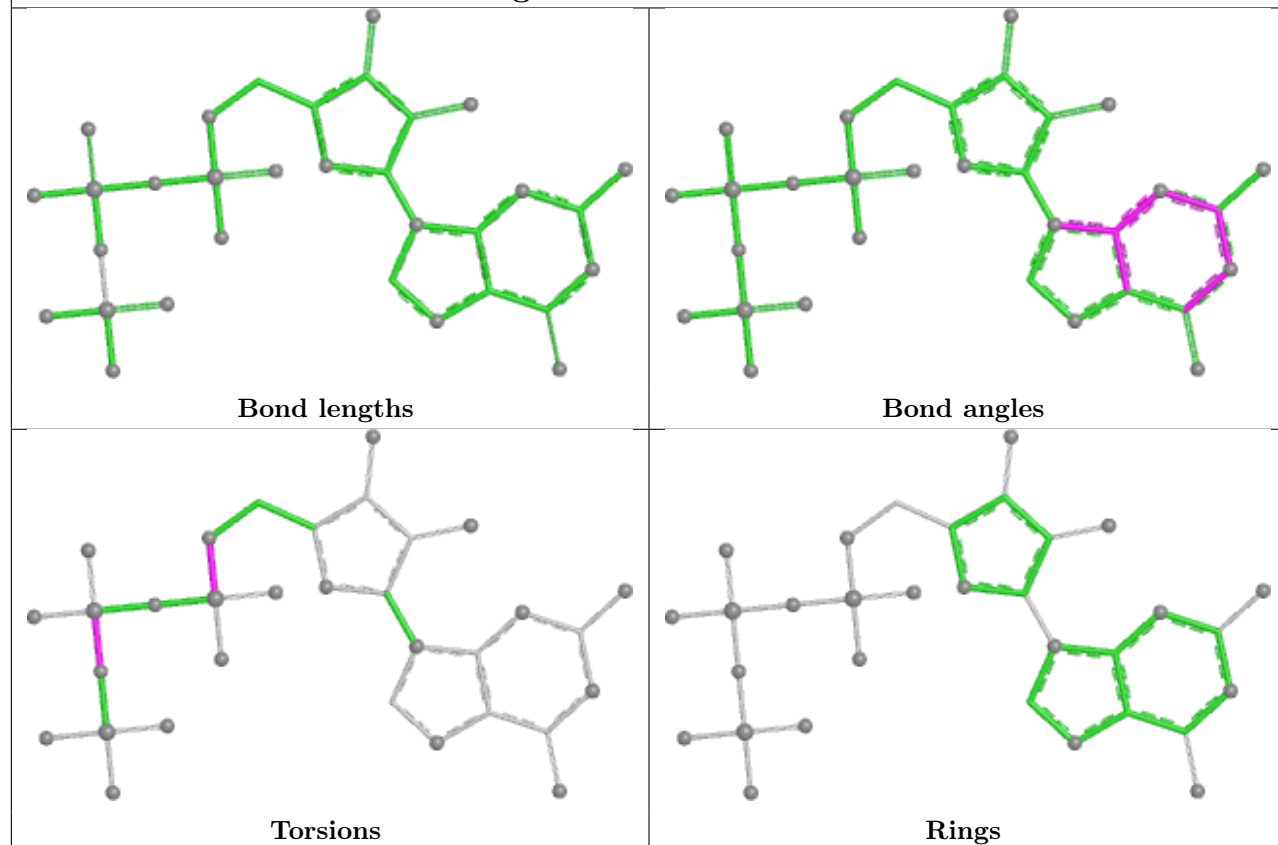




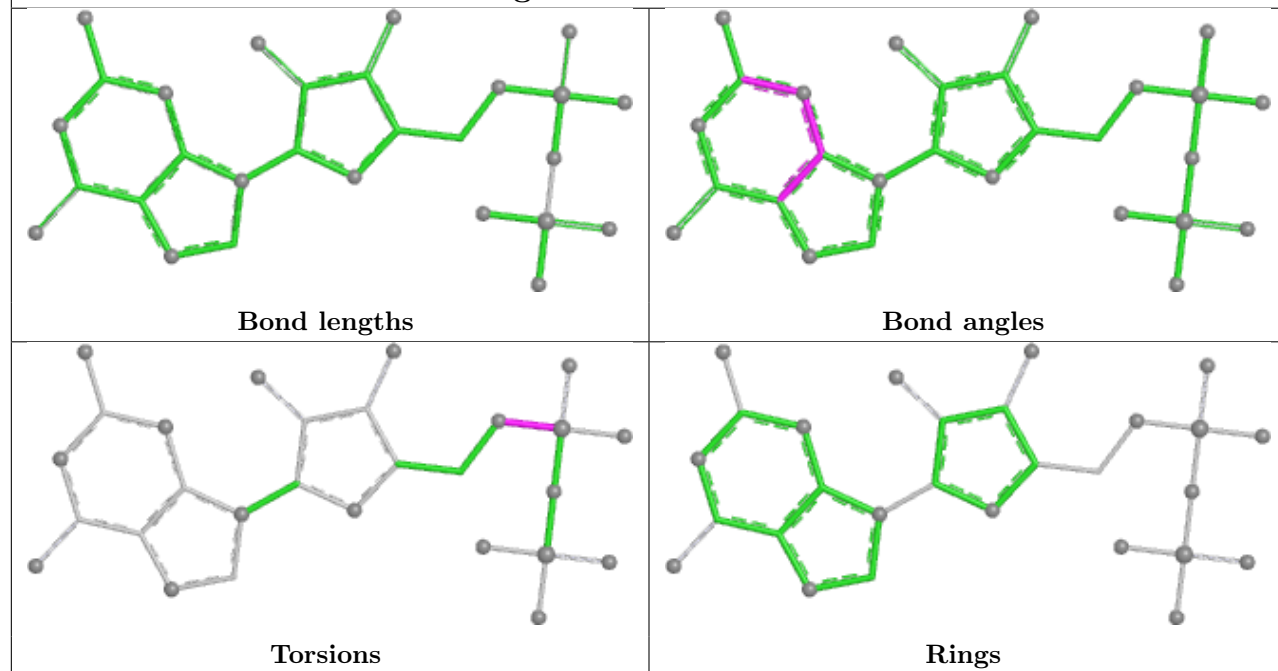


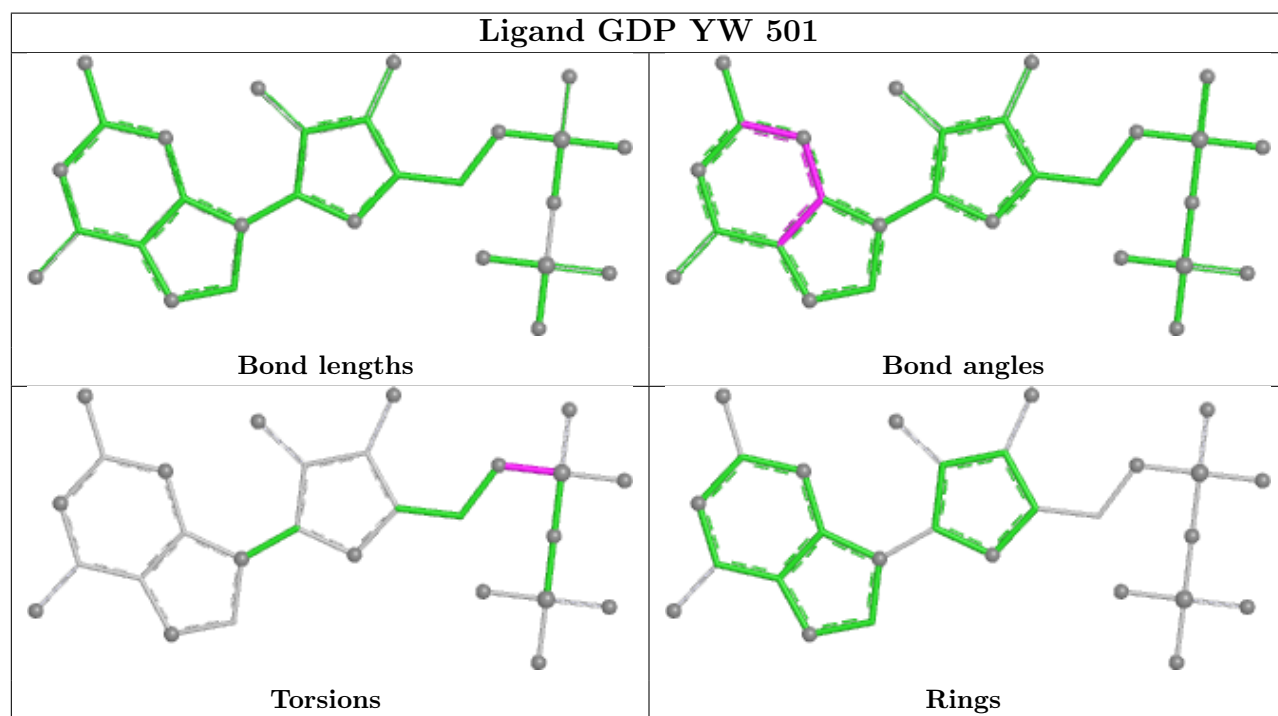
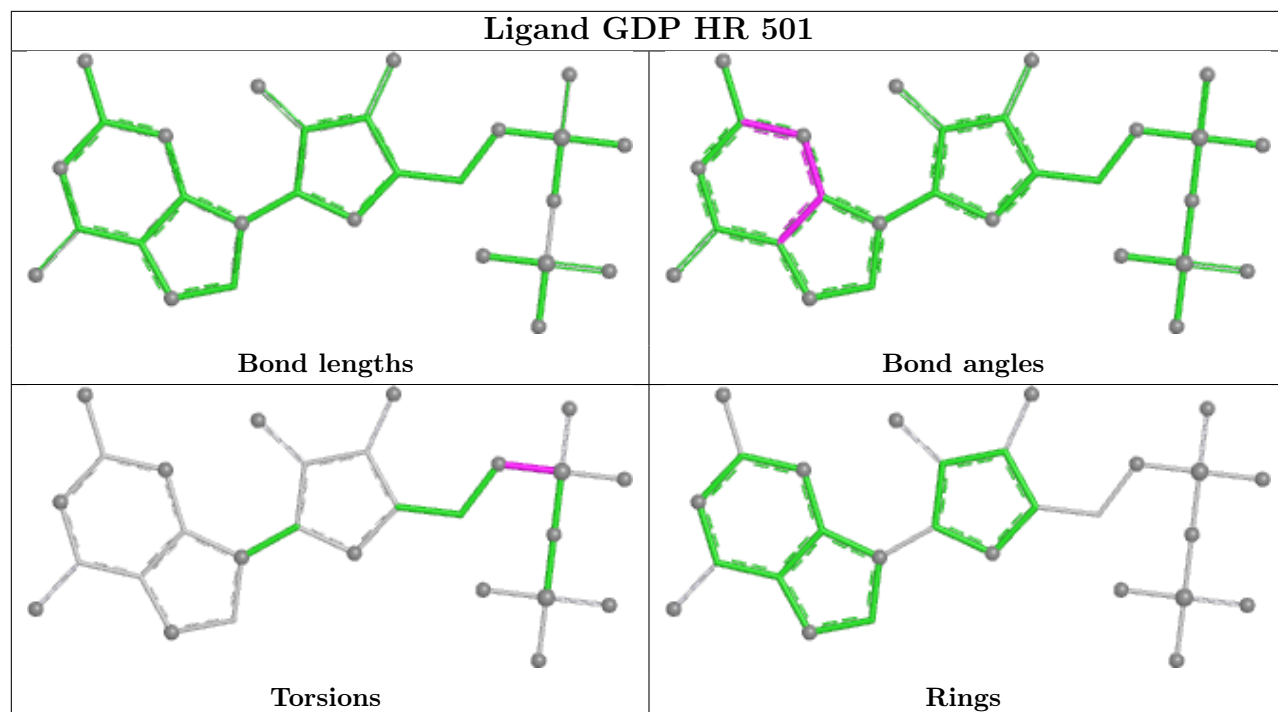


## Ligand GTP MH 501

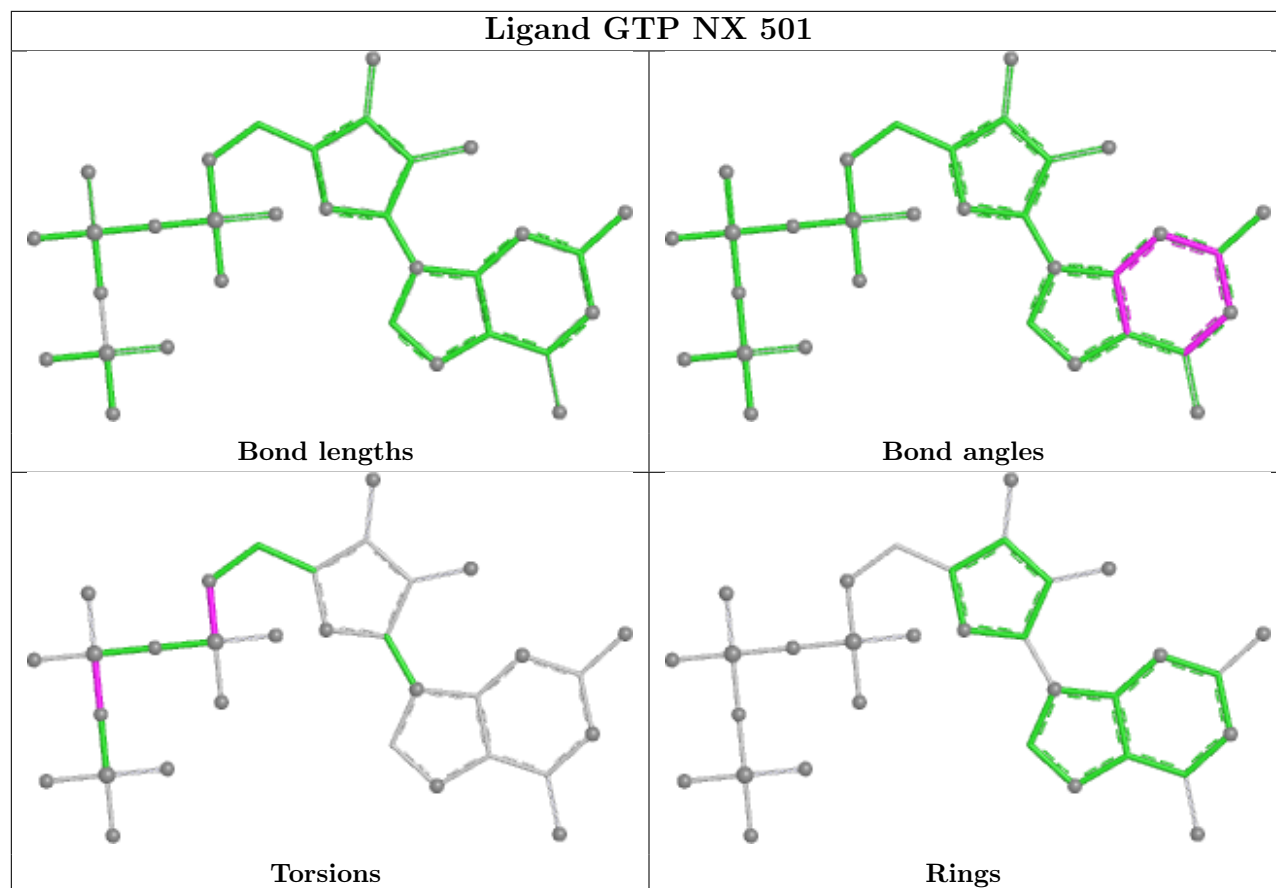


## Ligand GDP ME 501

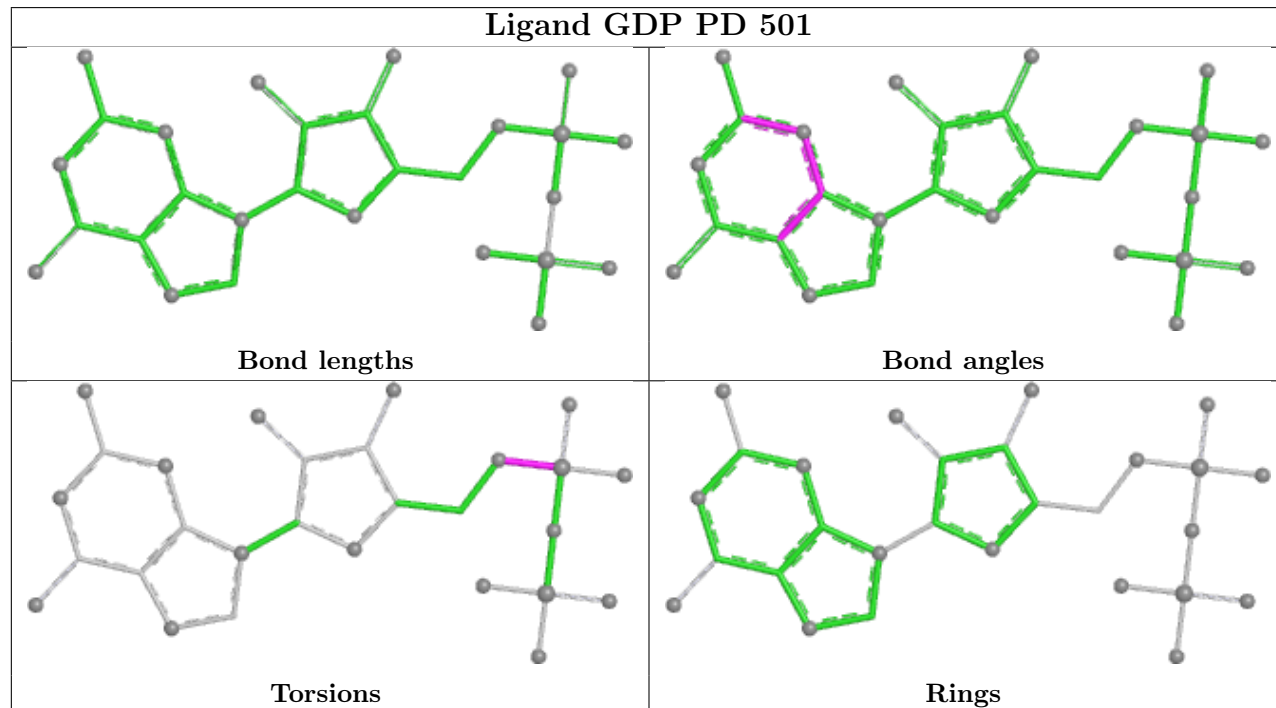


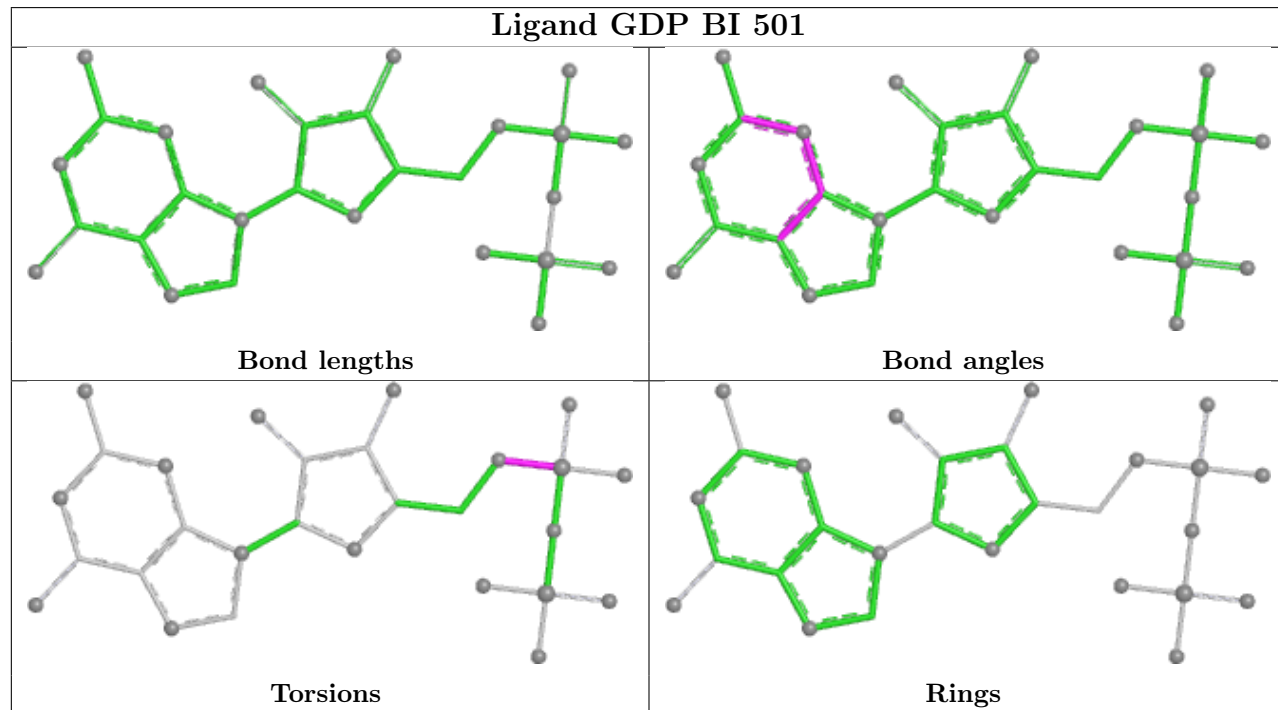
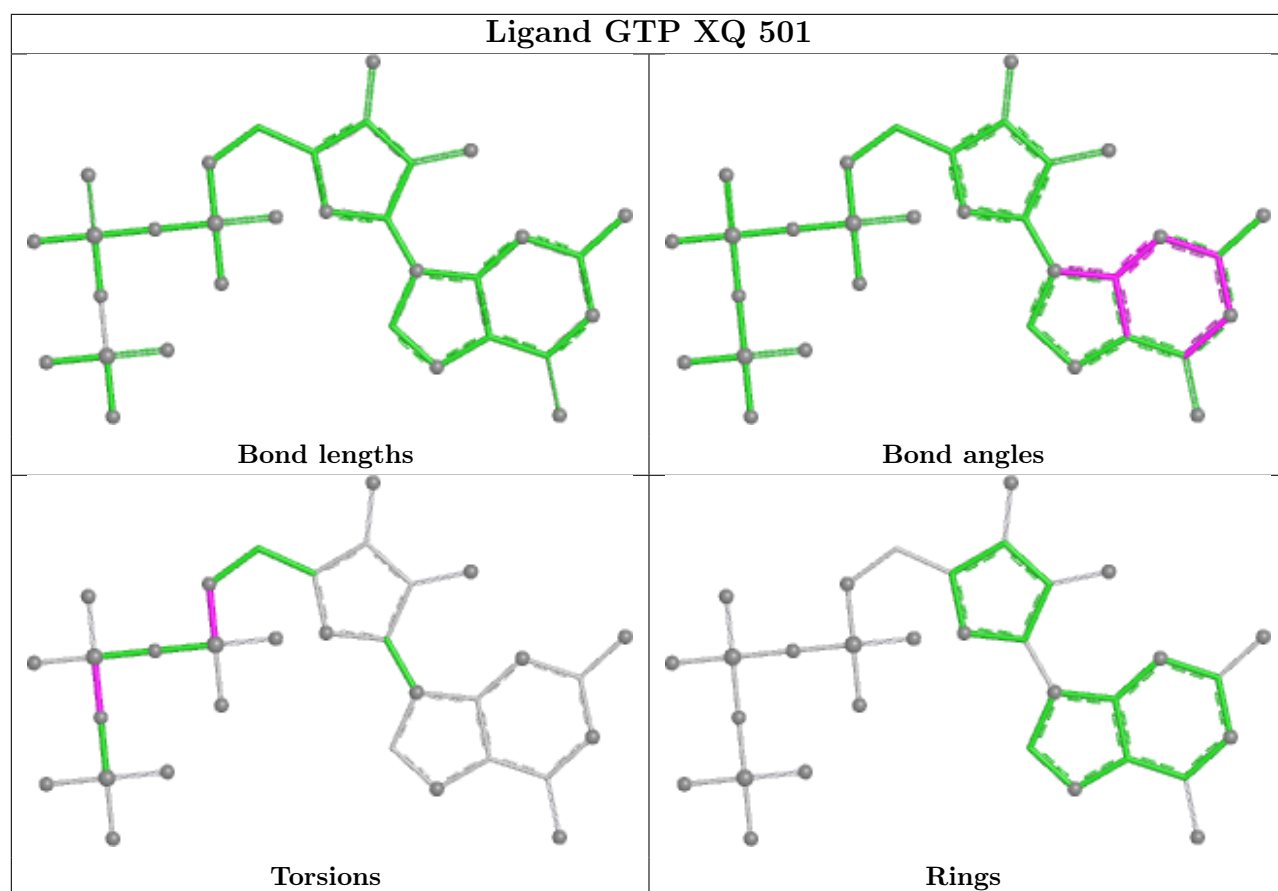


## Ligand GTP NX 501

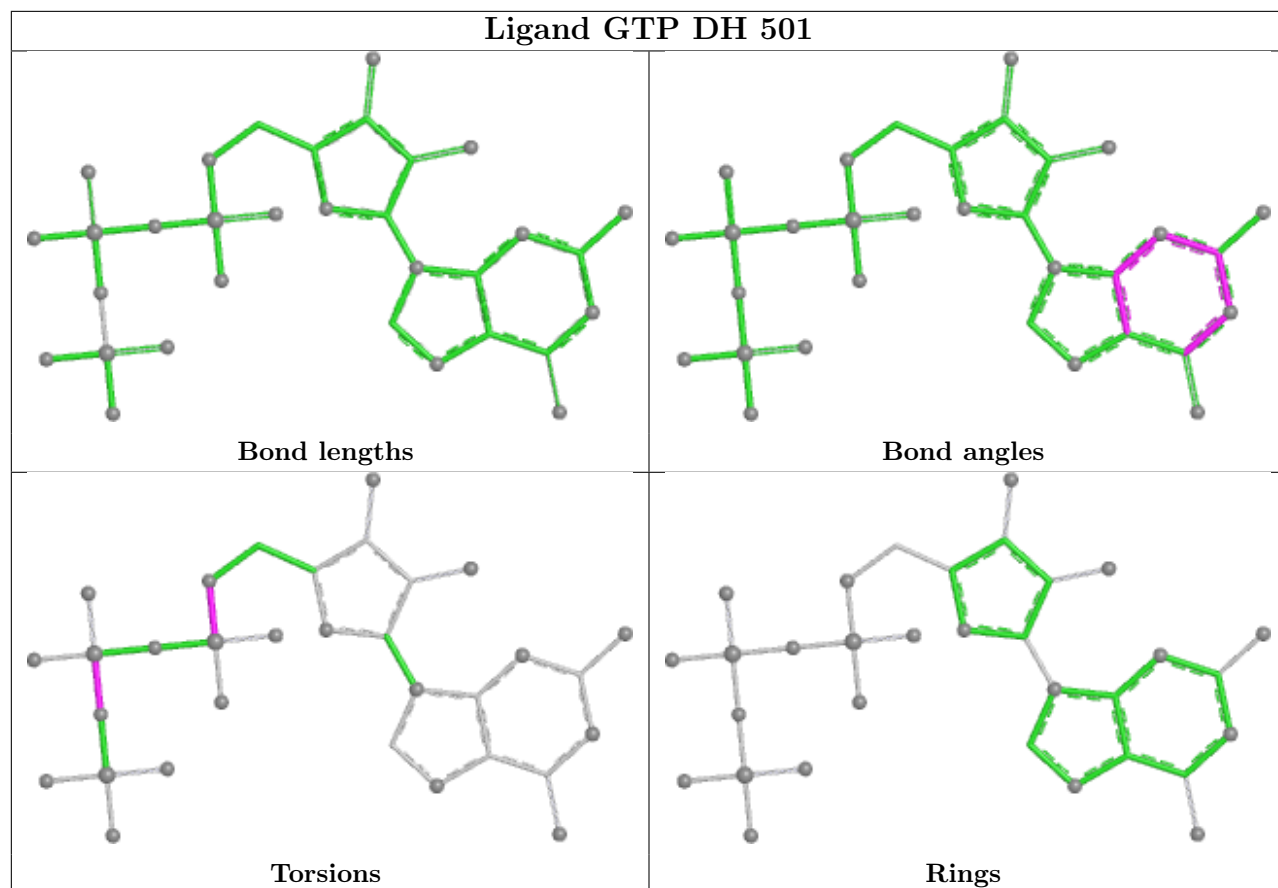


## Ligand GDP PD 501

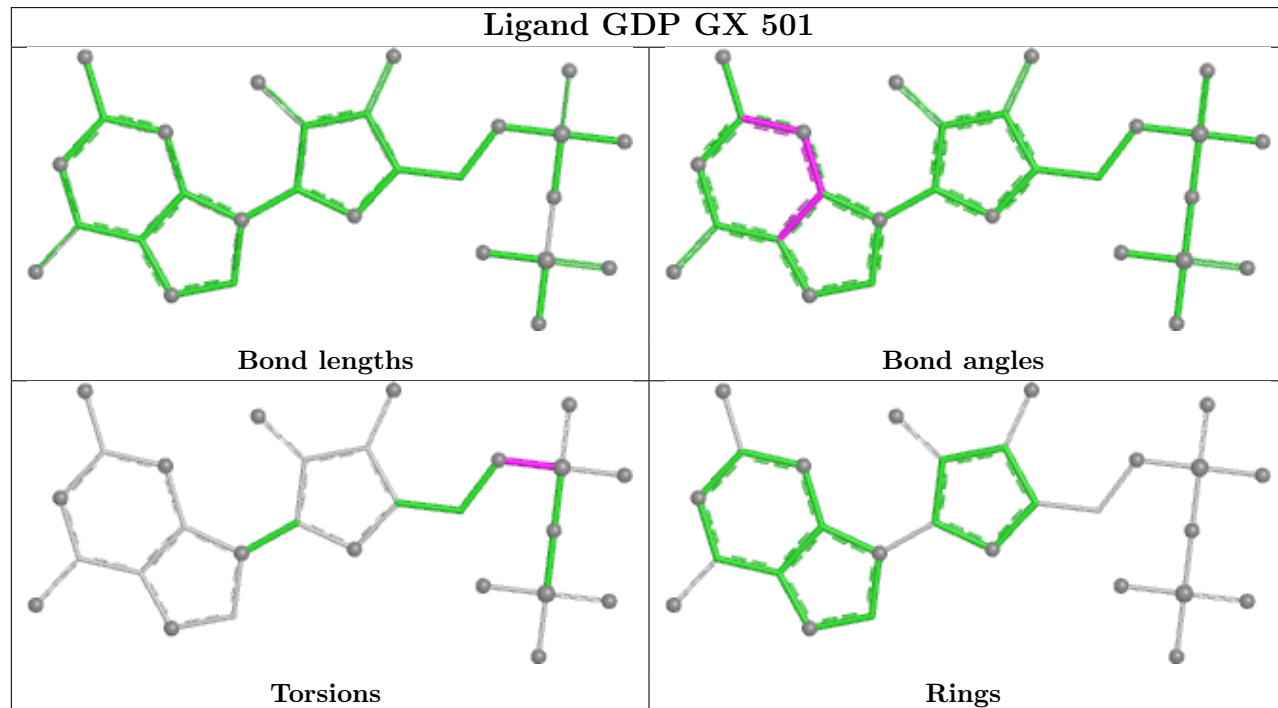




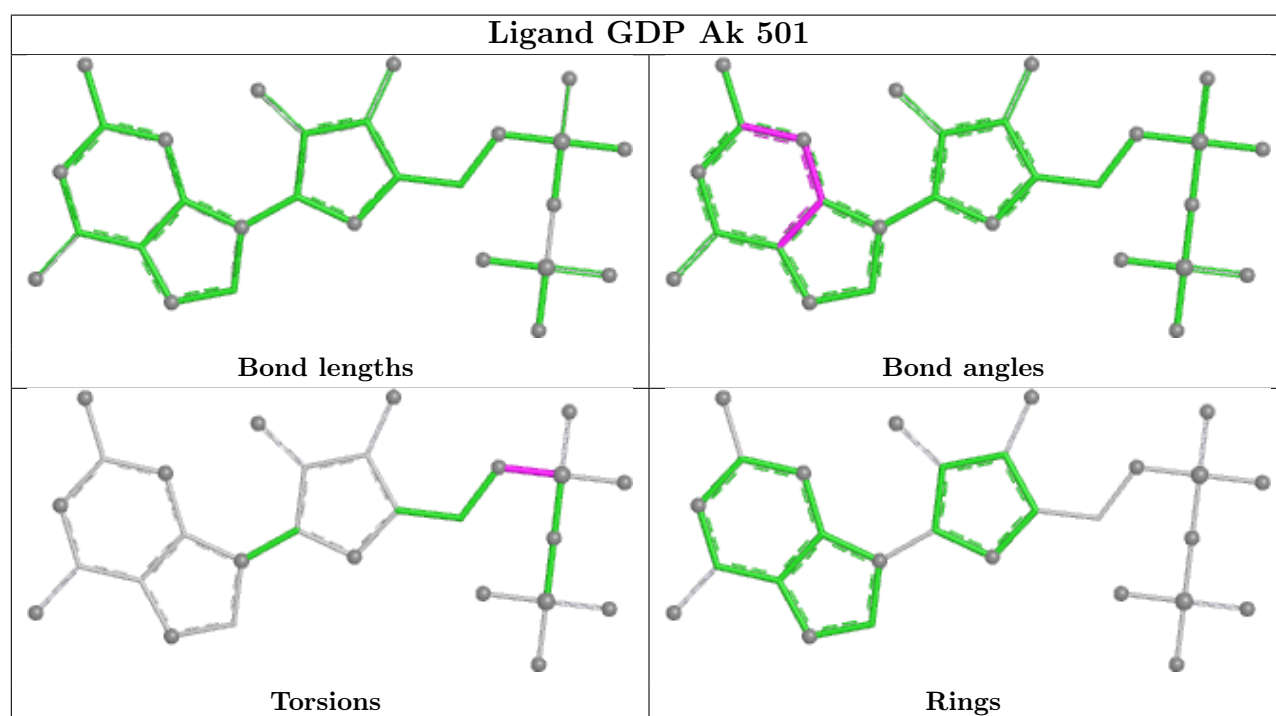
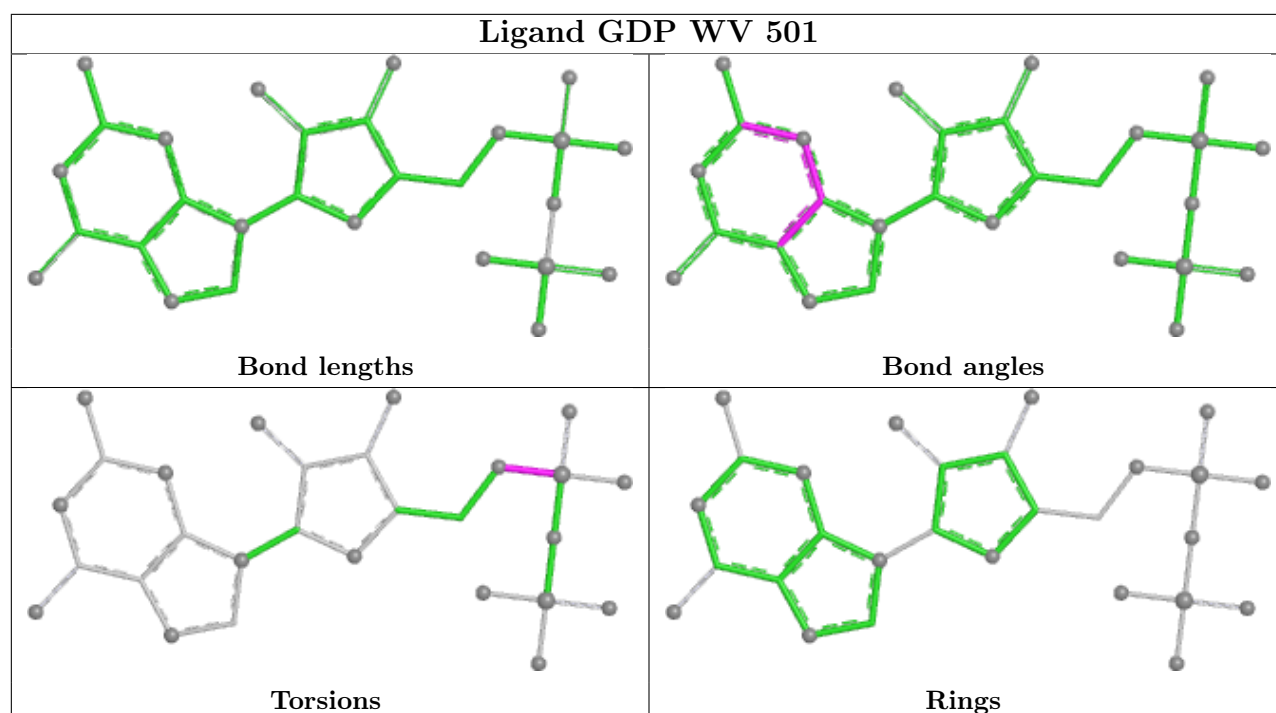
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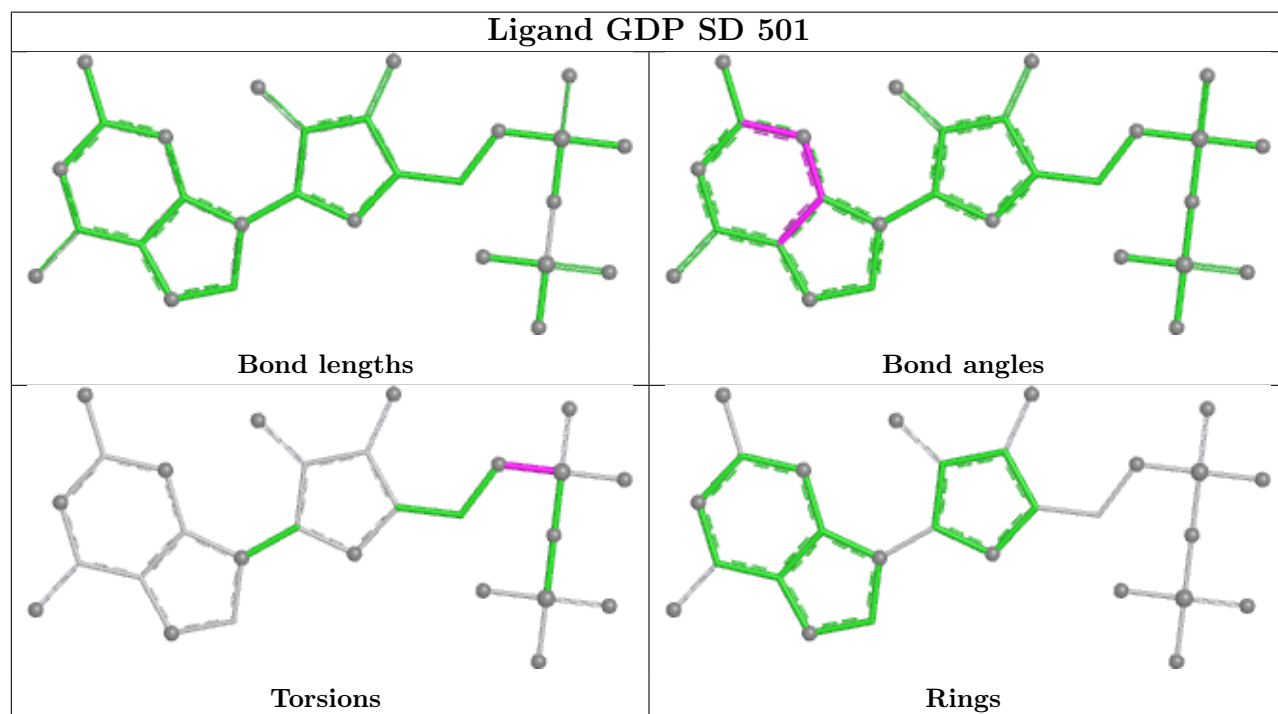
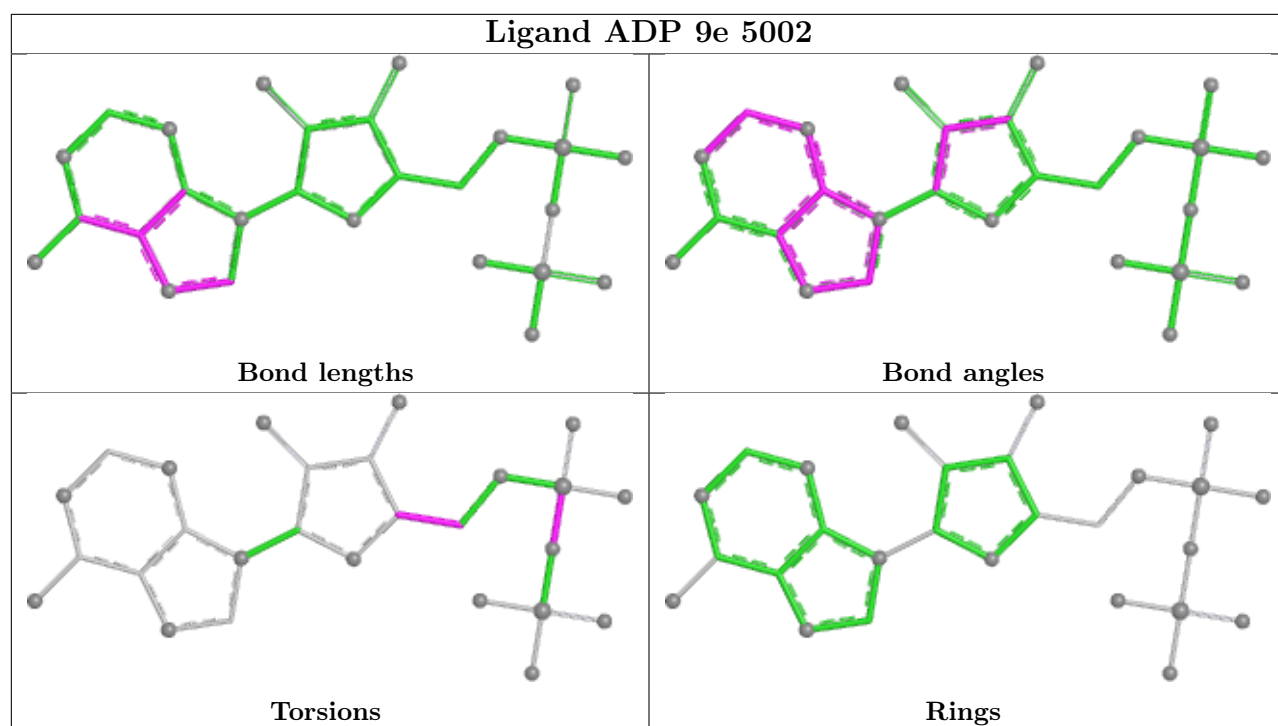


## Ligand GDP GX 501

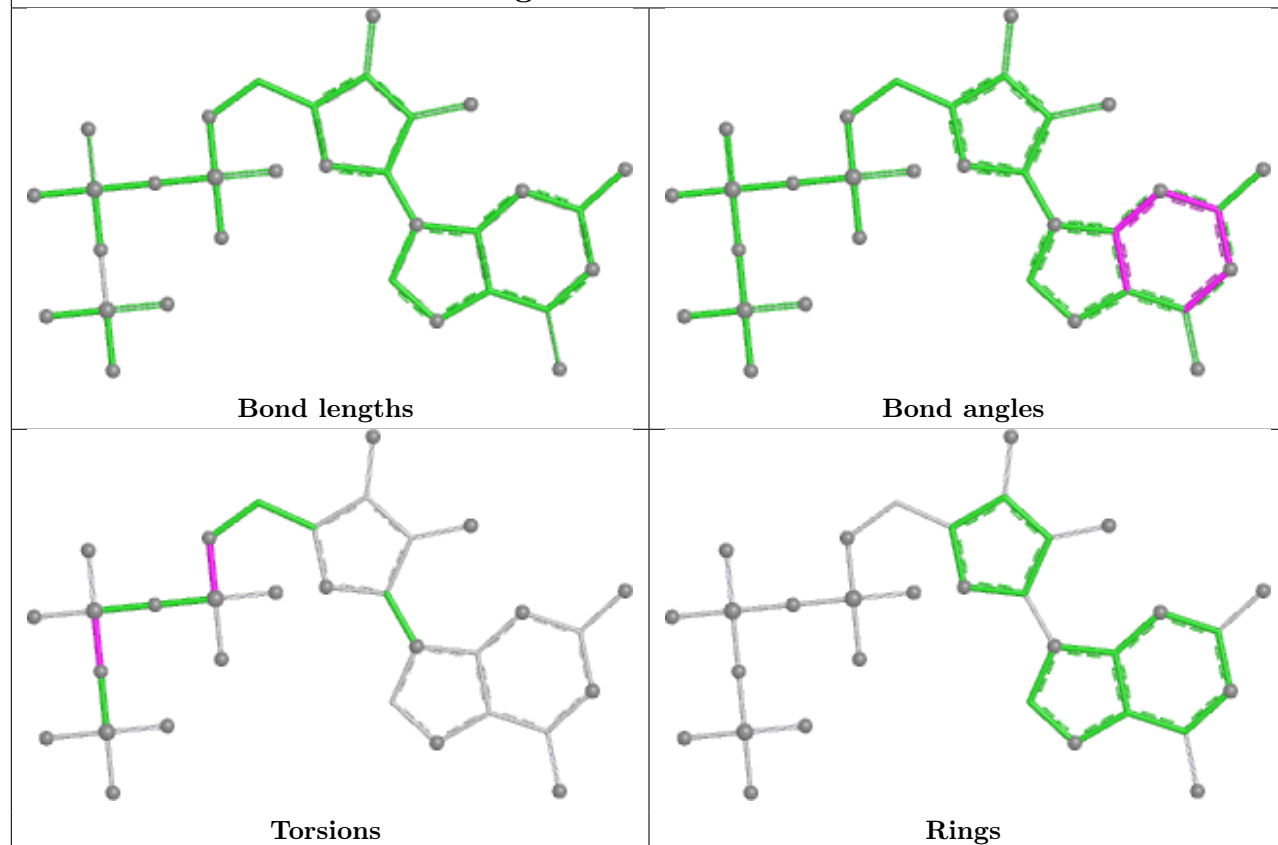




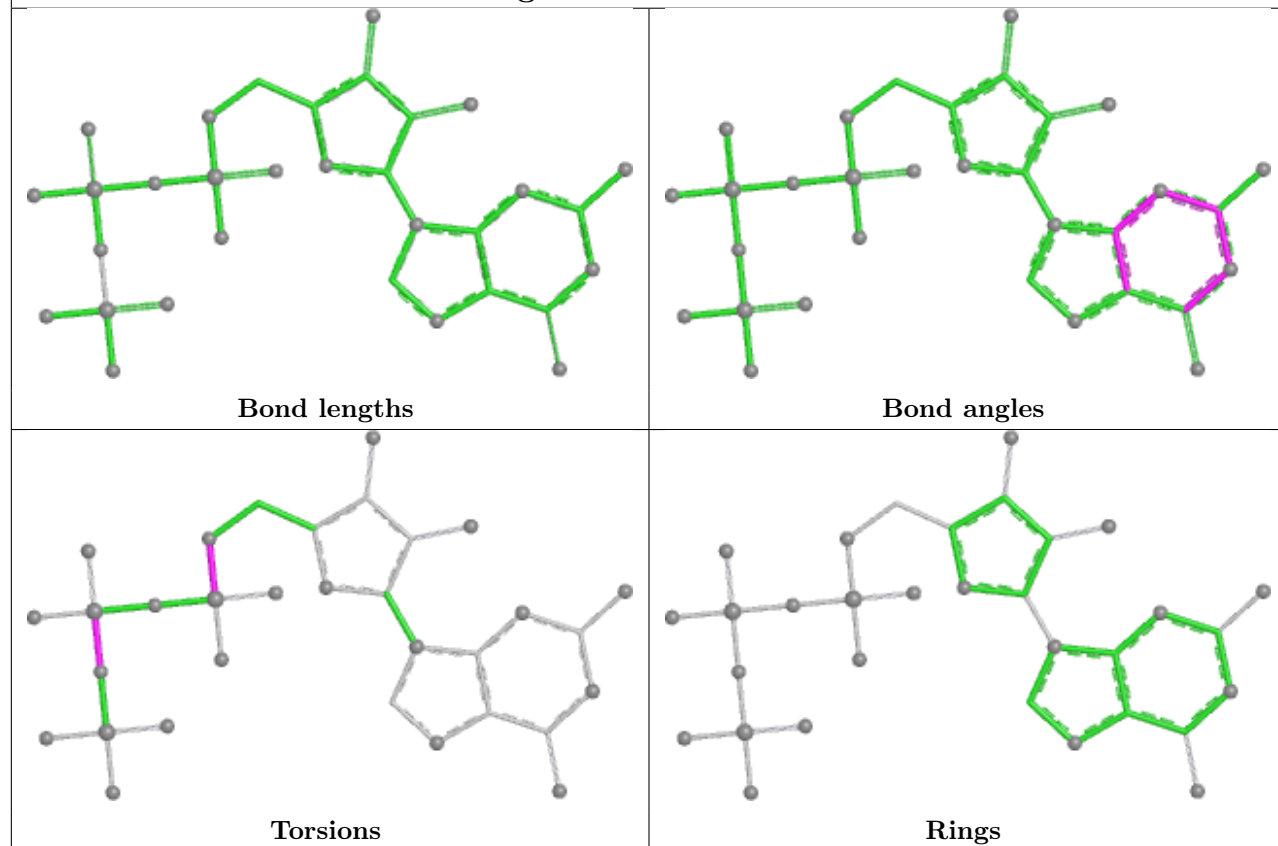


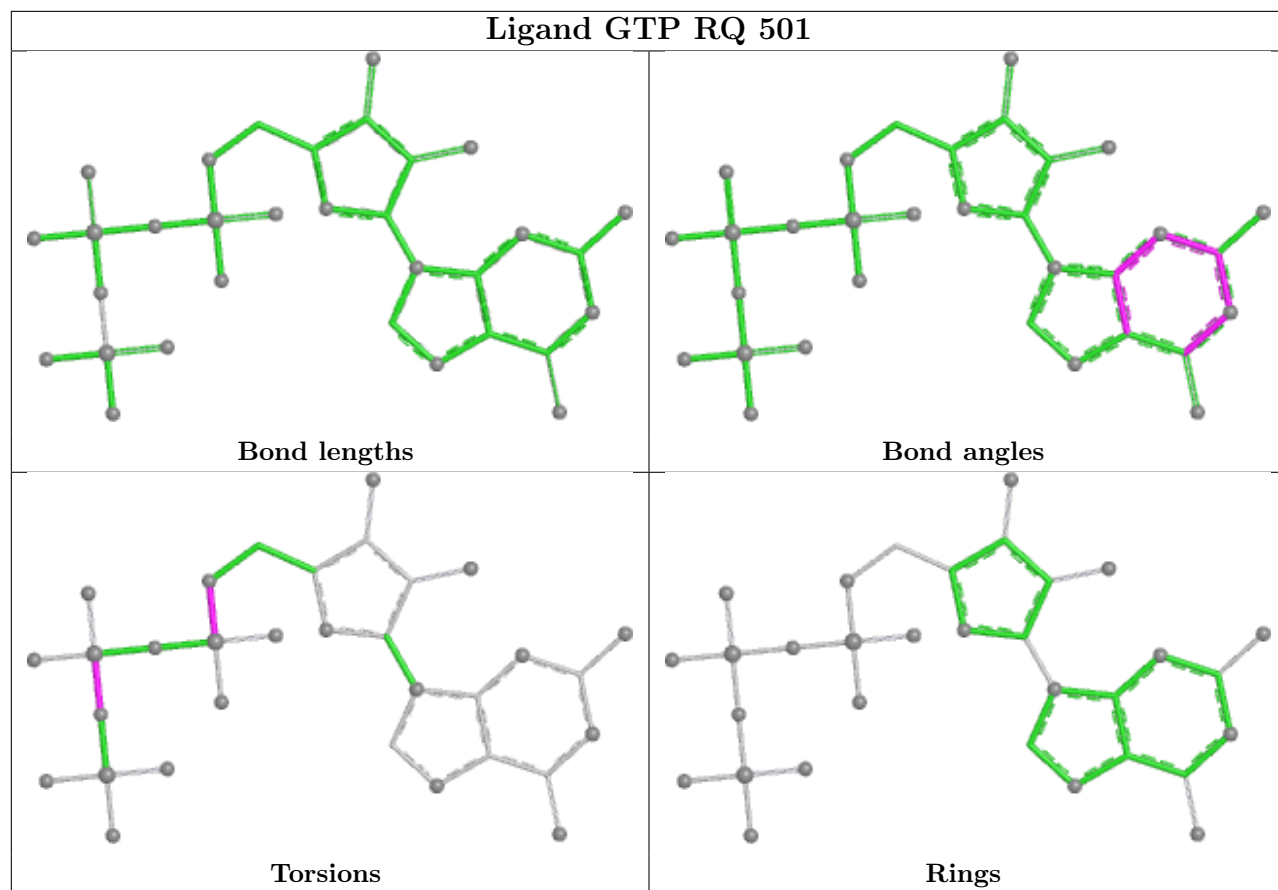


## Ligand GTP EM 501

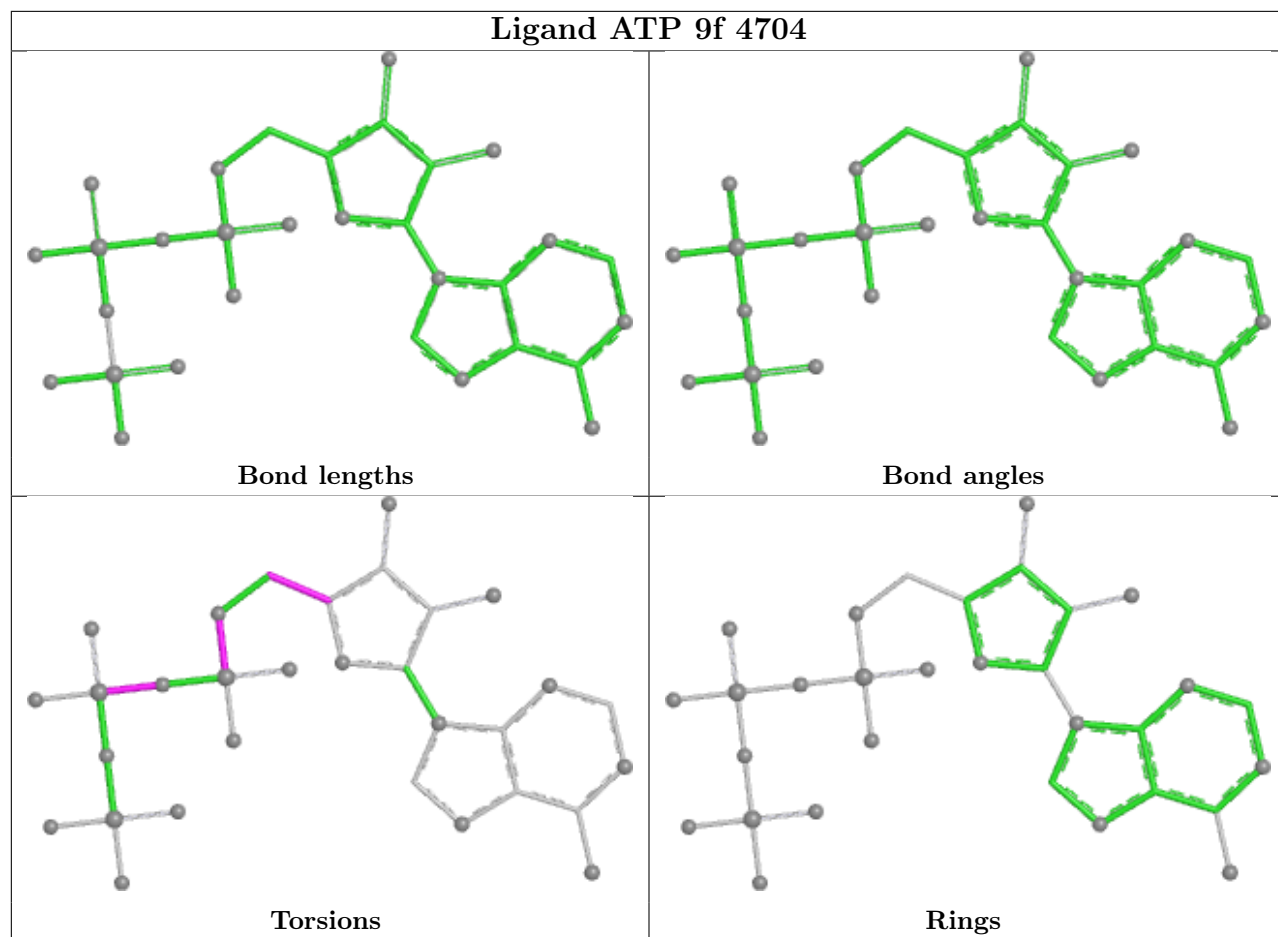


## Ligand GTP GE 602

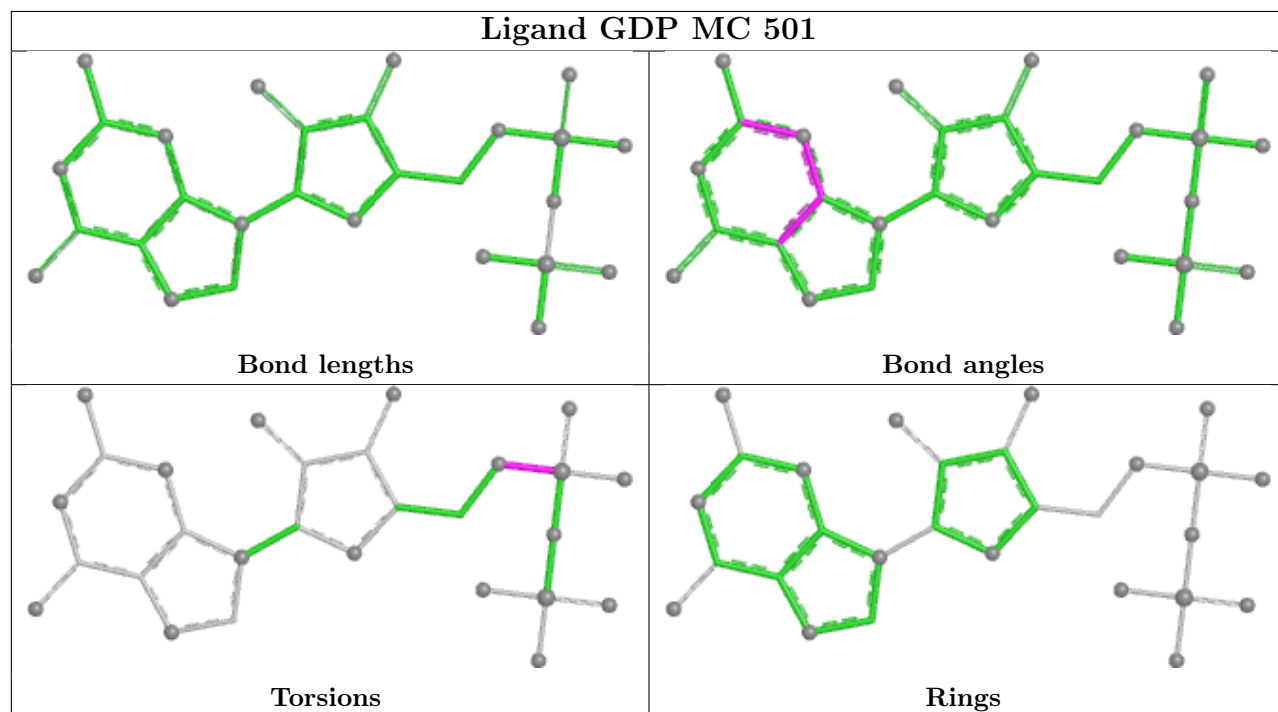


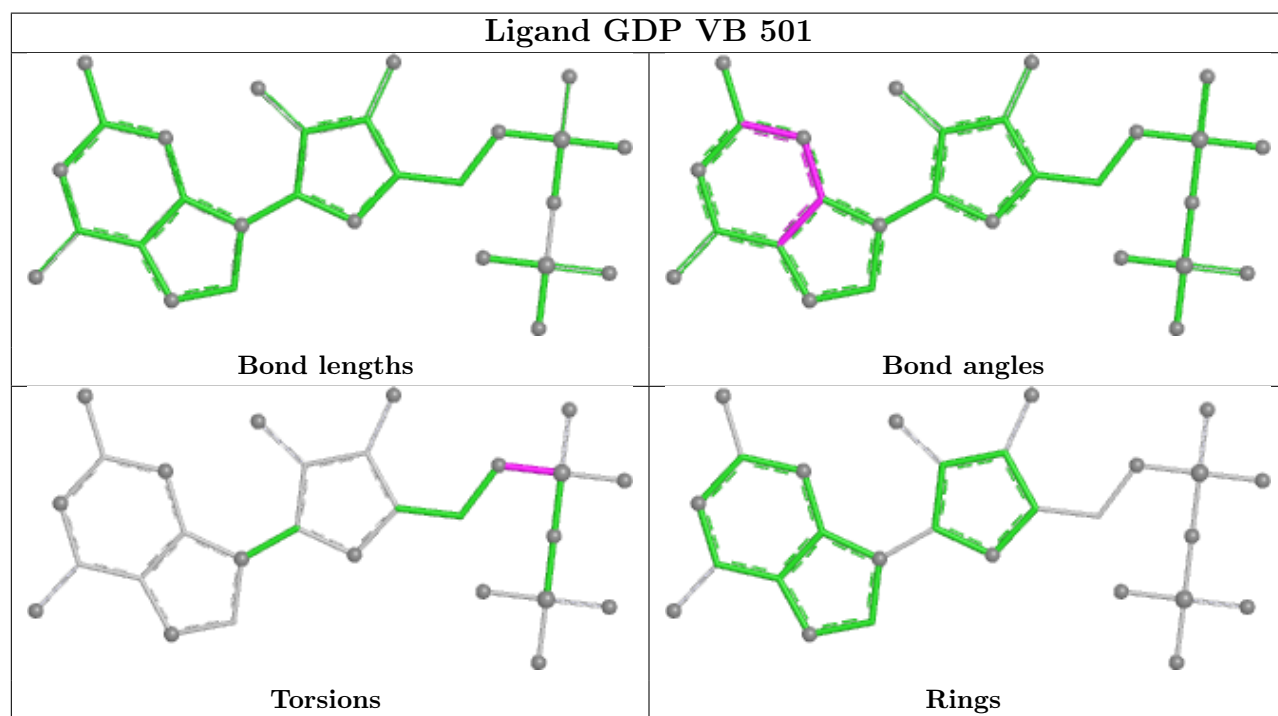
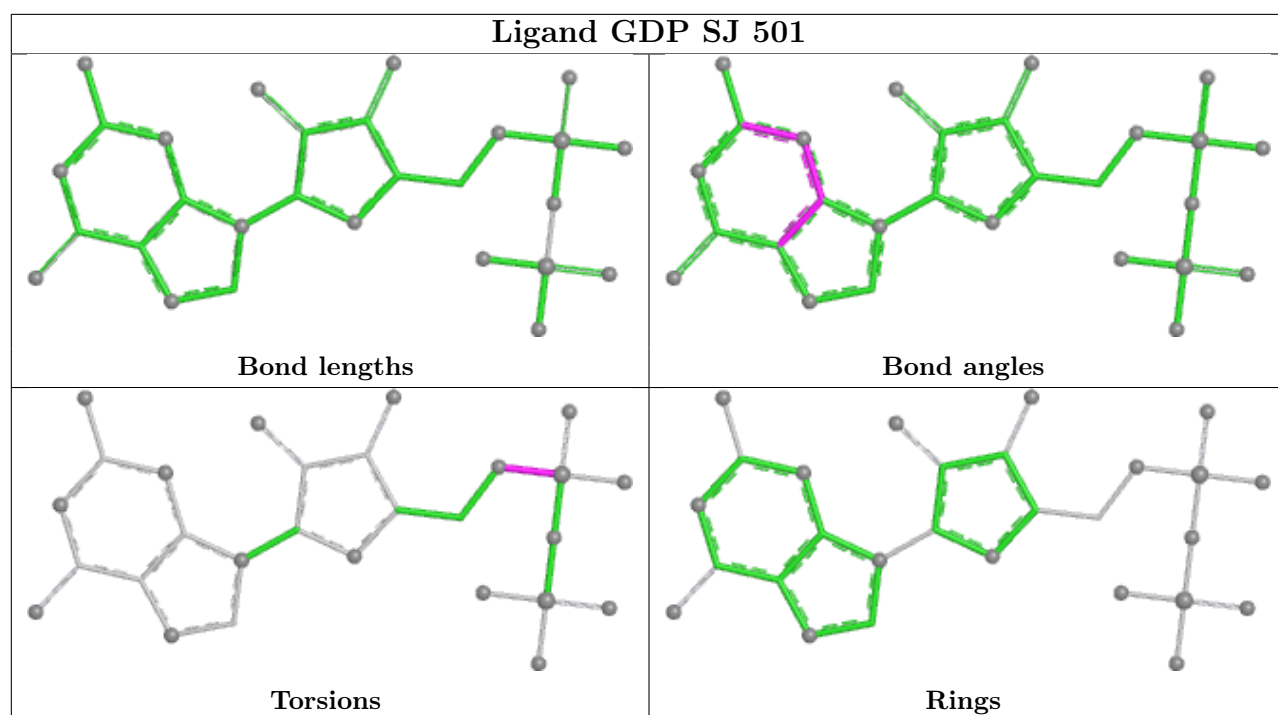


## Ligand ATP 9f 4704

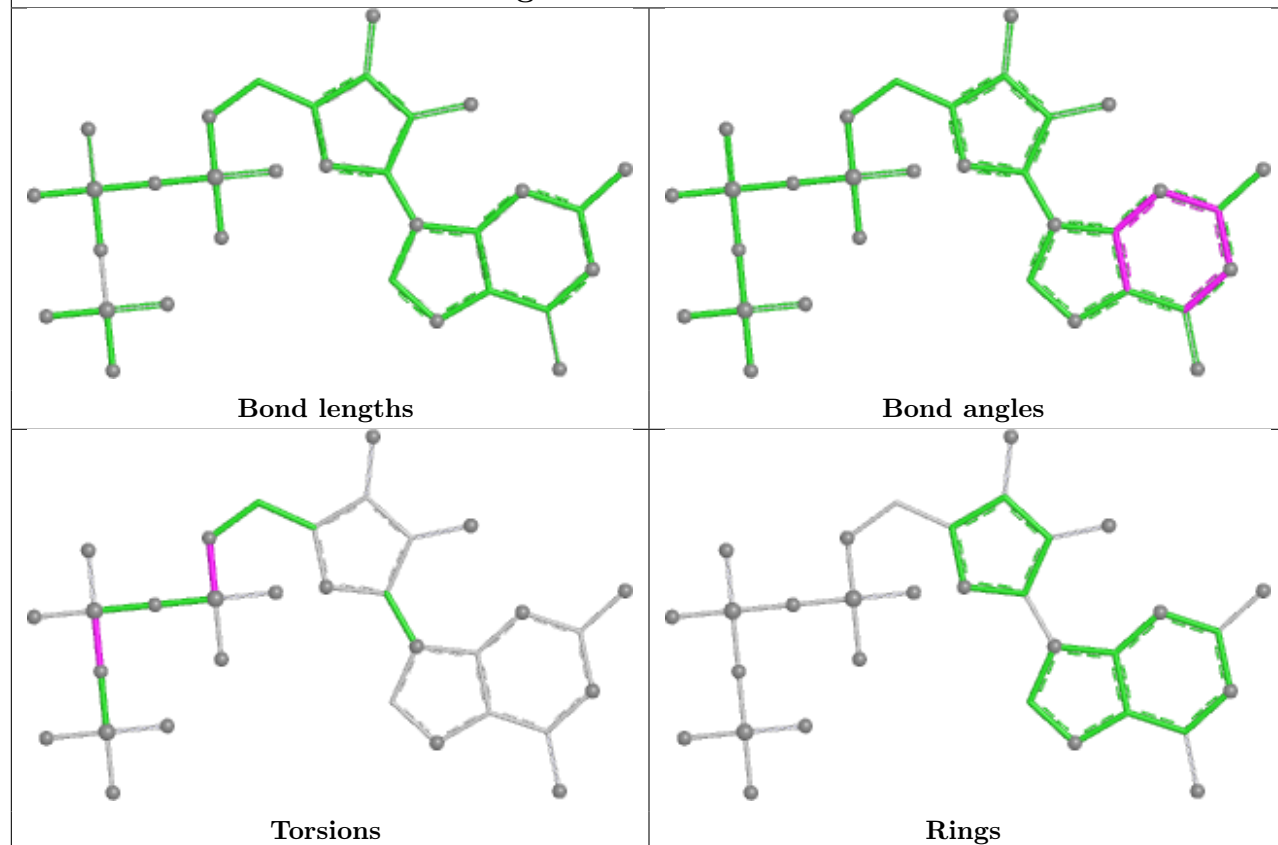


## Ligand GDP MC 501

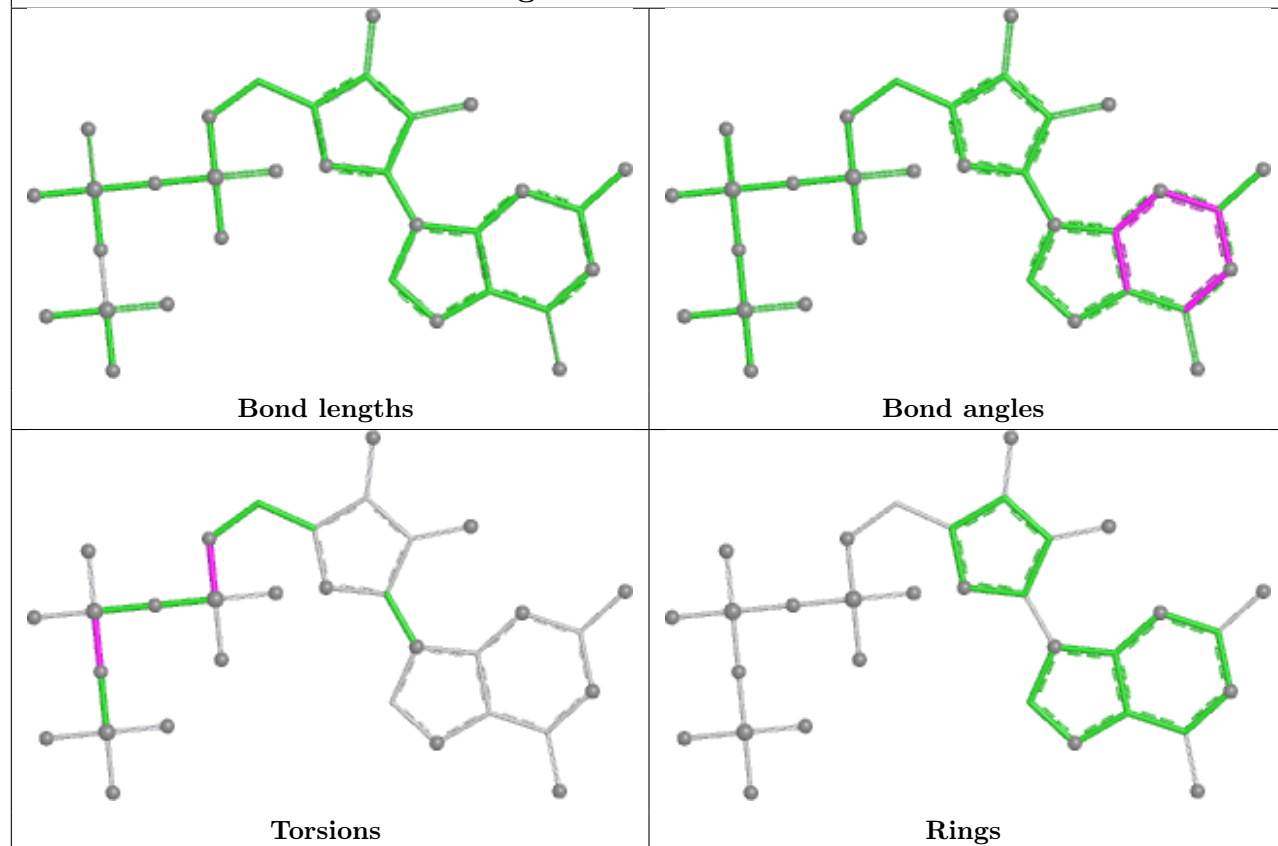


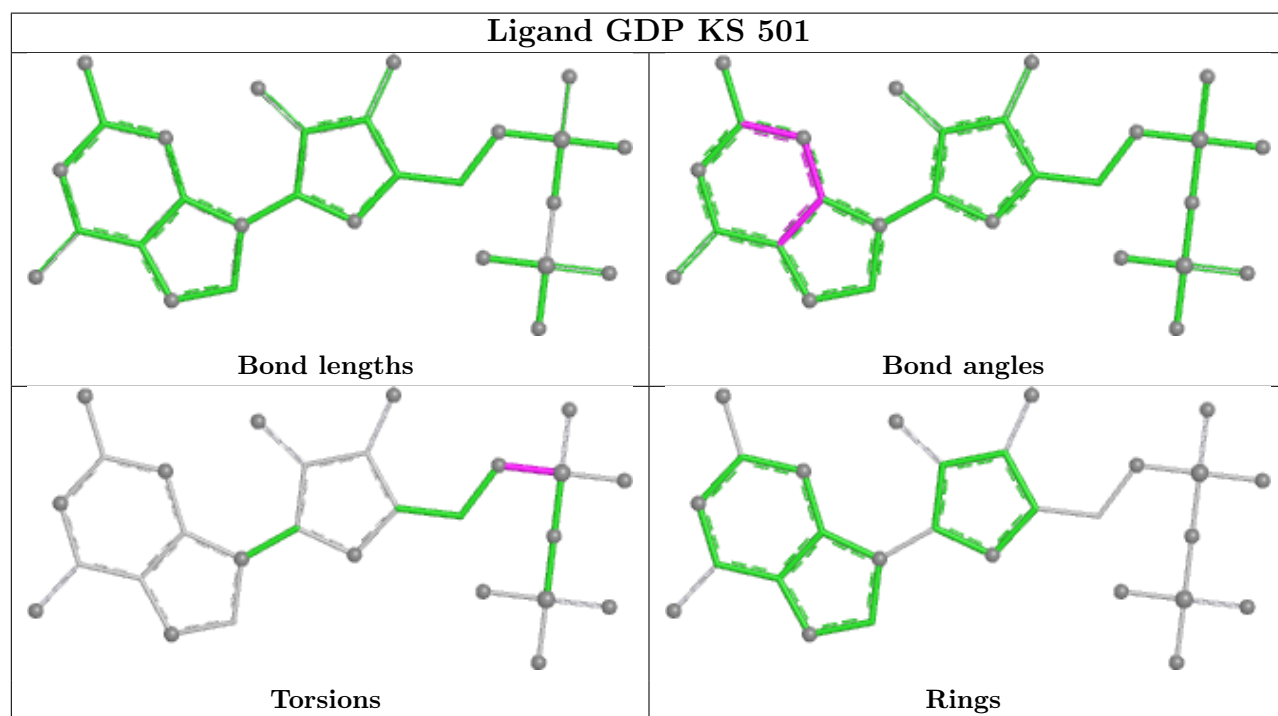
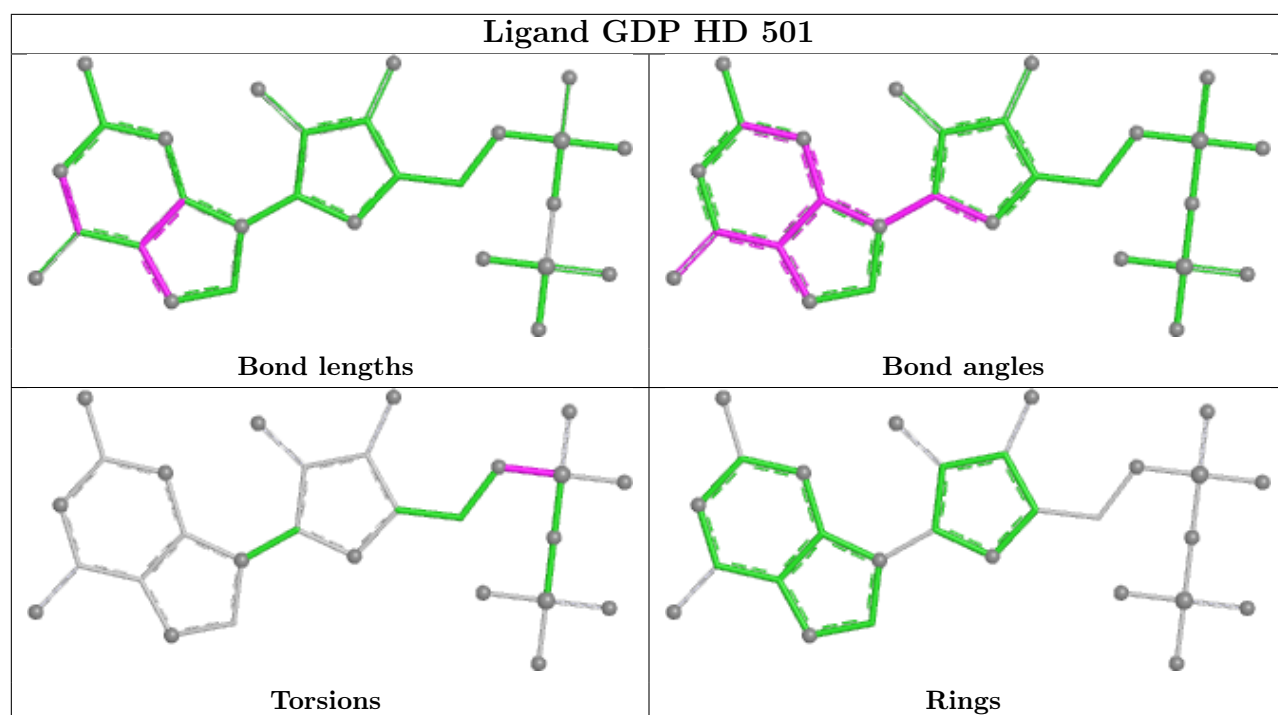


## Ligand GTP VG 501



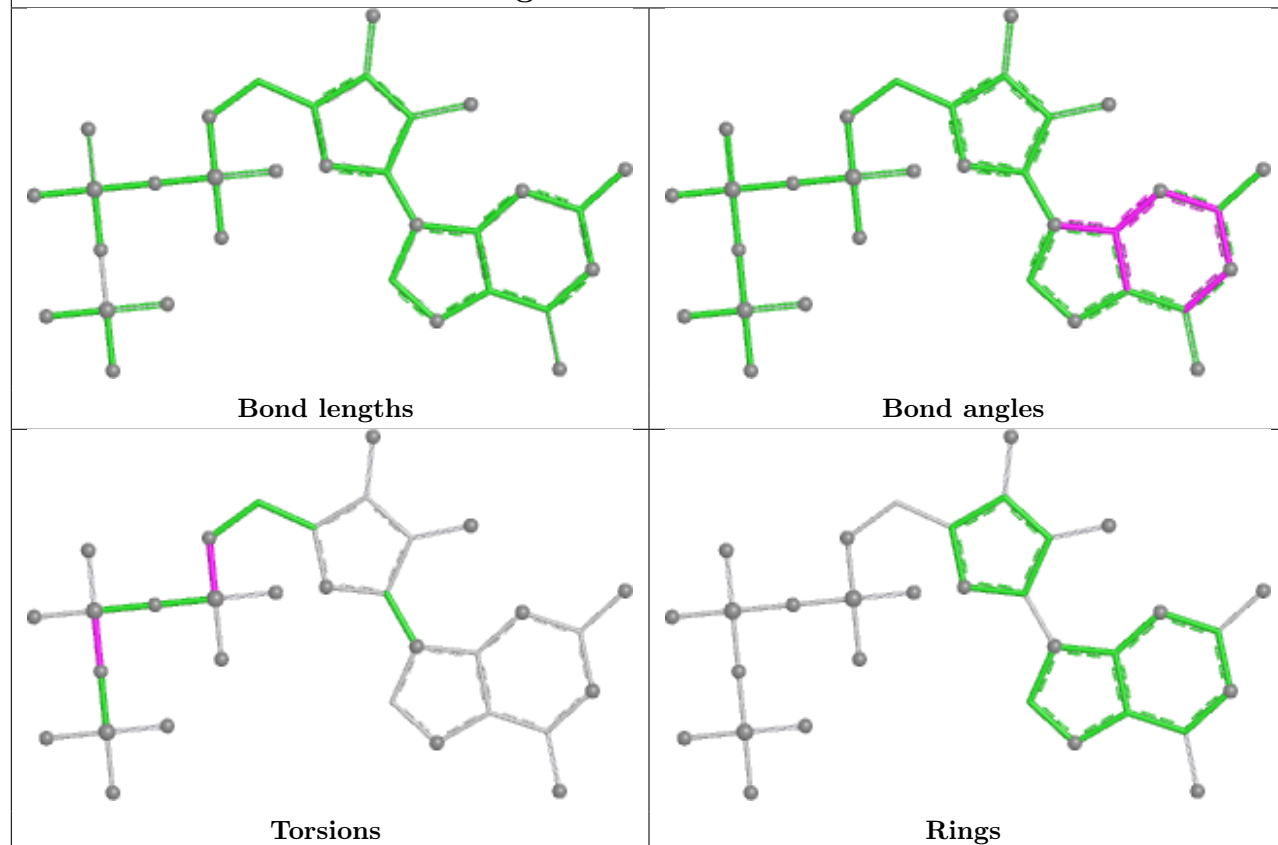
## Ligand GTP XC 602



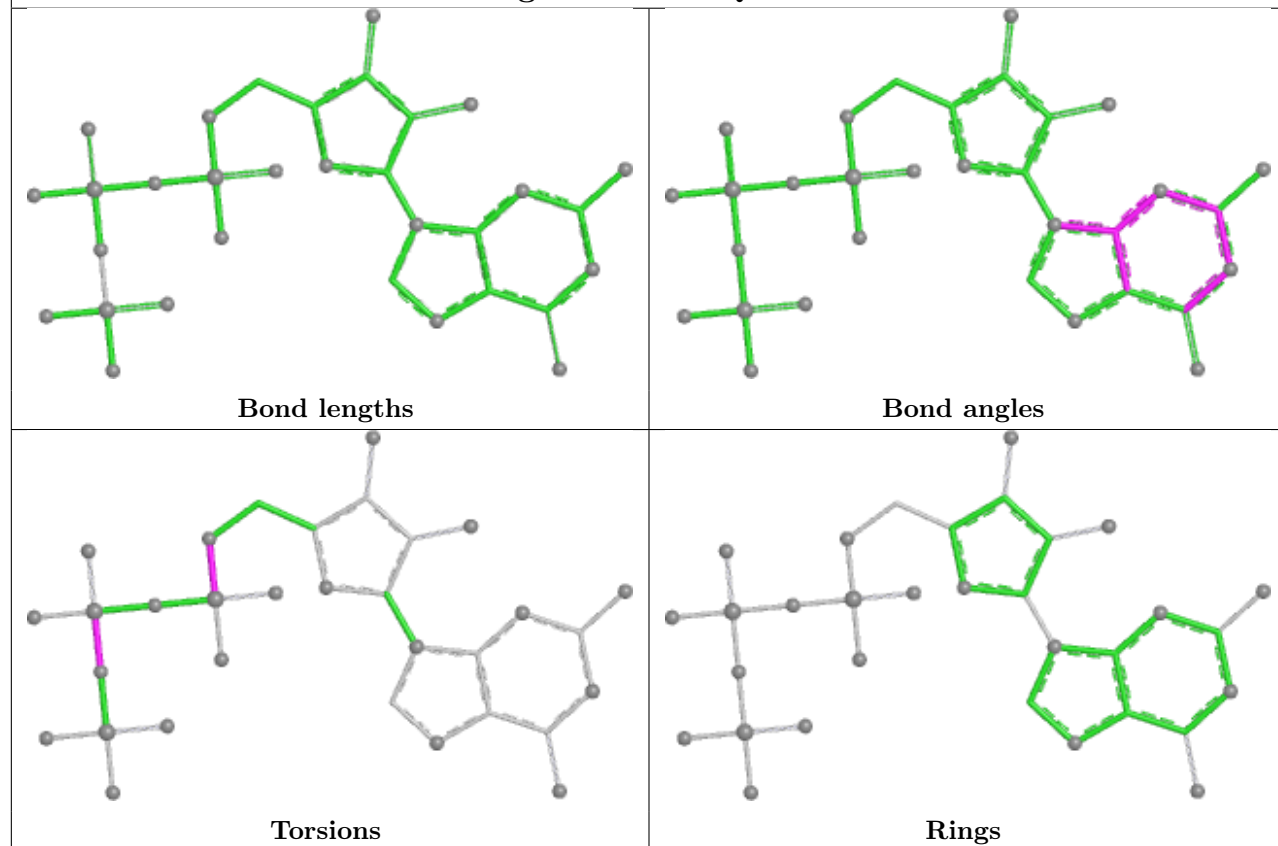


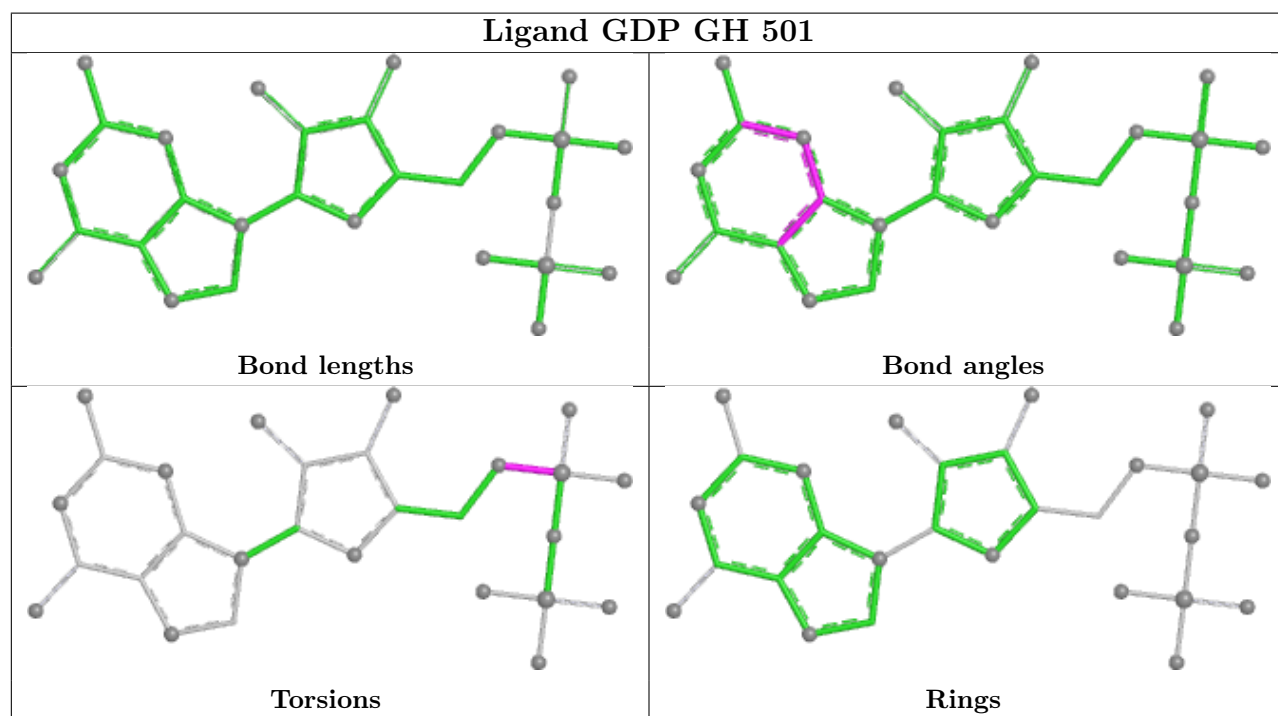
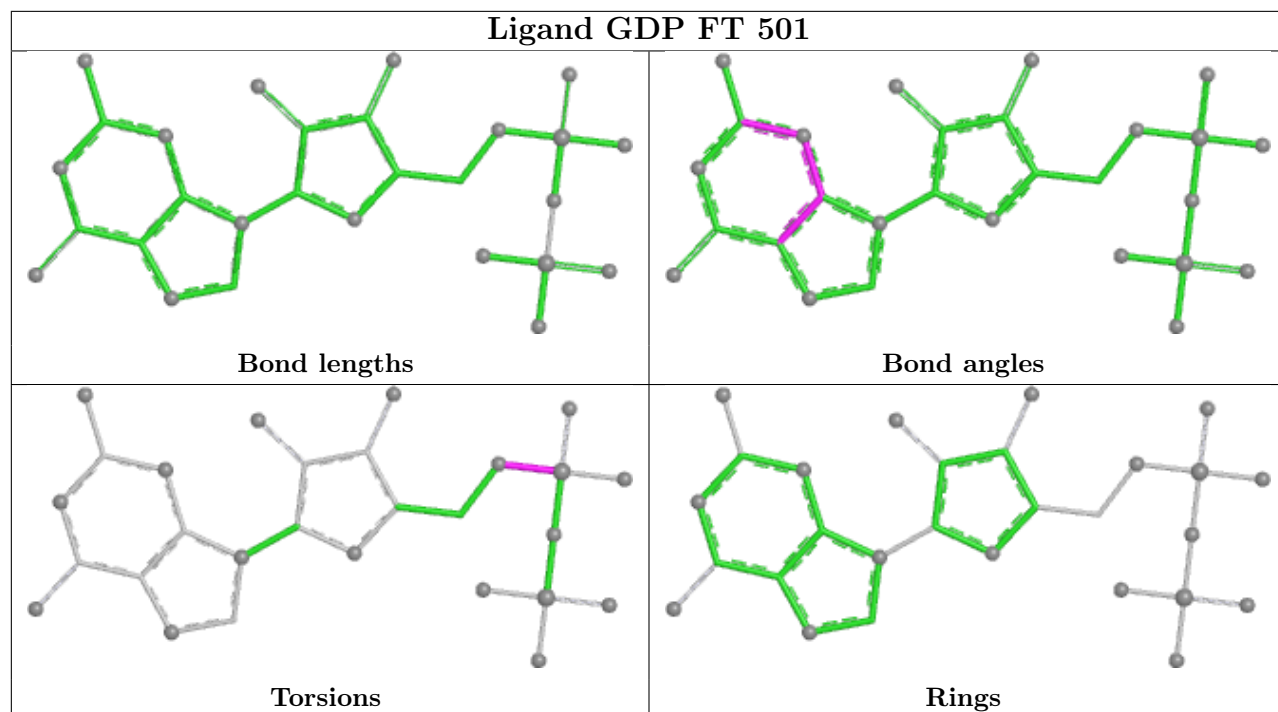


## Ligand GTP KD 501

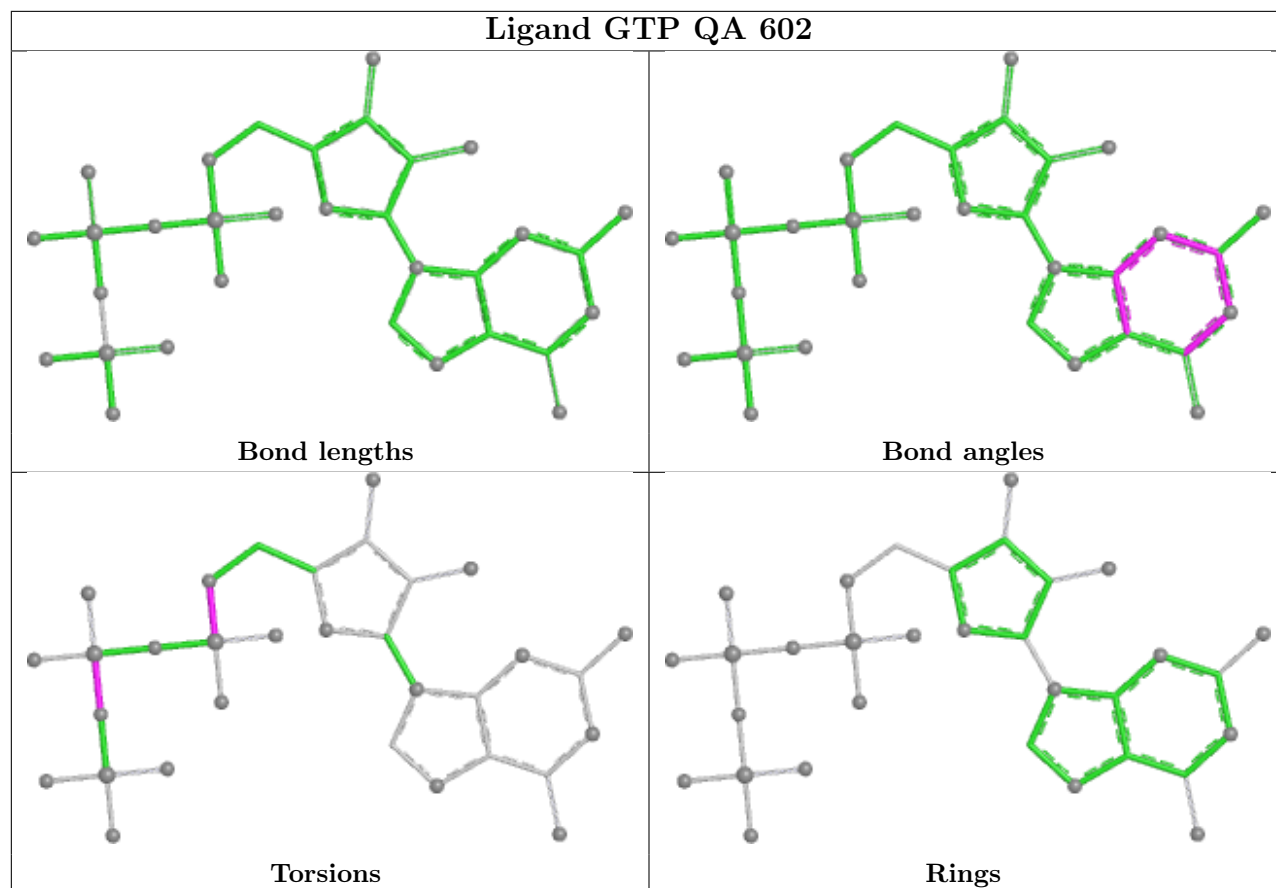


## Ligand GTP PQ 501

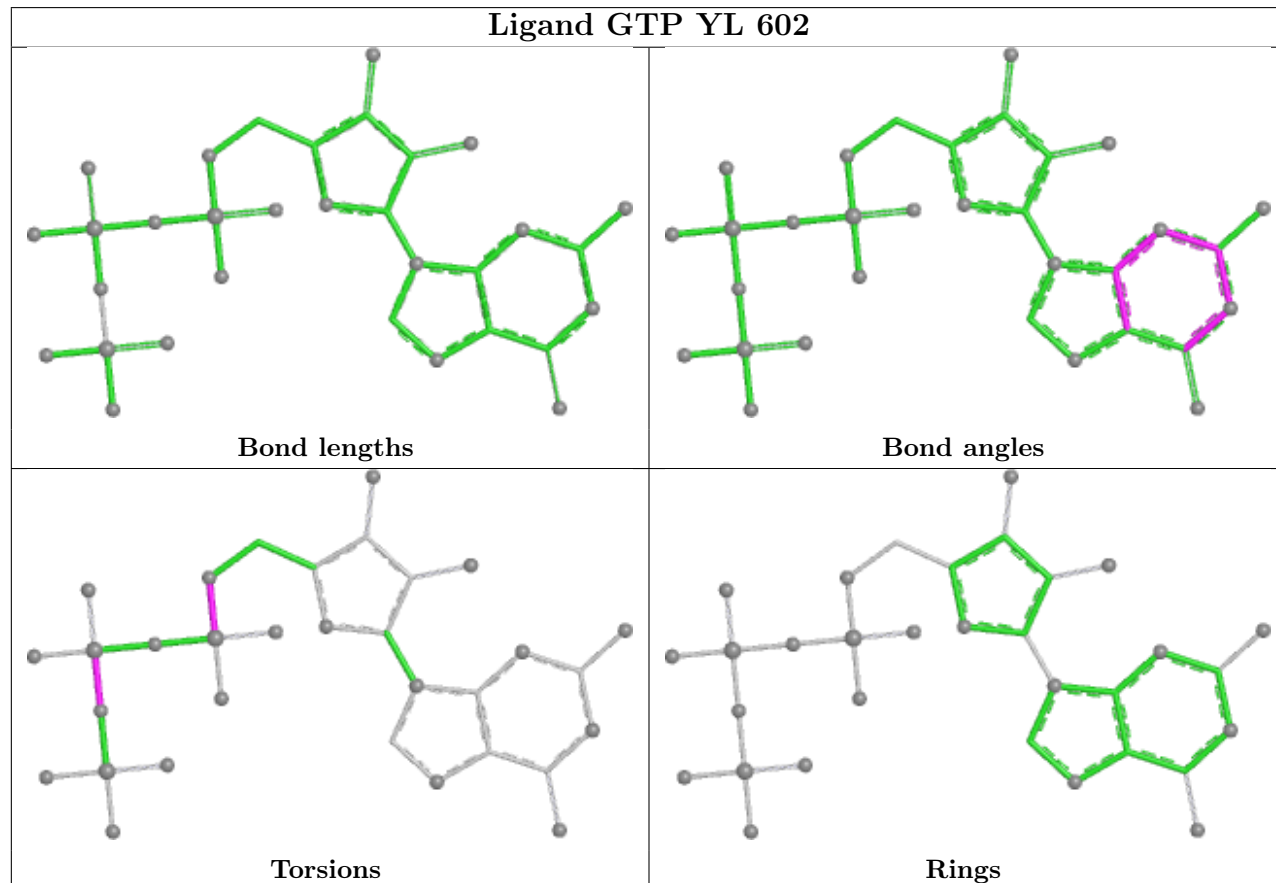




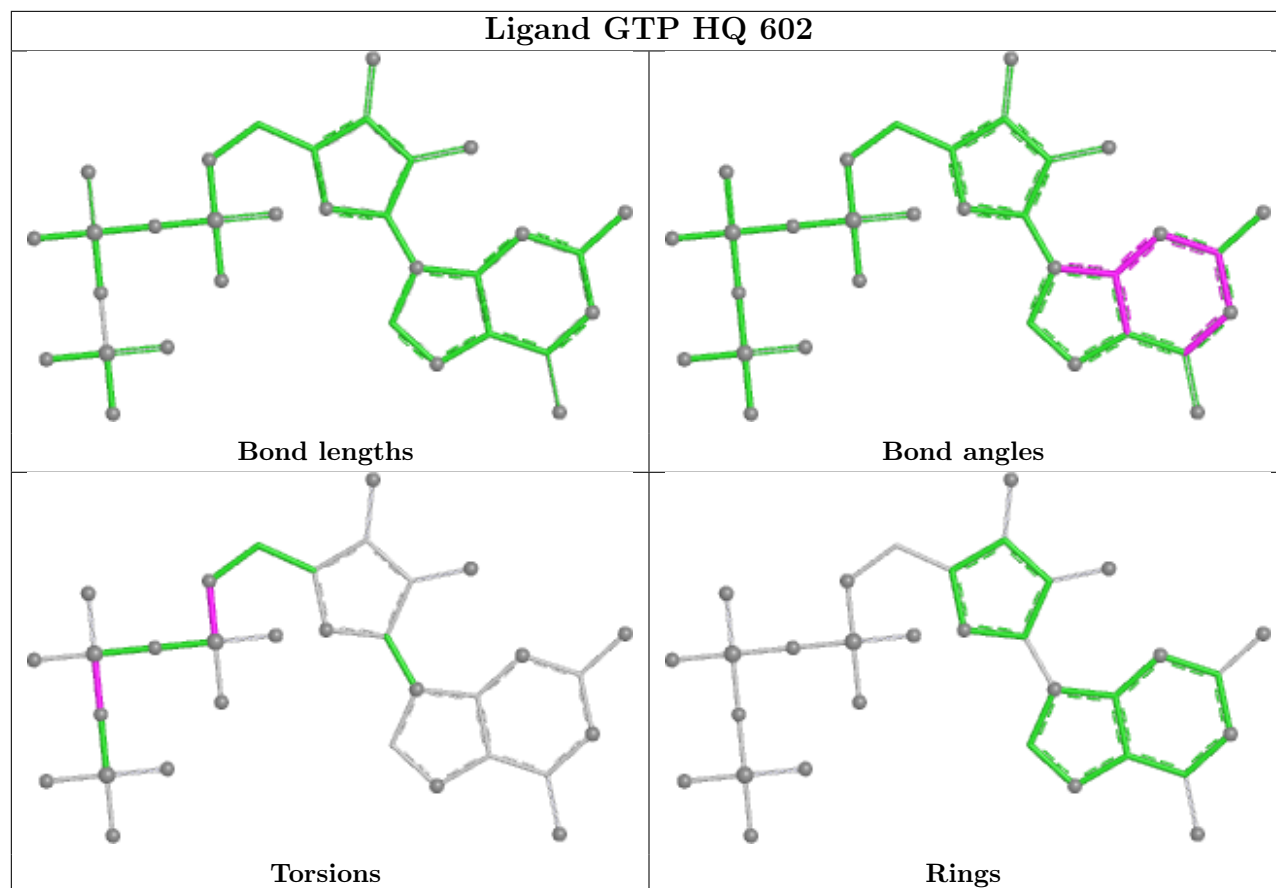
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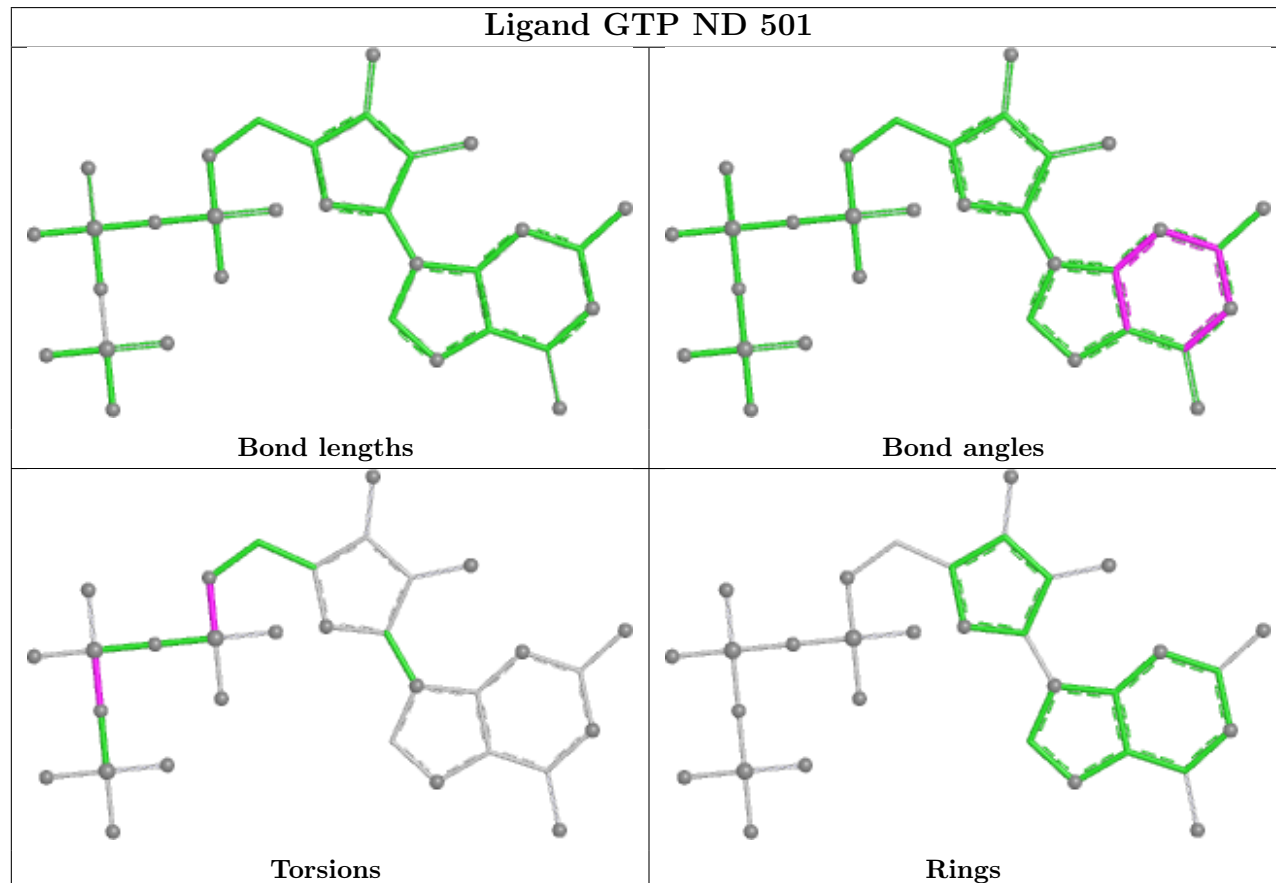
## Ligand GTP YL 602



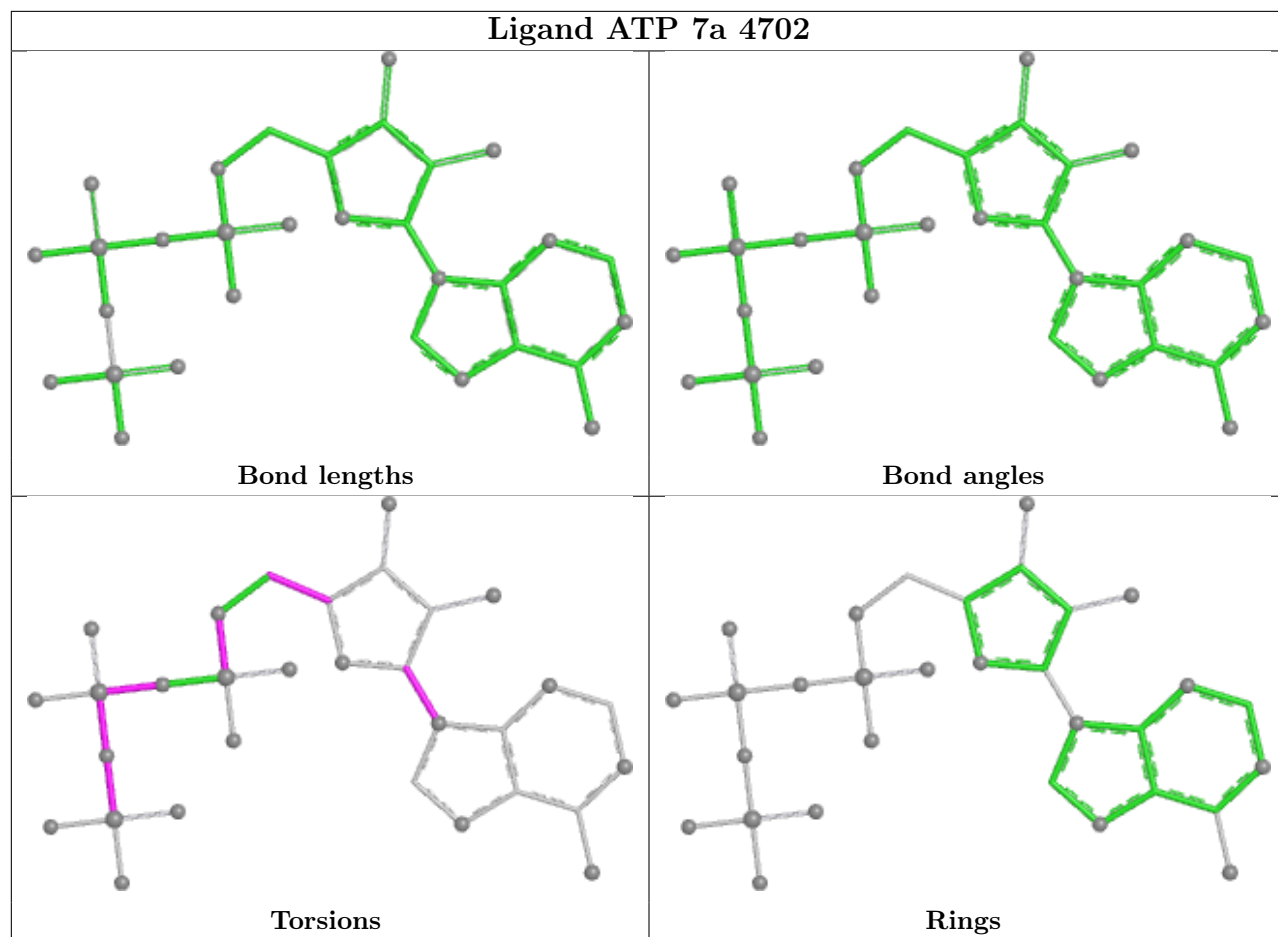
## Ligand GTP HQ 602



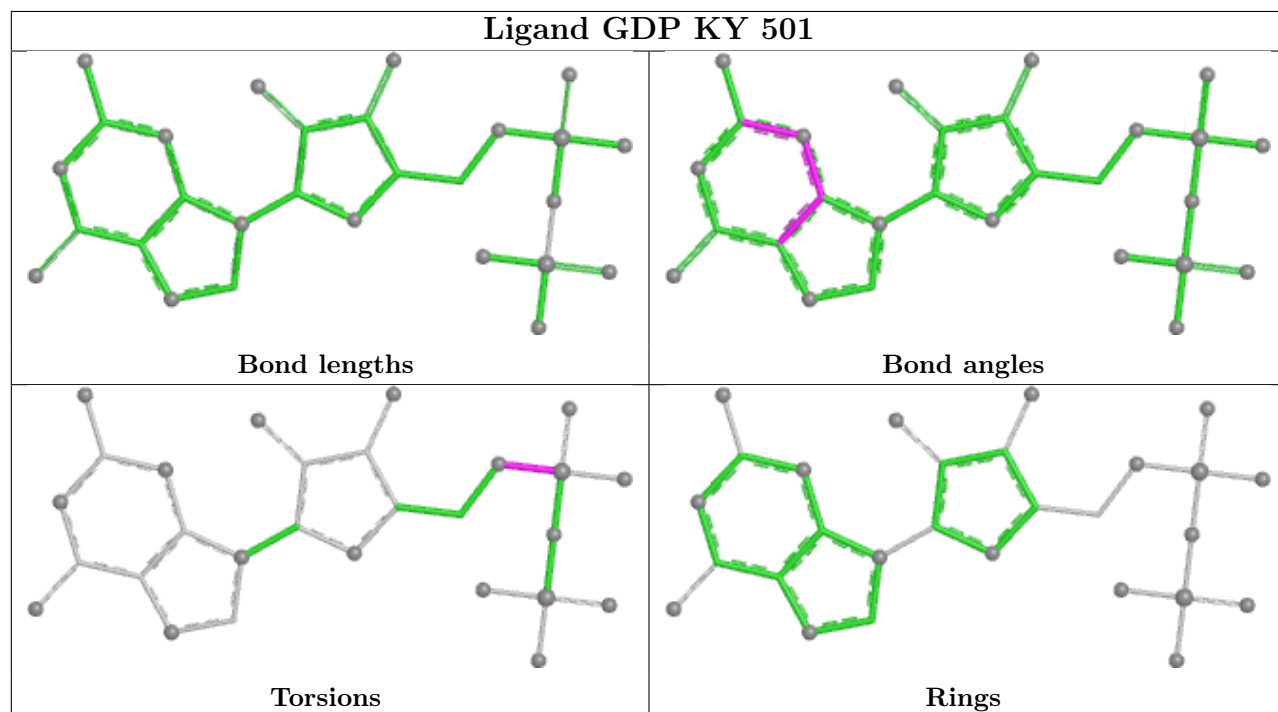
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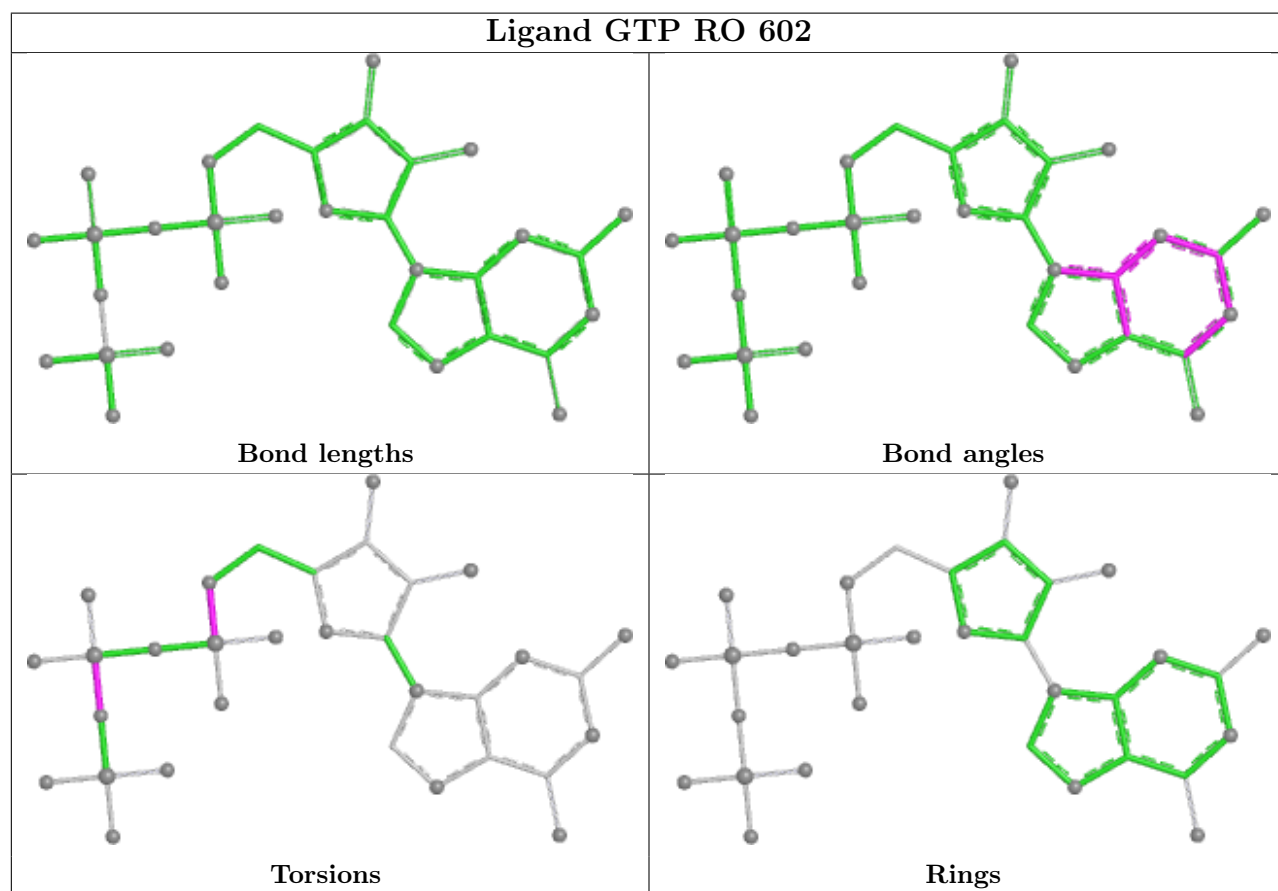
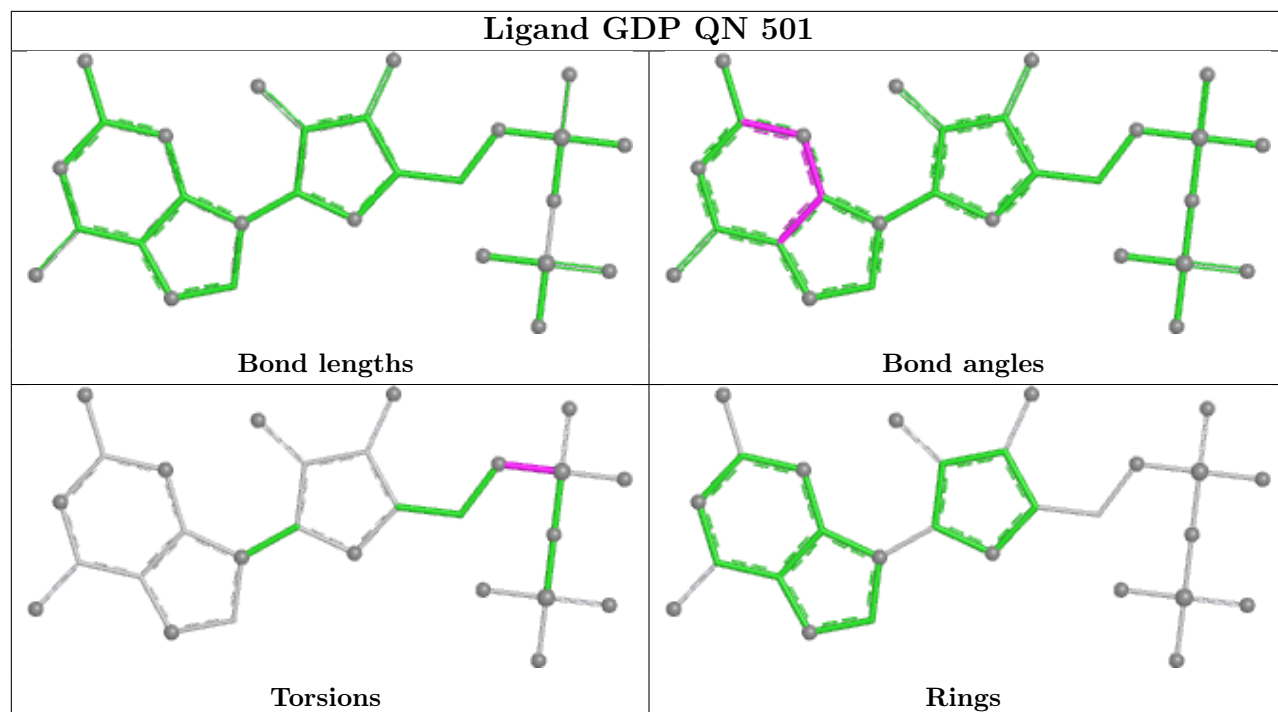


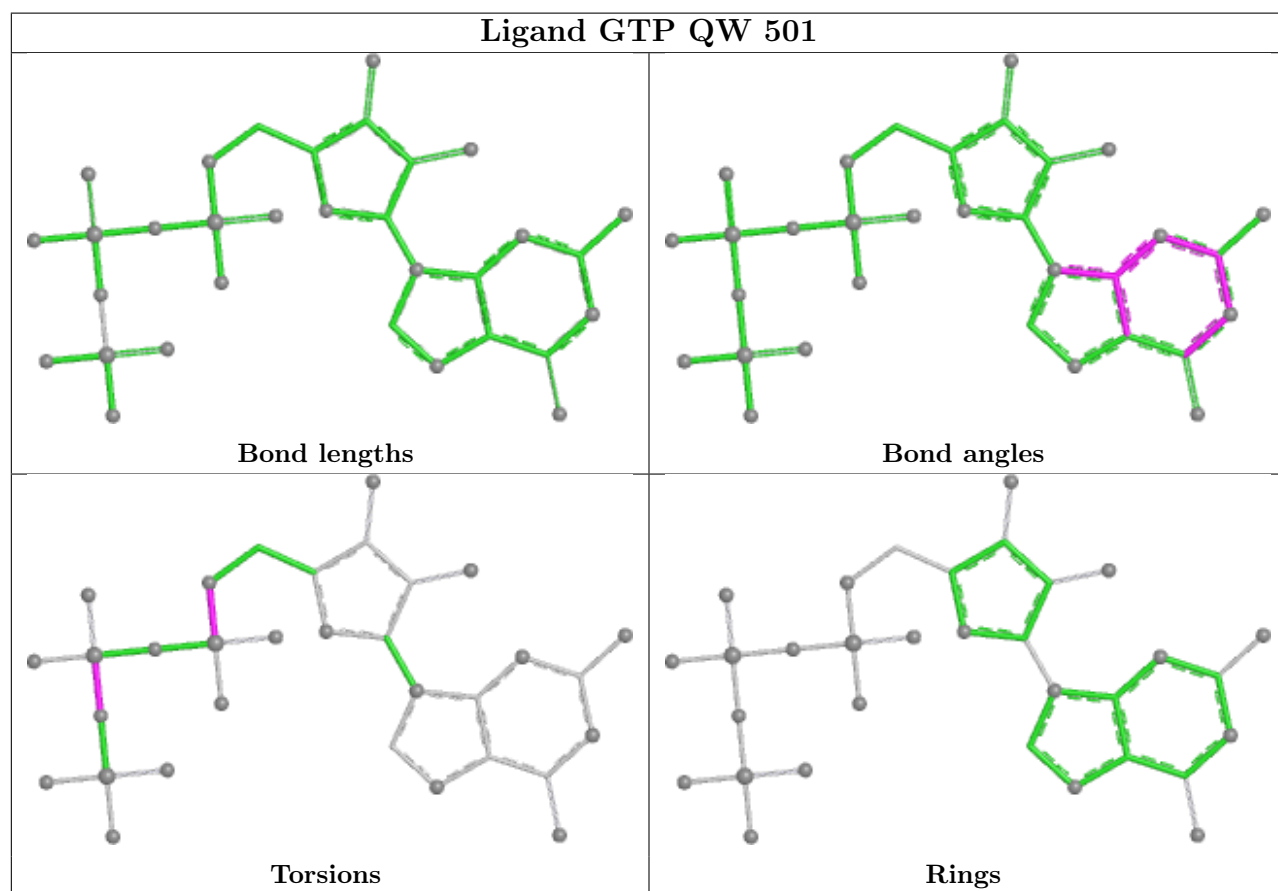
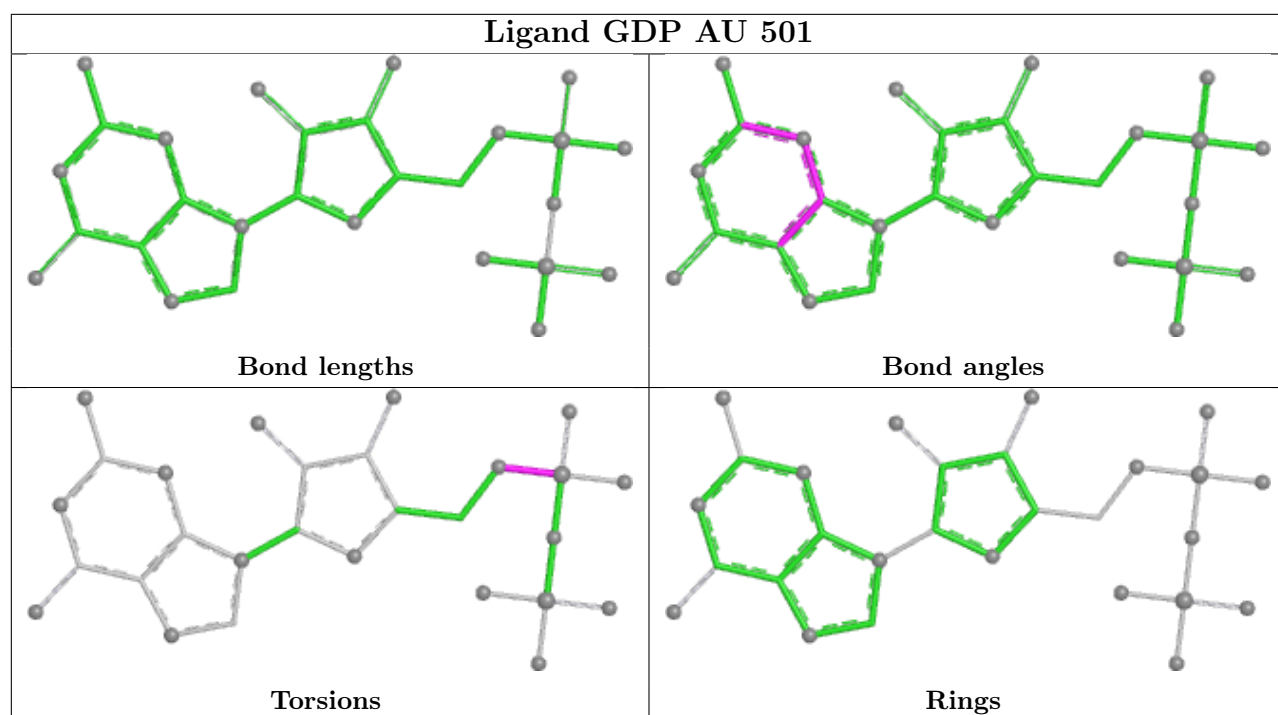
## Ligand ATP 7a 4702



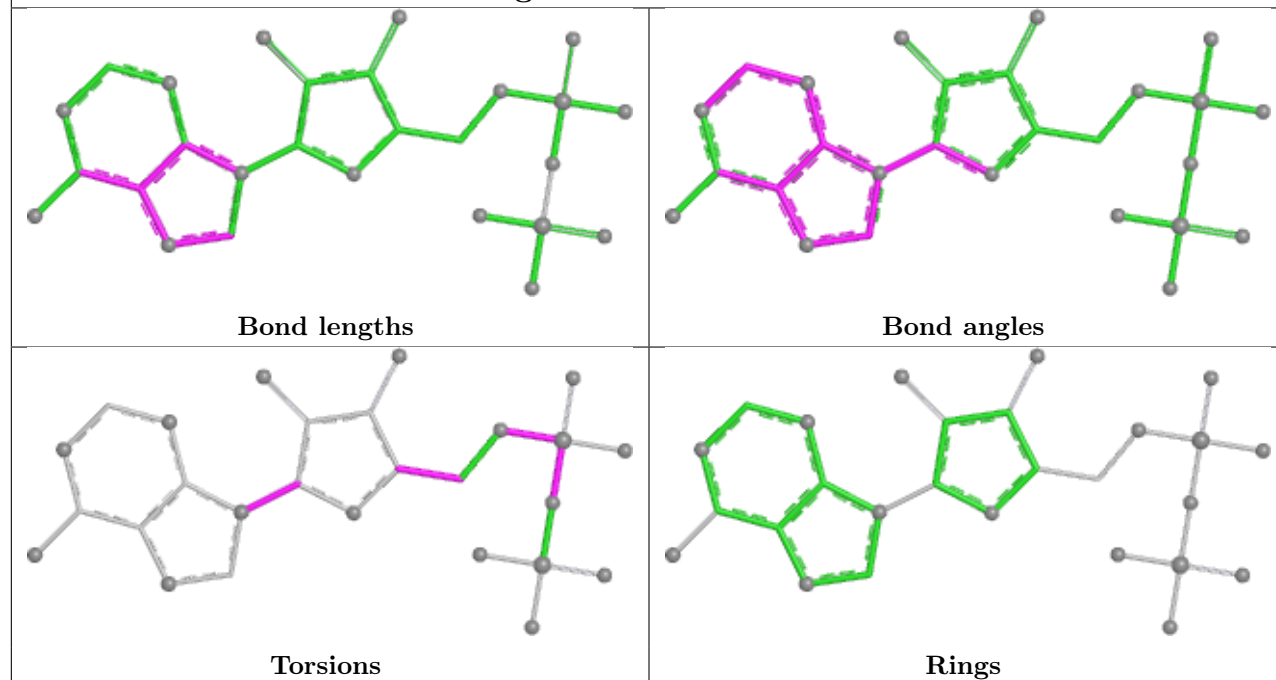
## Ligand GDP KY 501



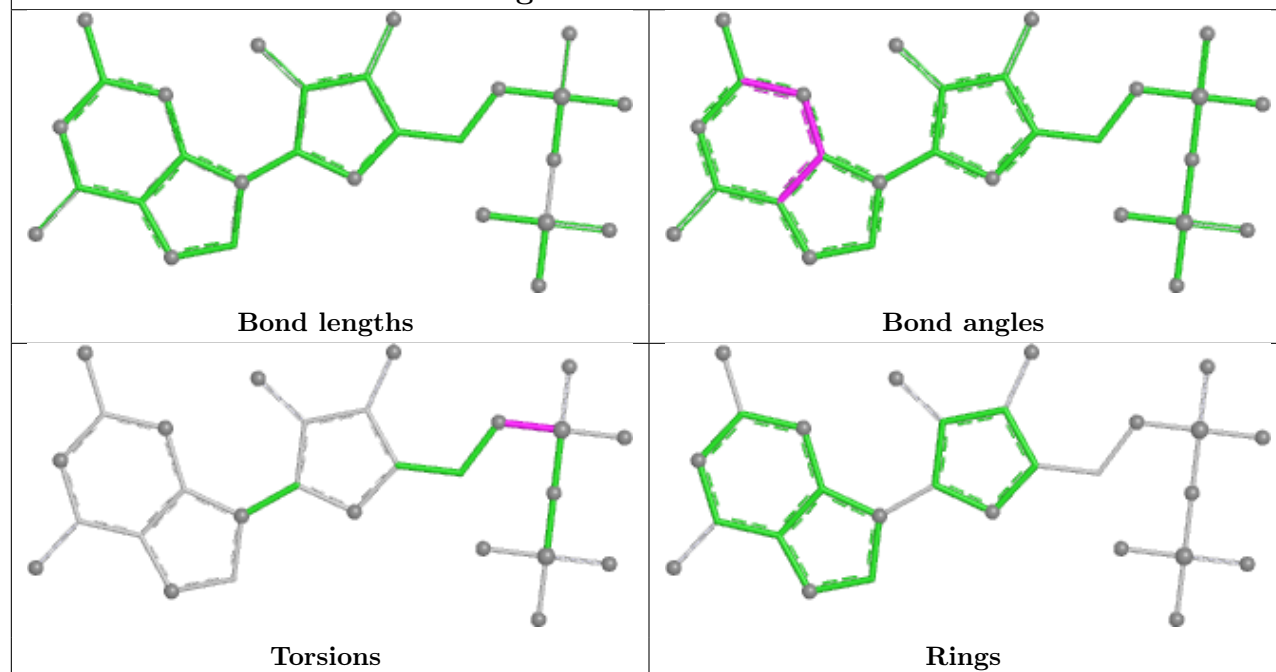




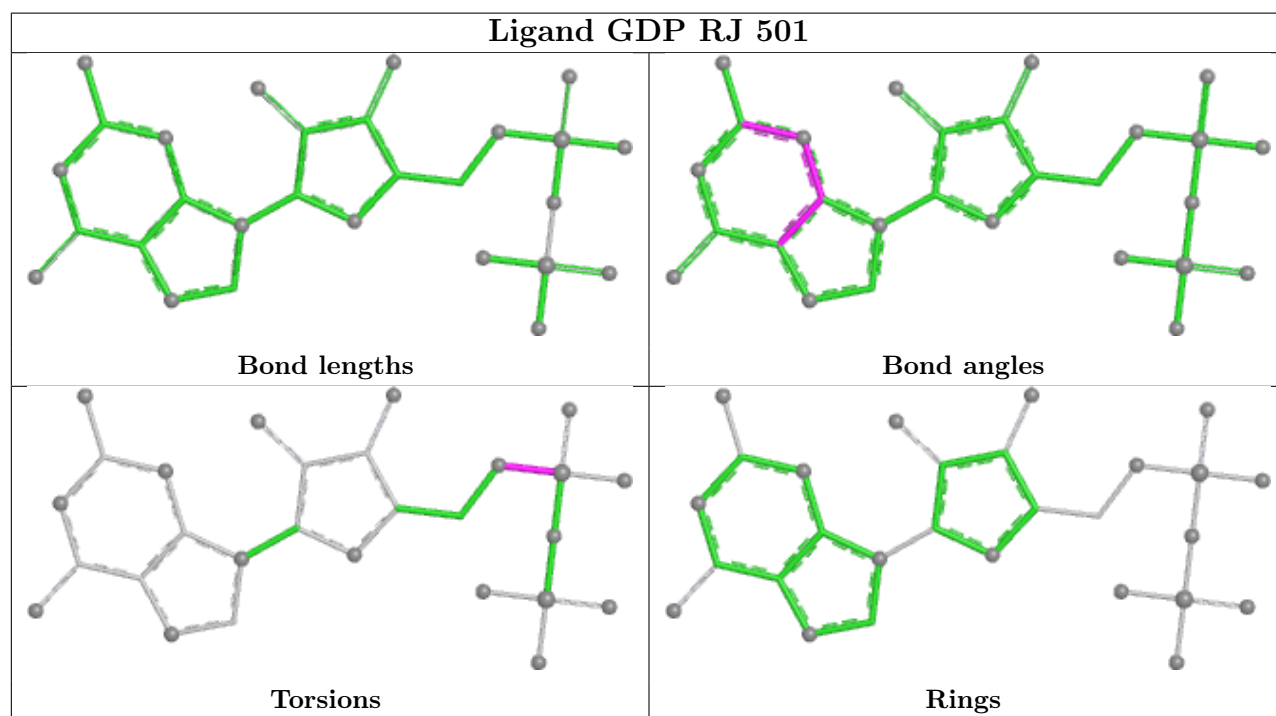
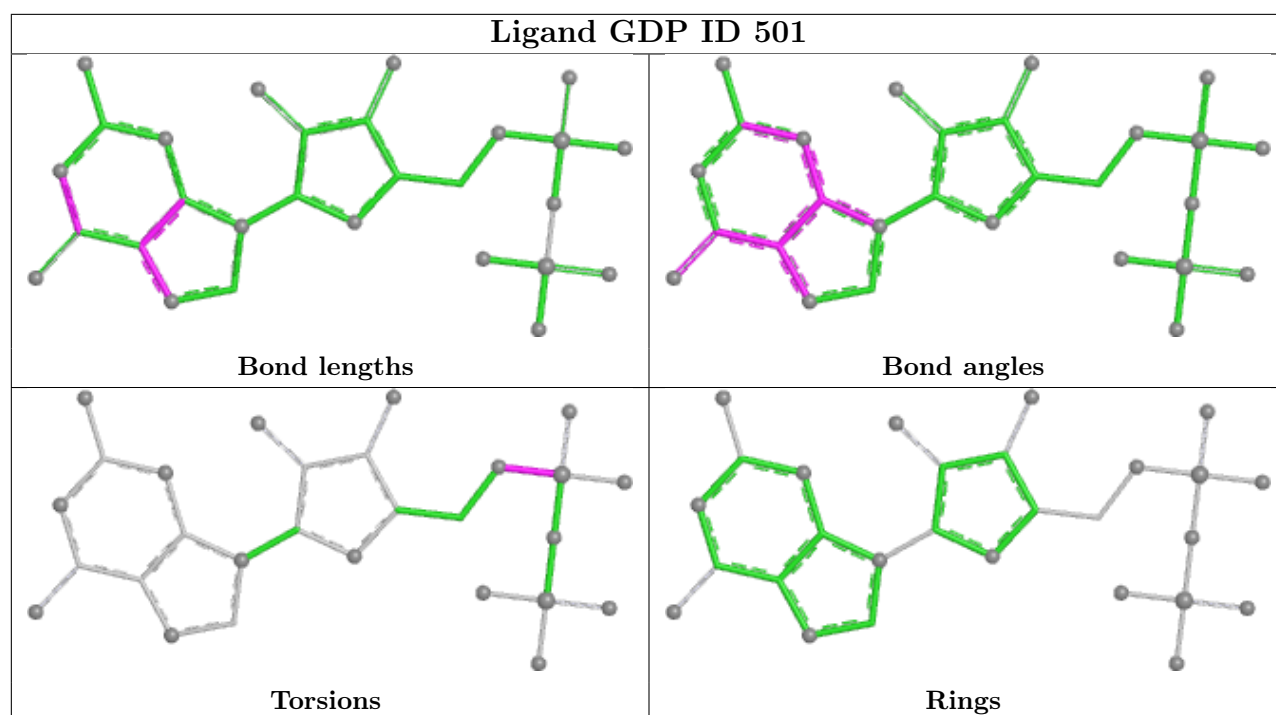
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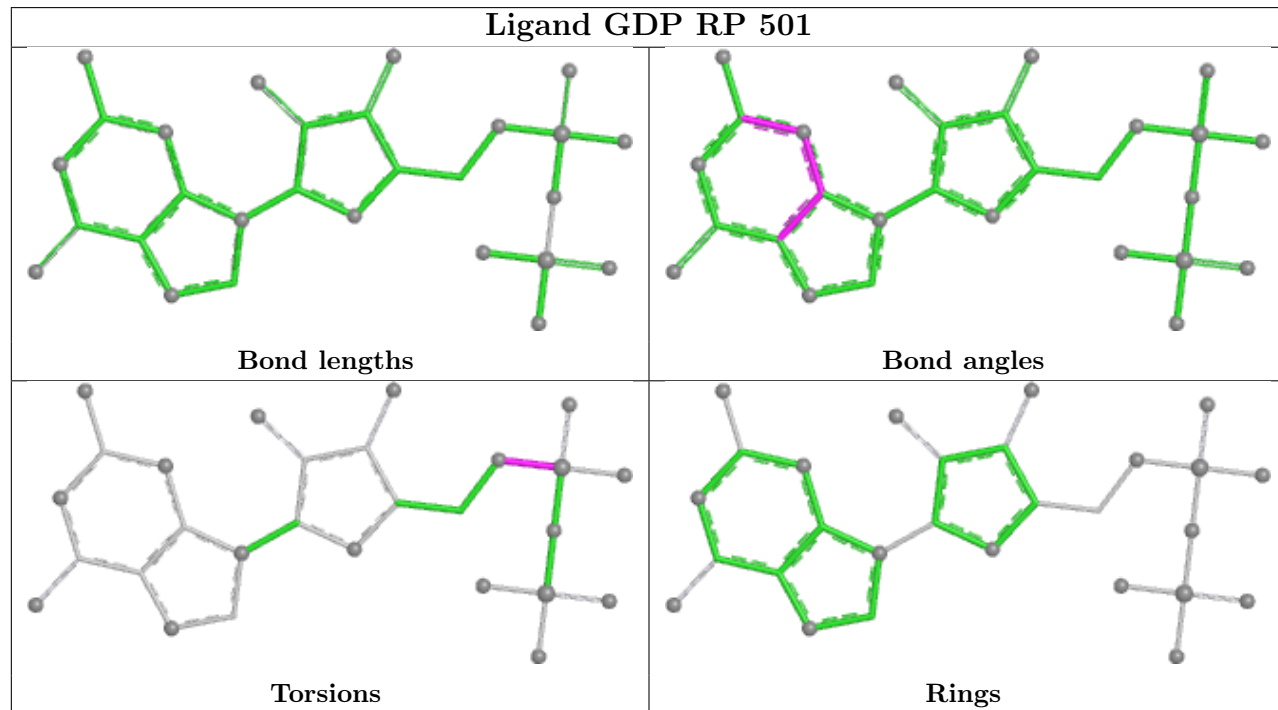
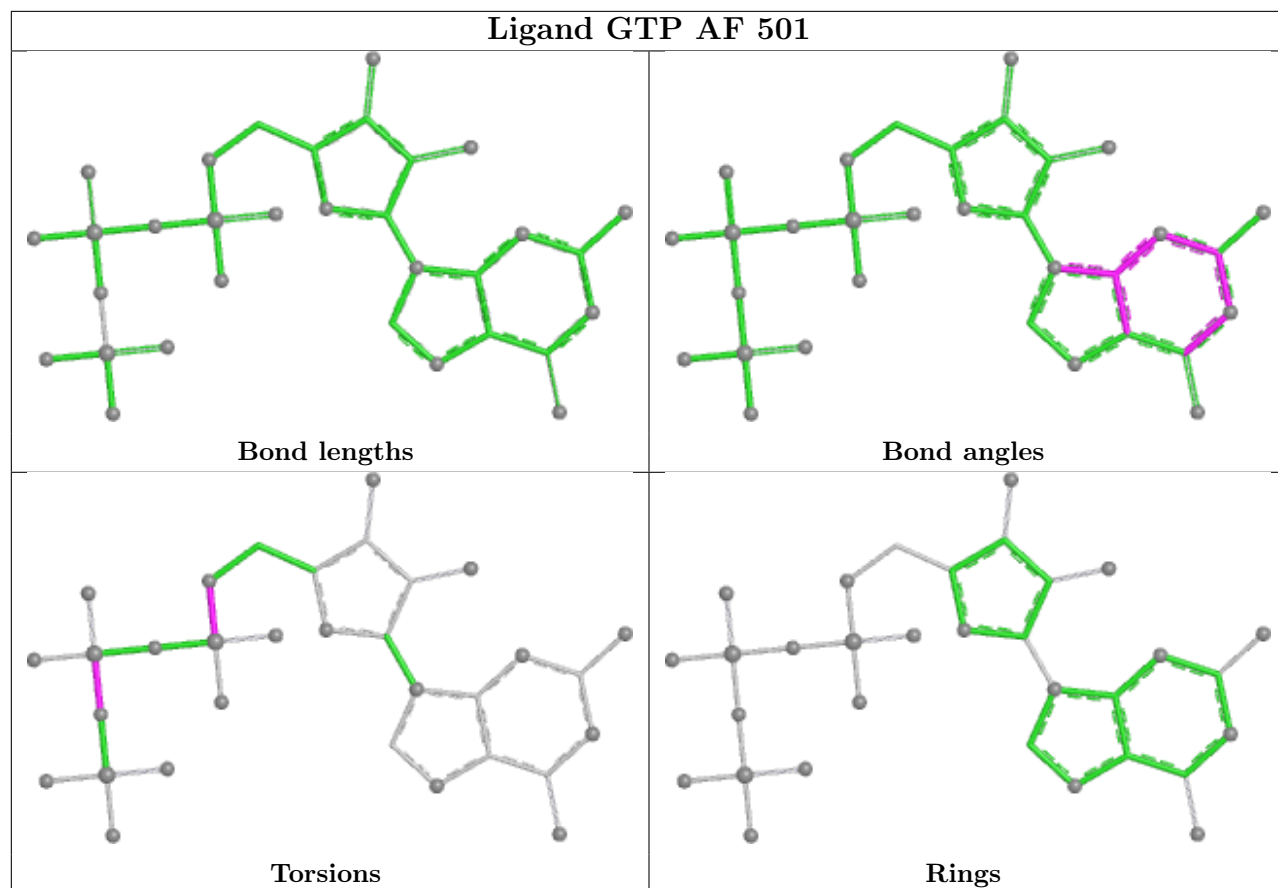


## Ligand GDP JM 501

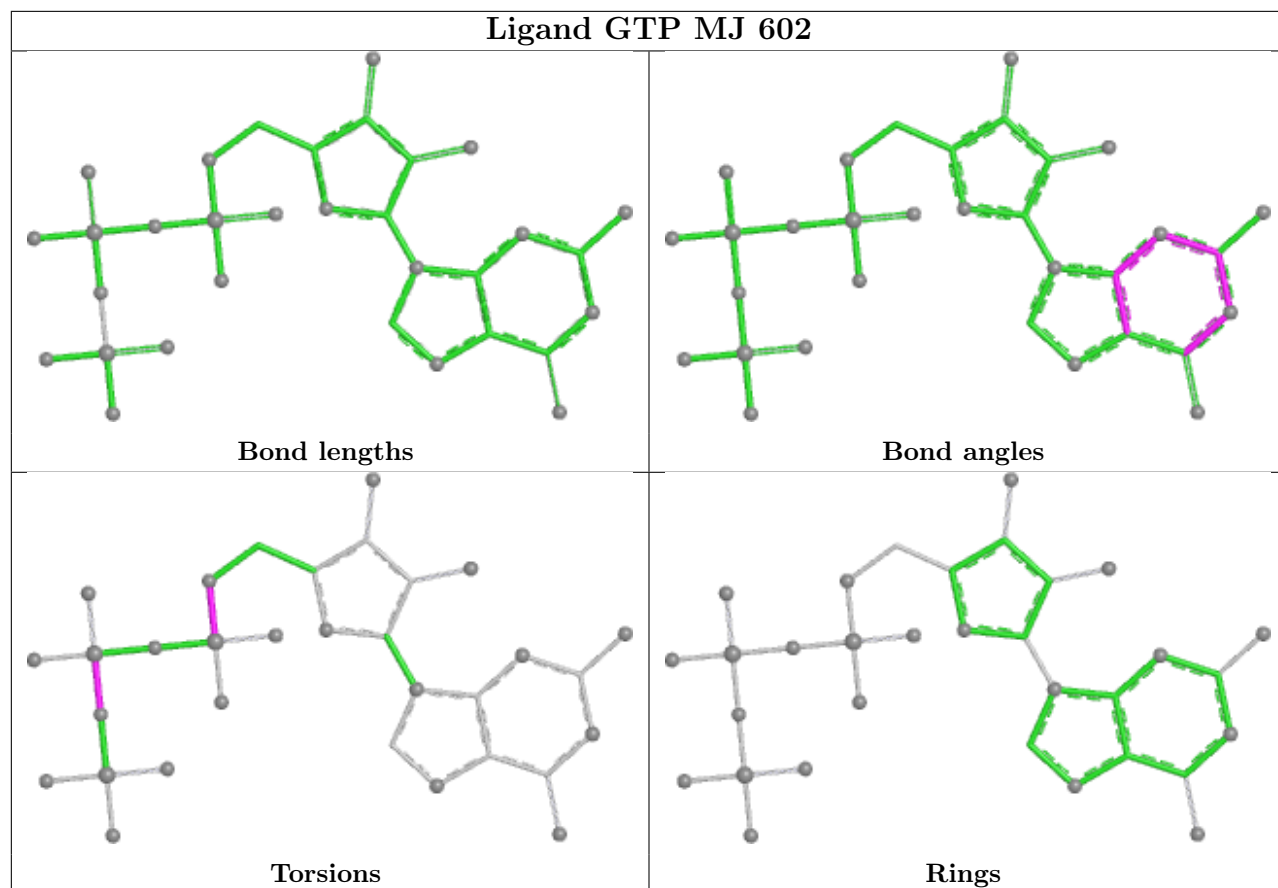




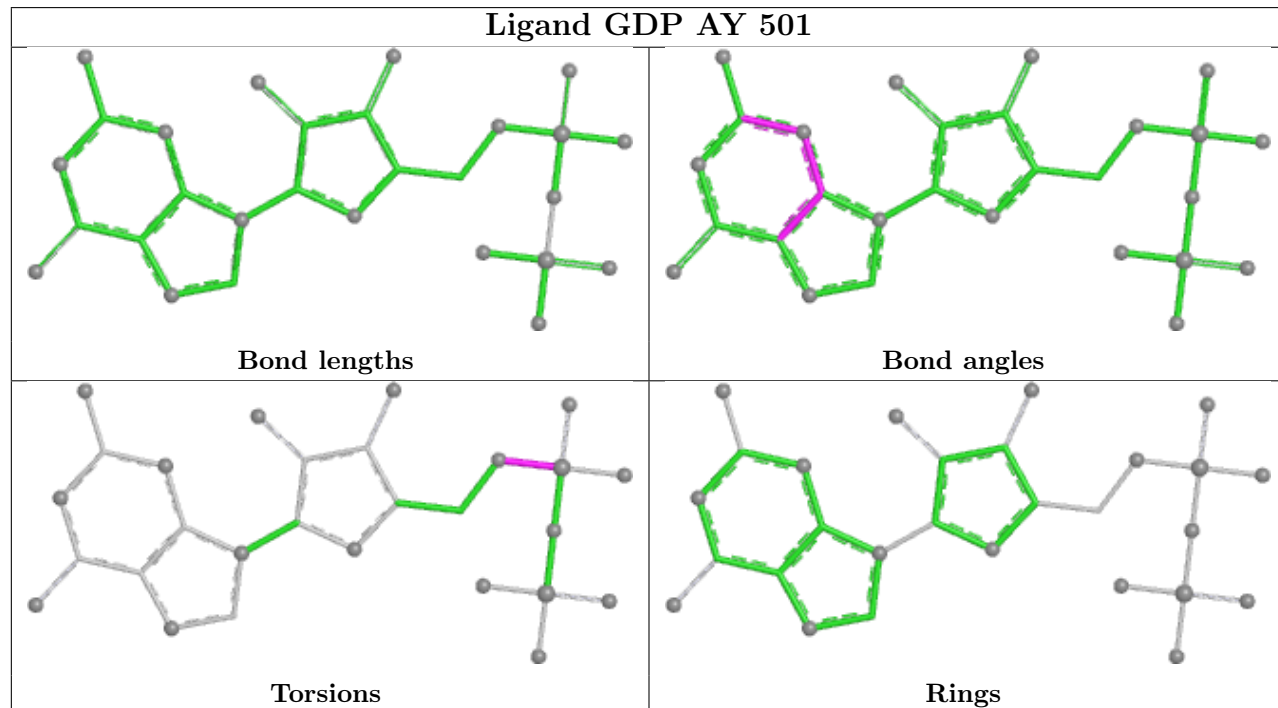


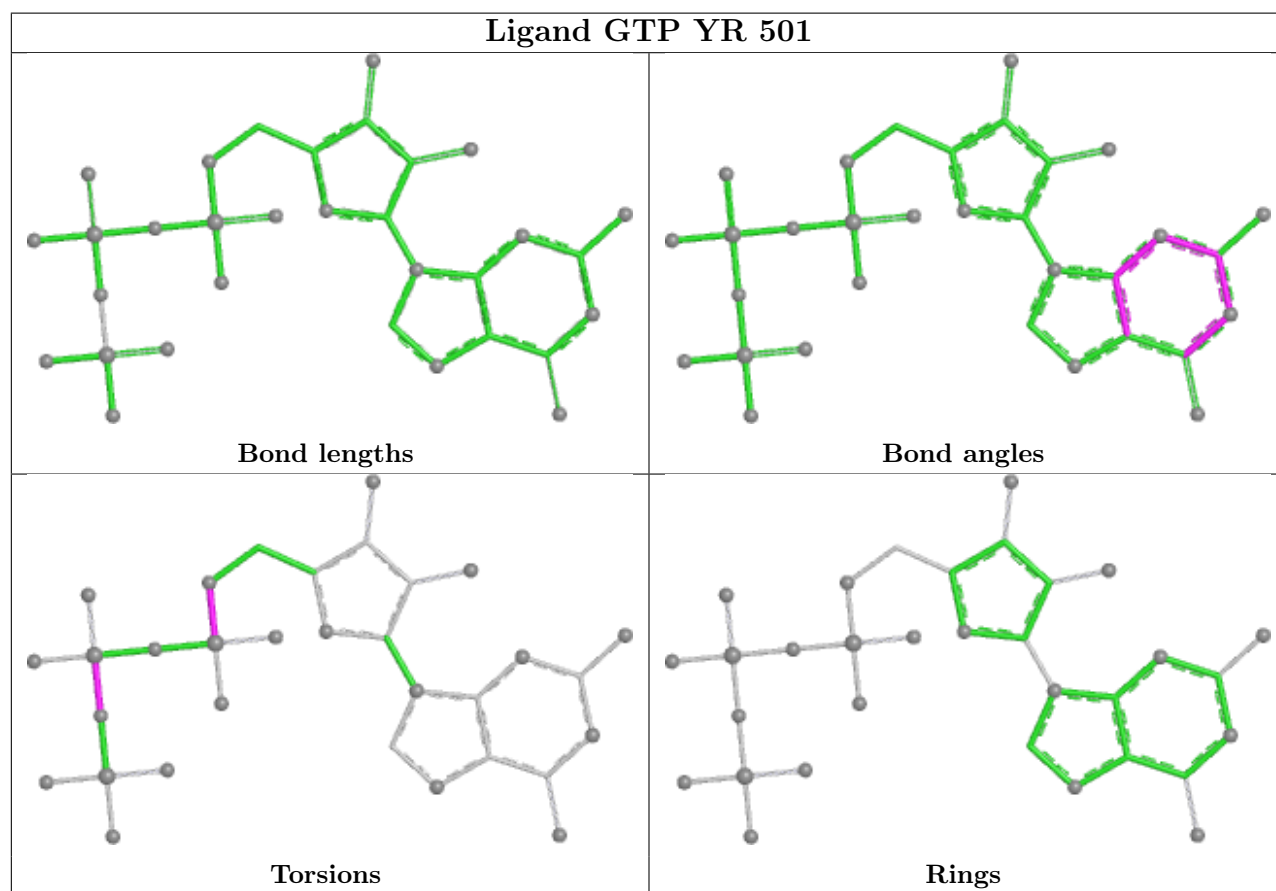
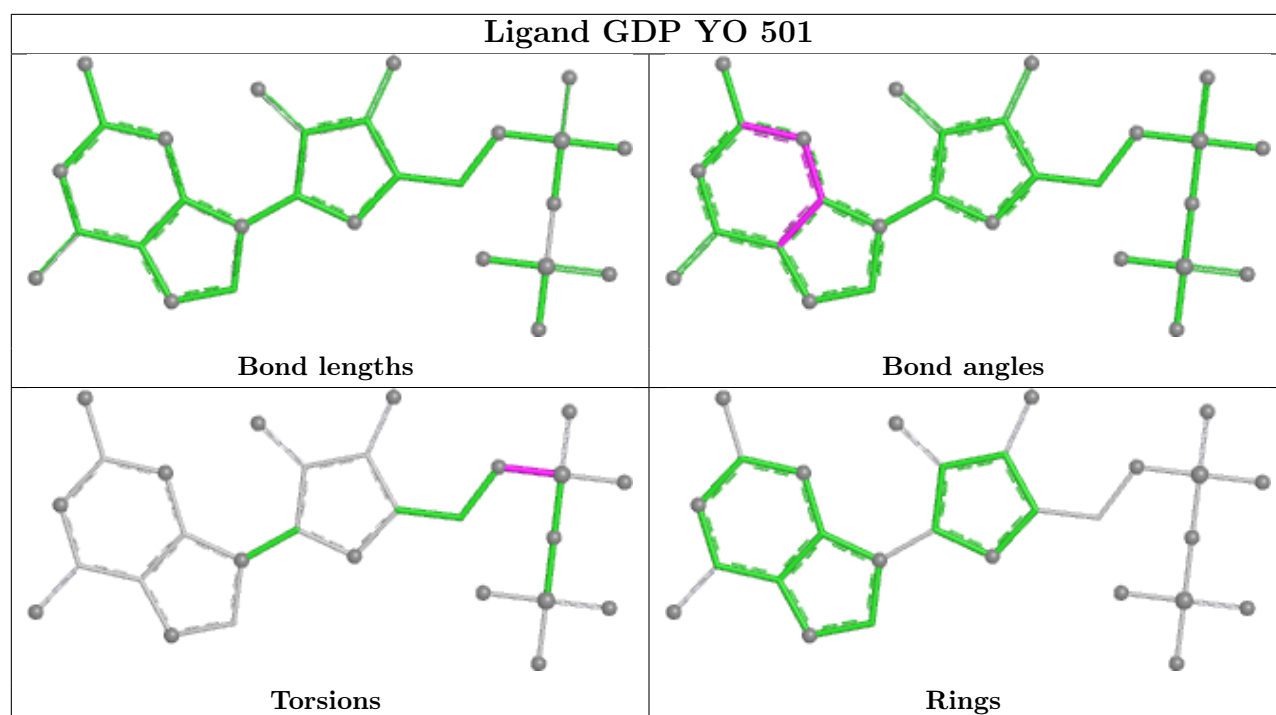


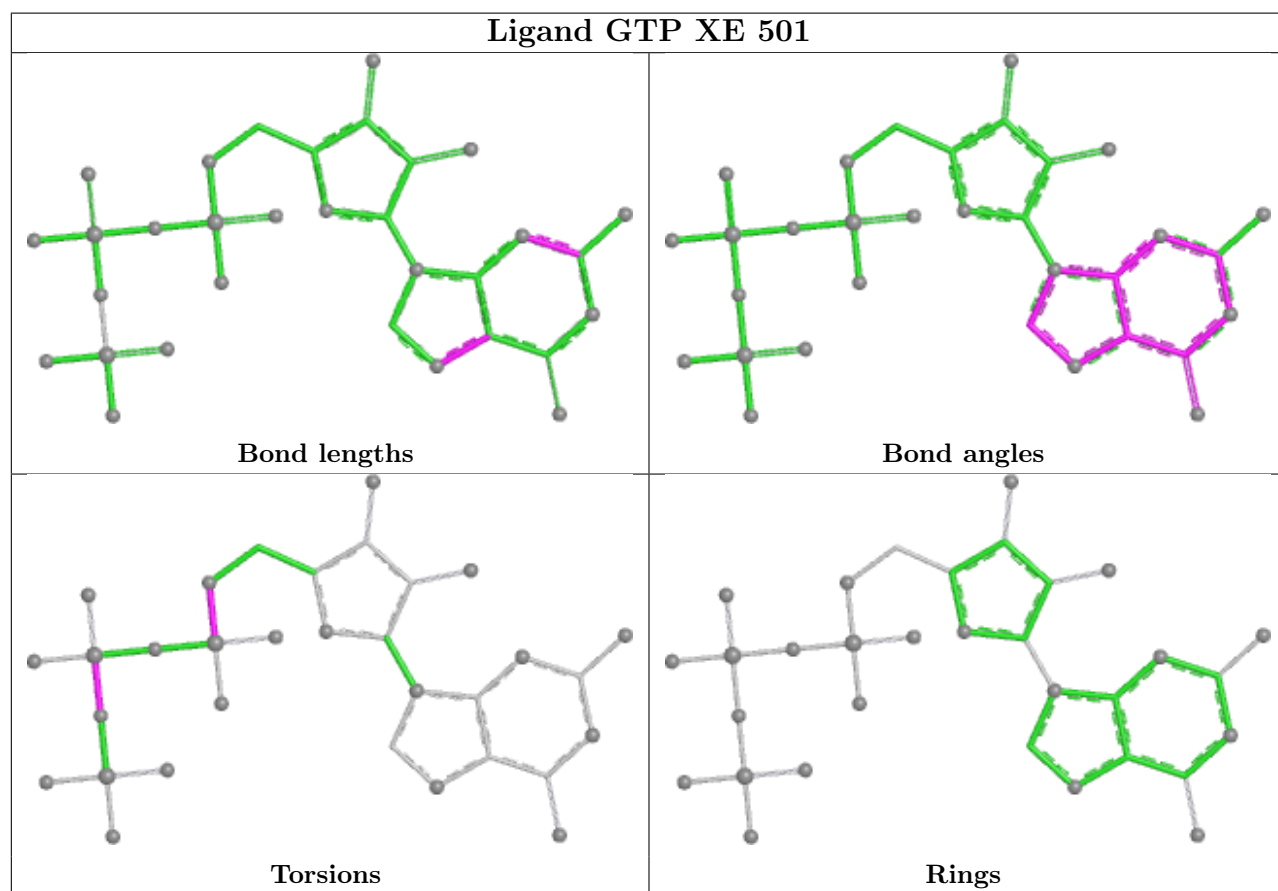
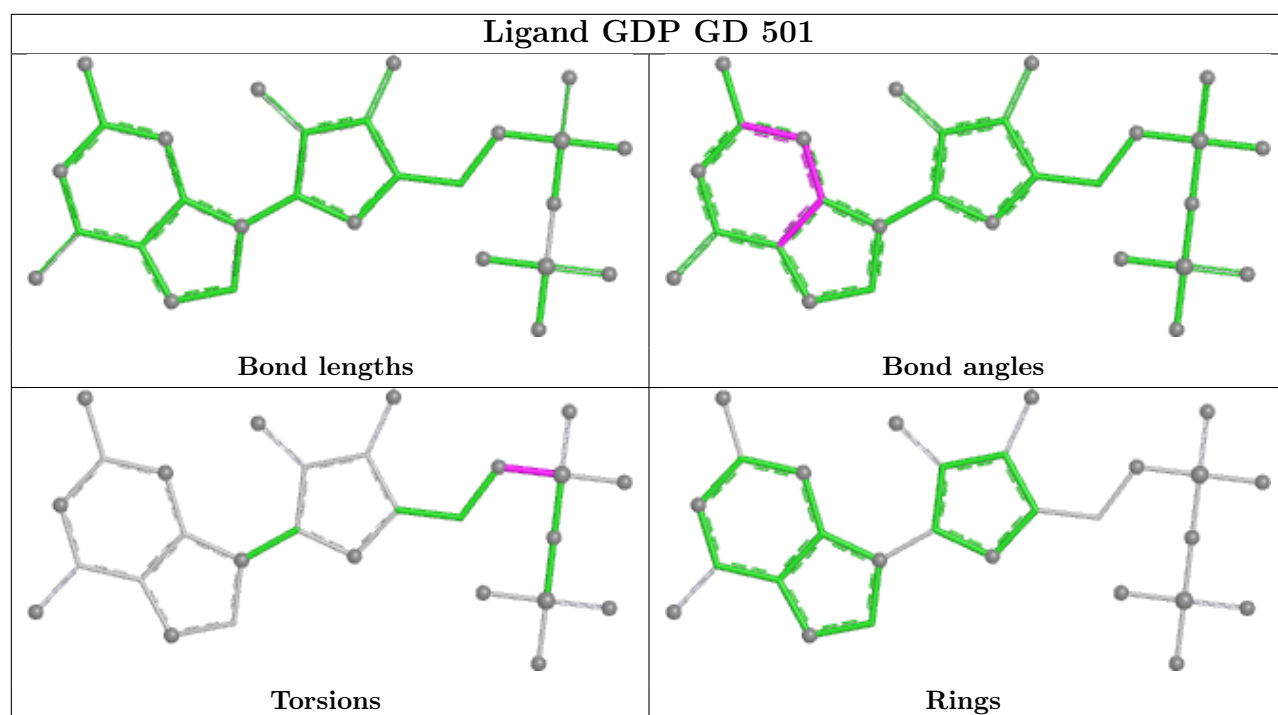
## Ligand GTP MJ 602



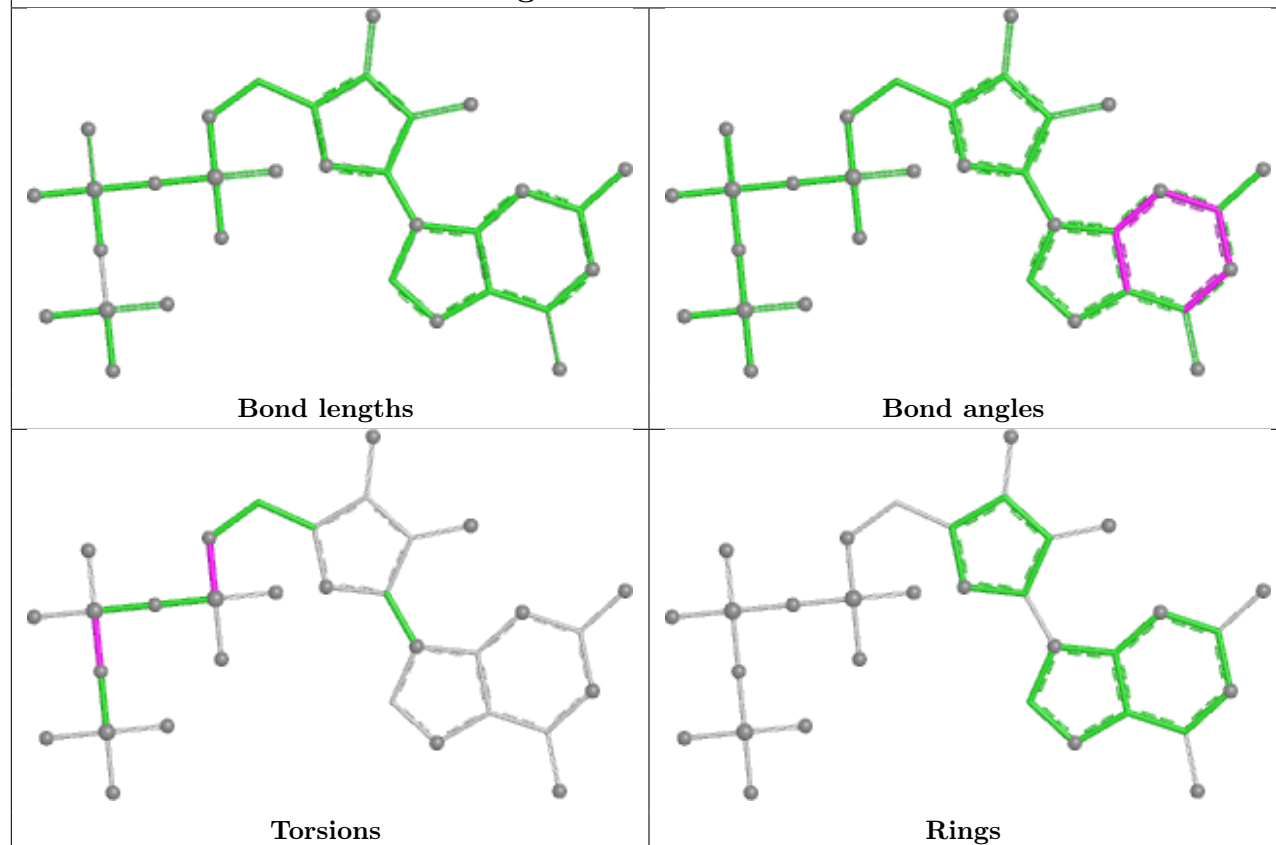
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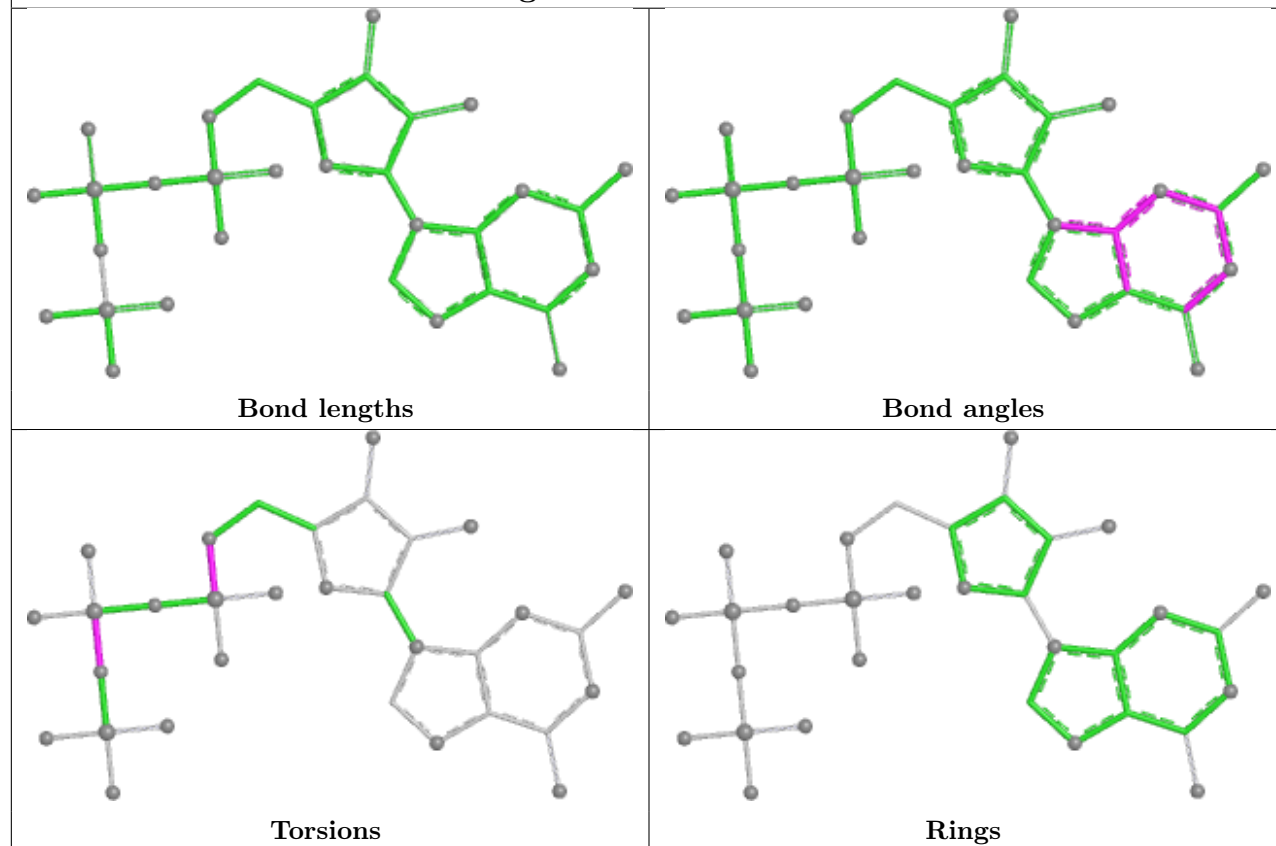




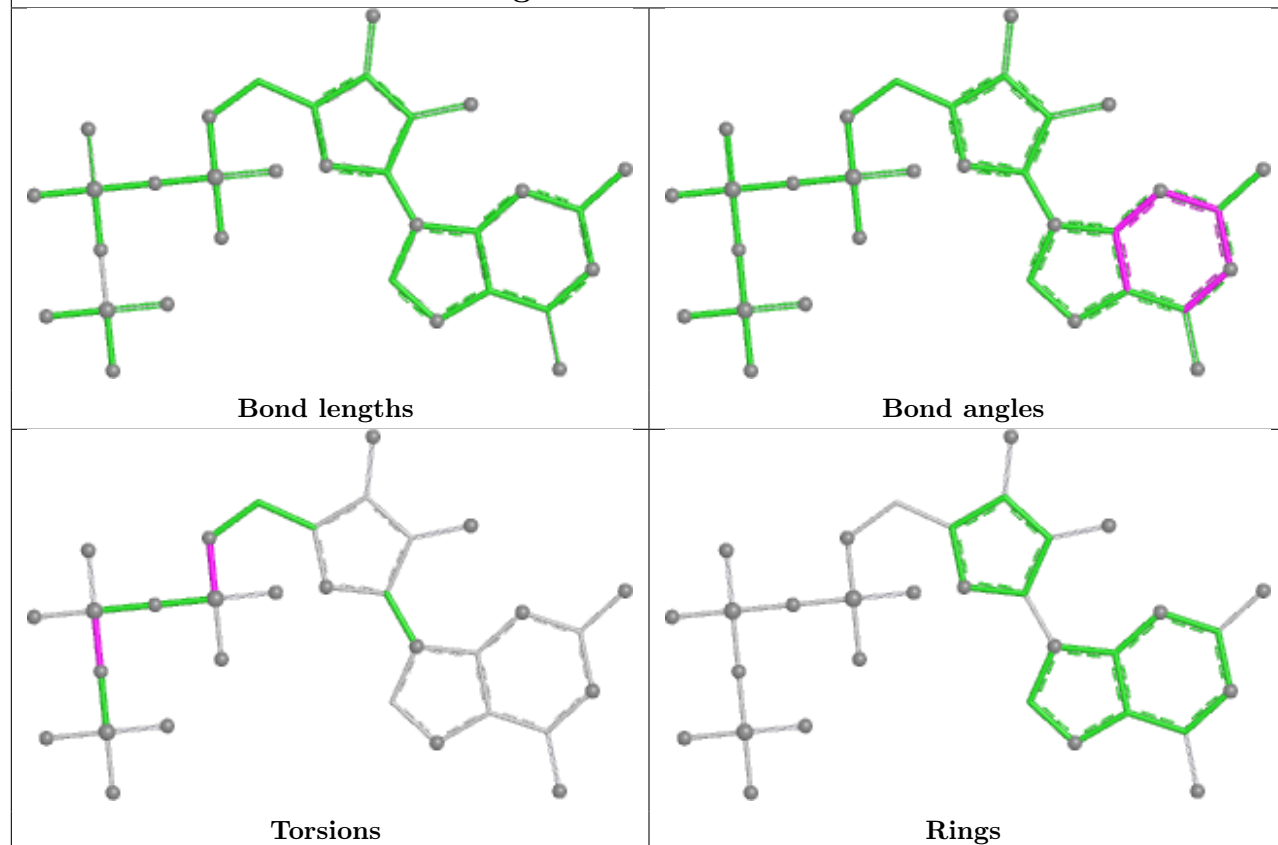
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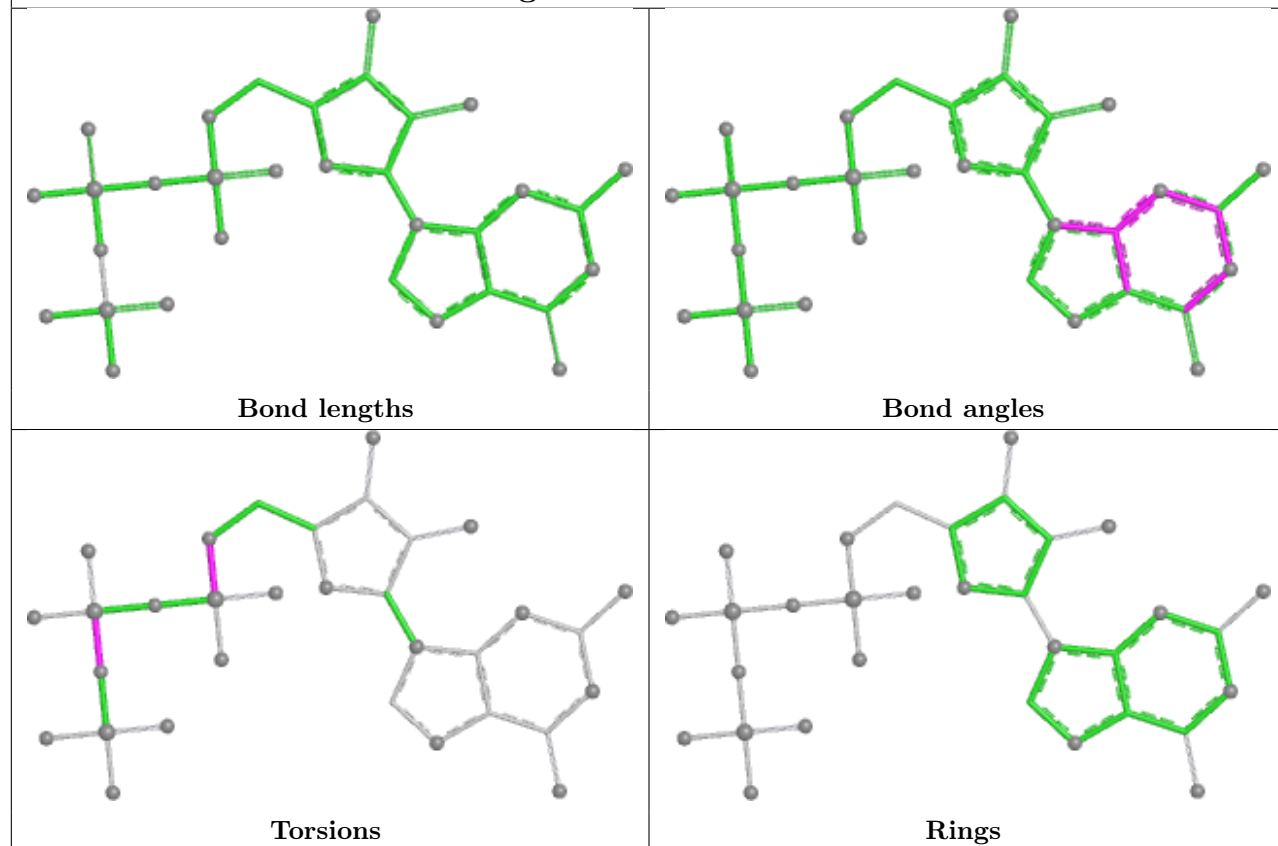
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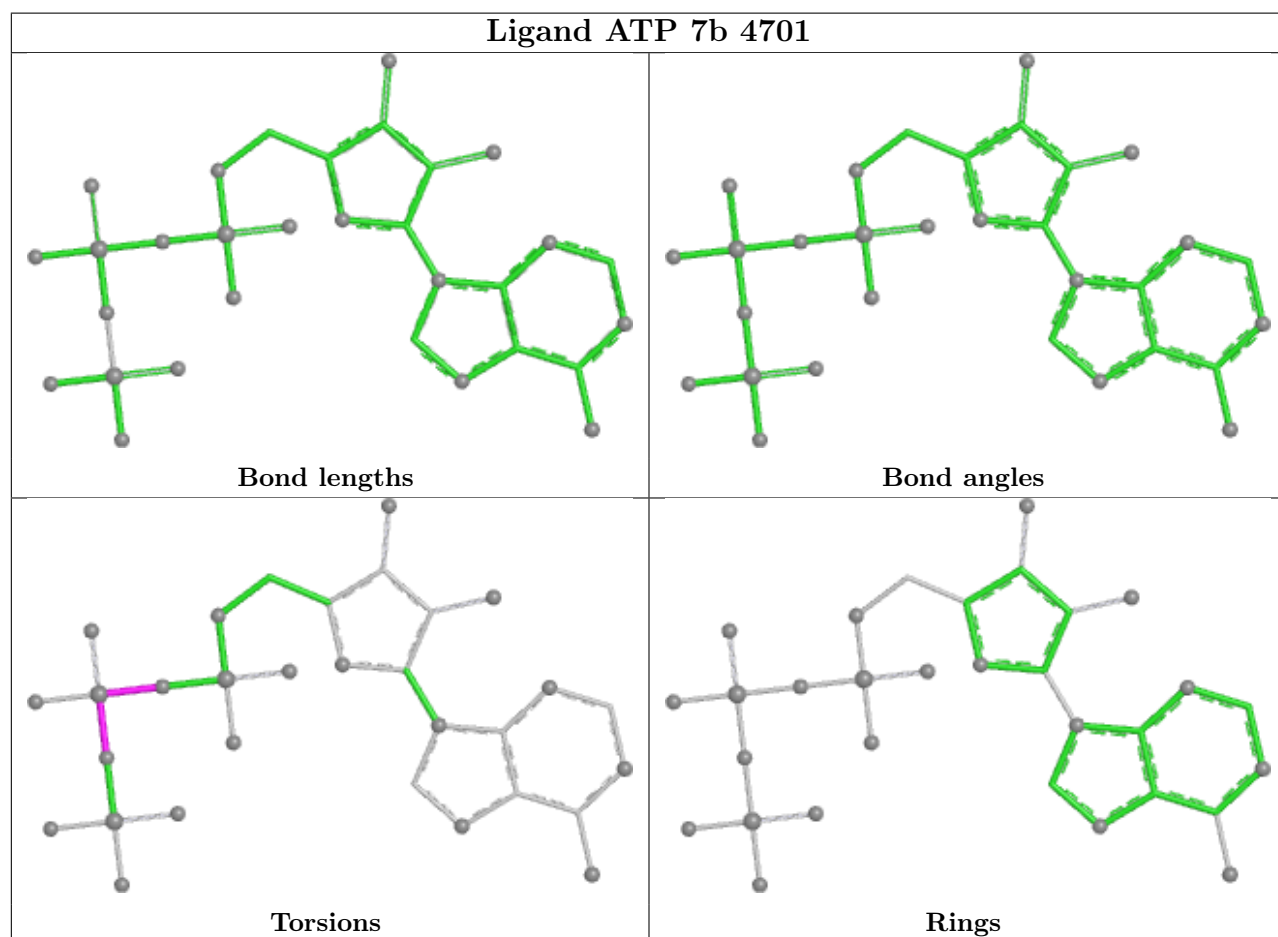
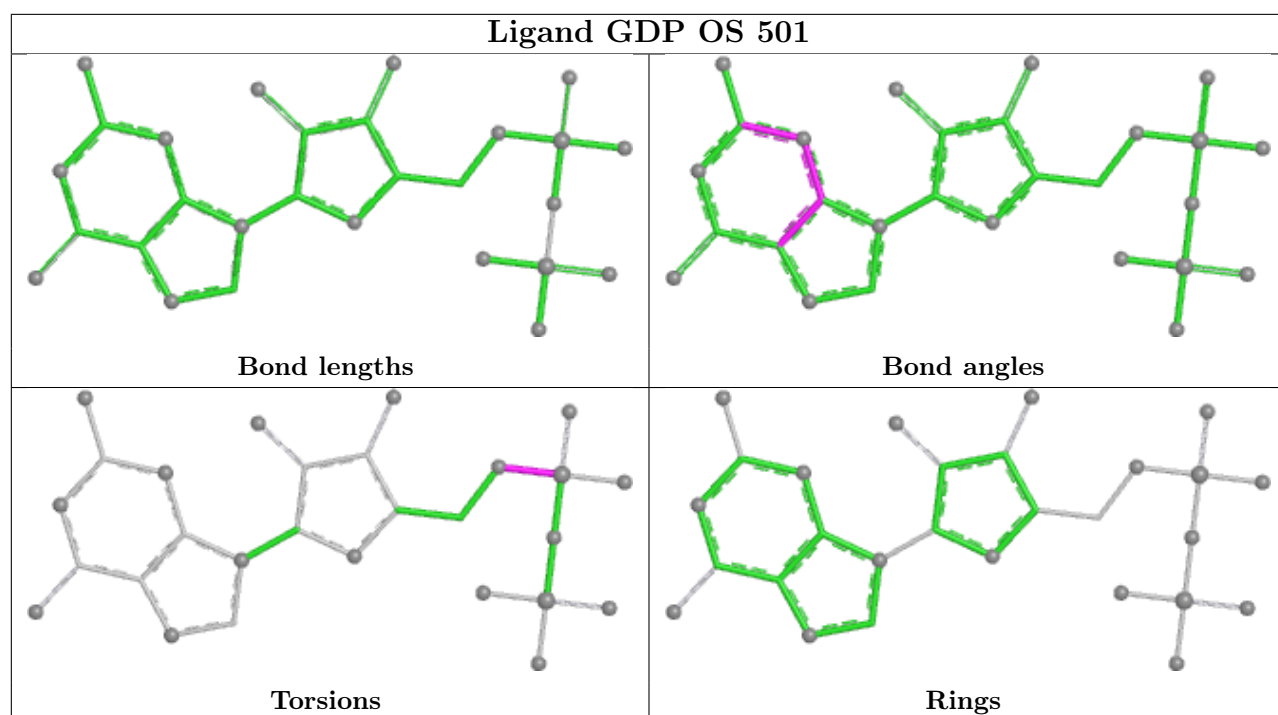


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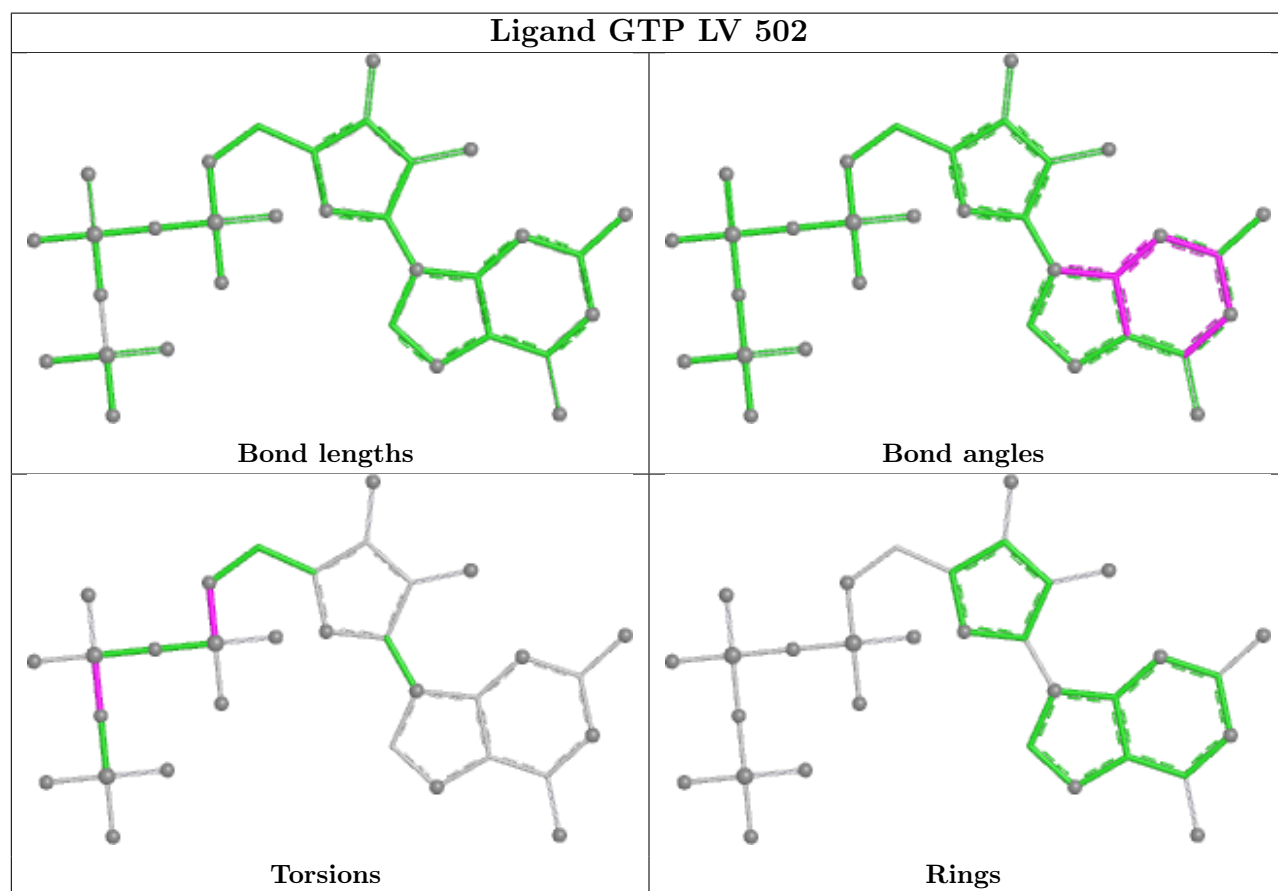
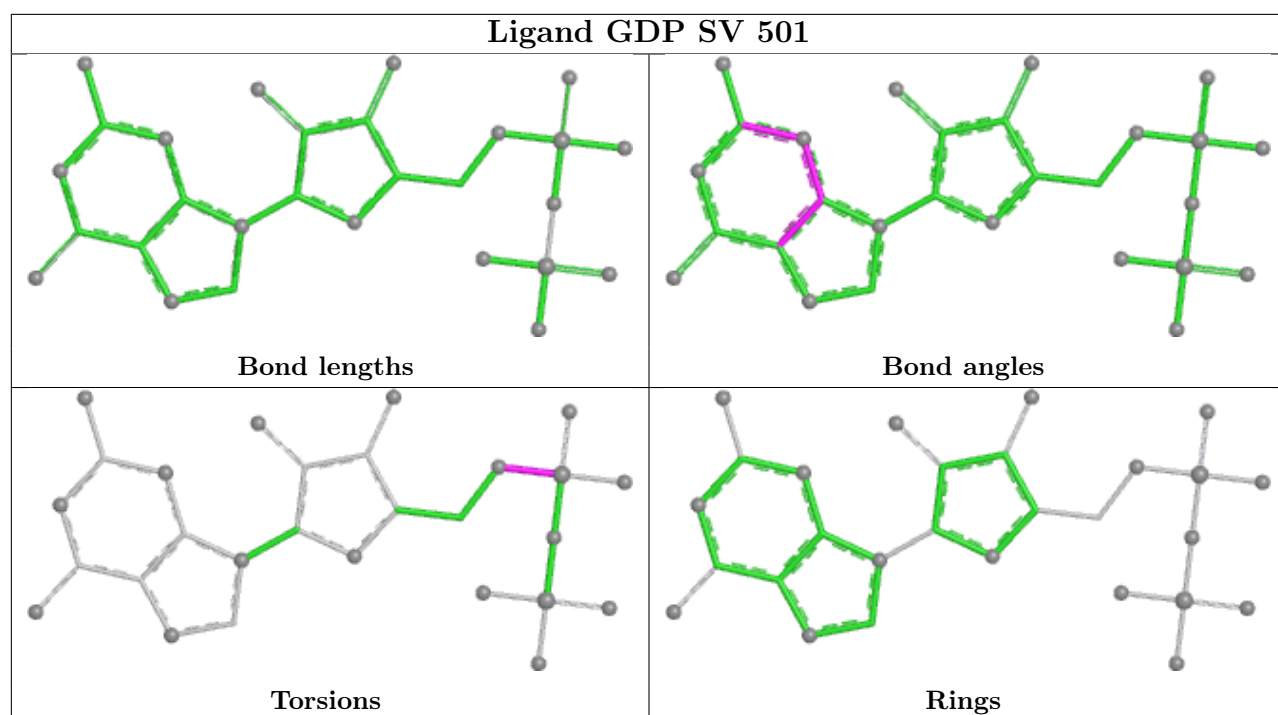


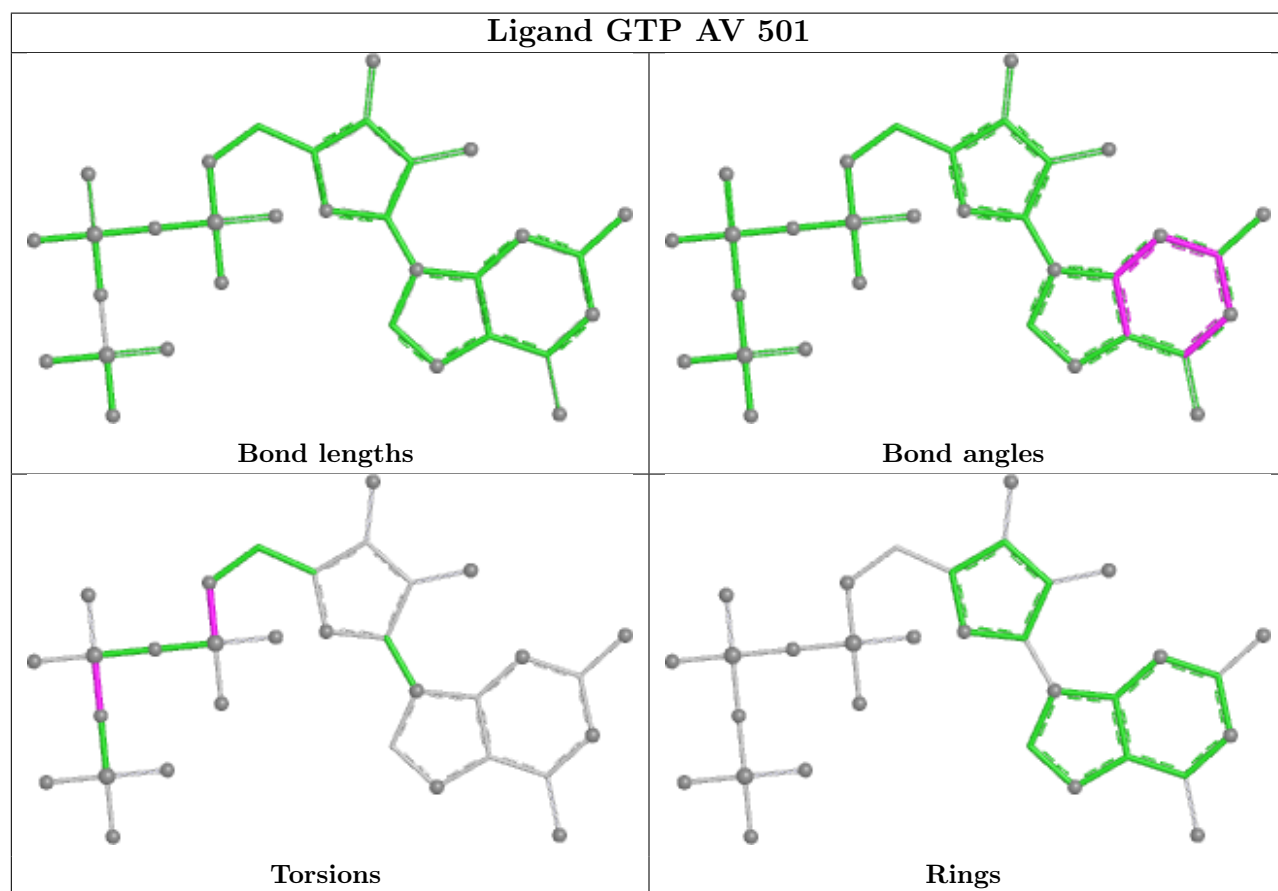
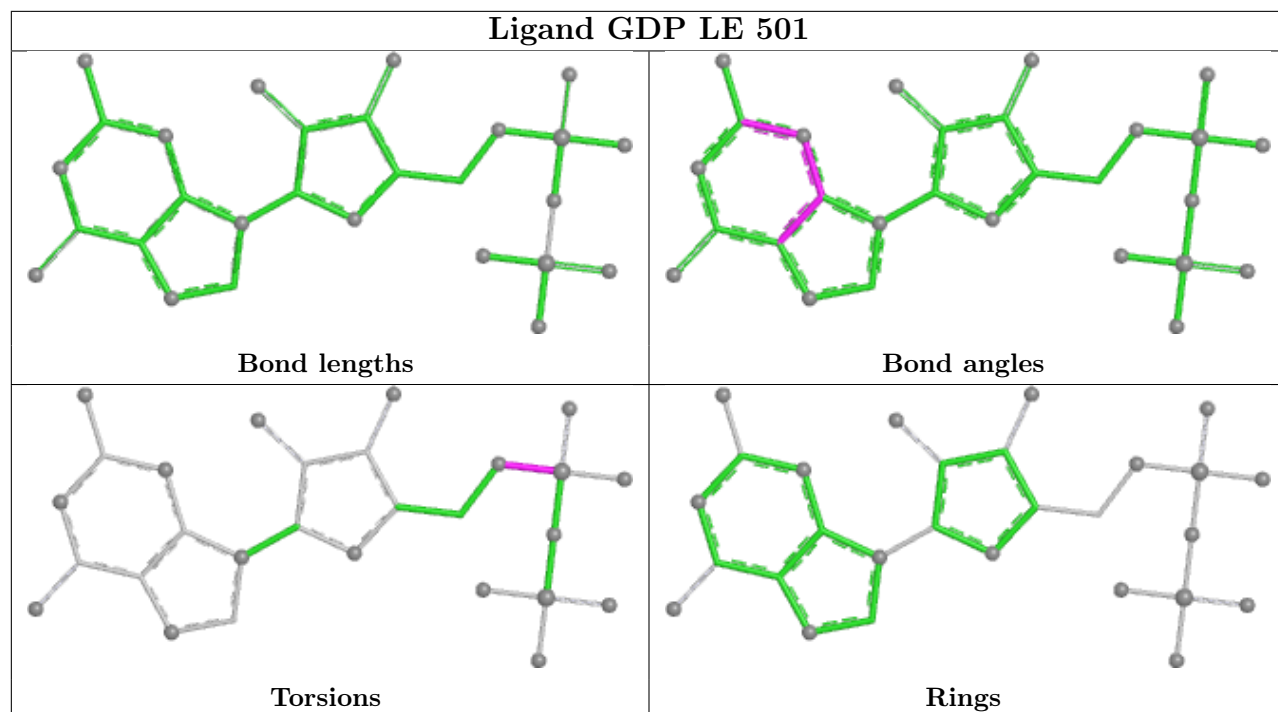
## Ligand GTP AZ 501



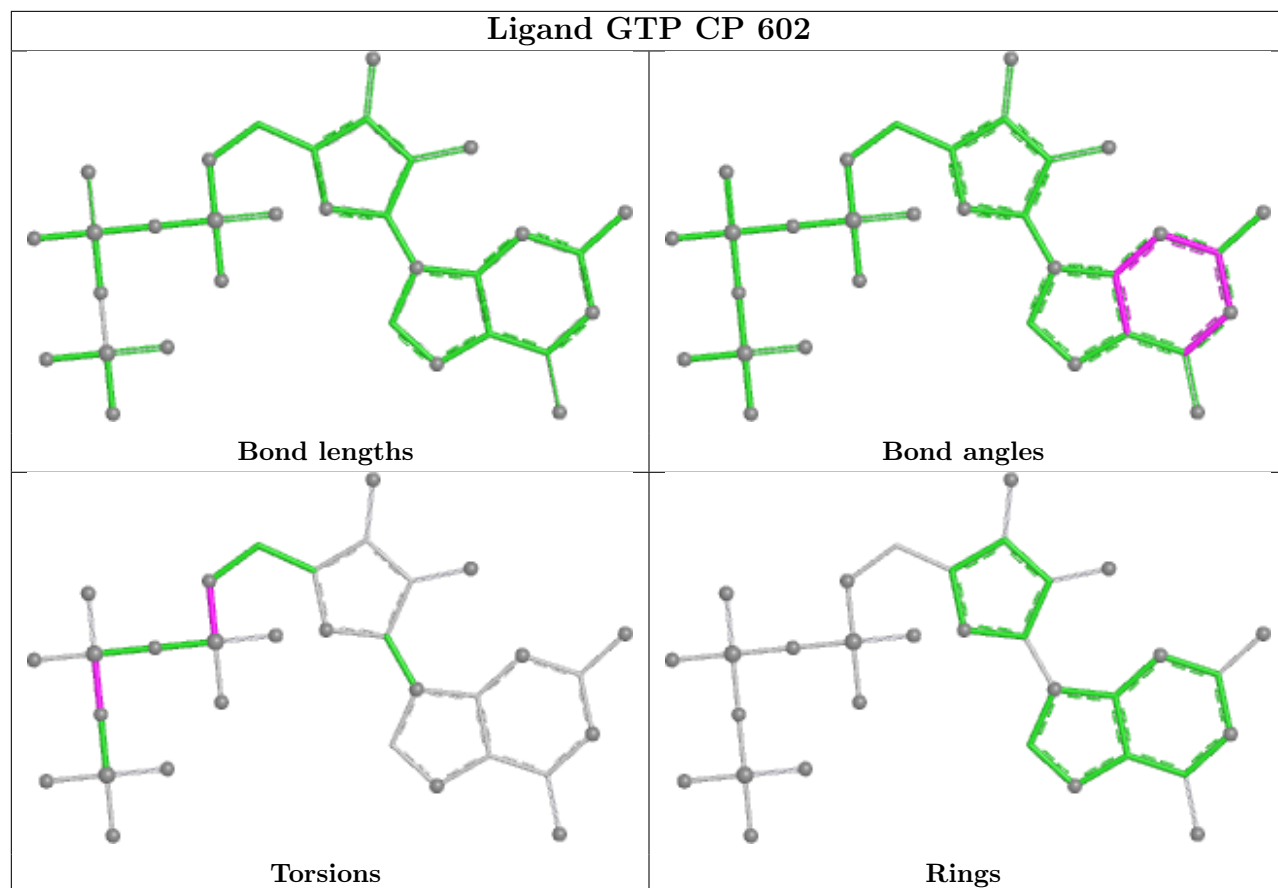




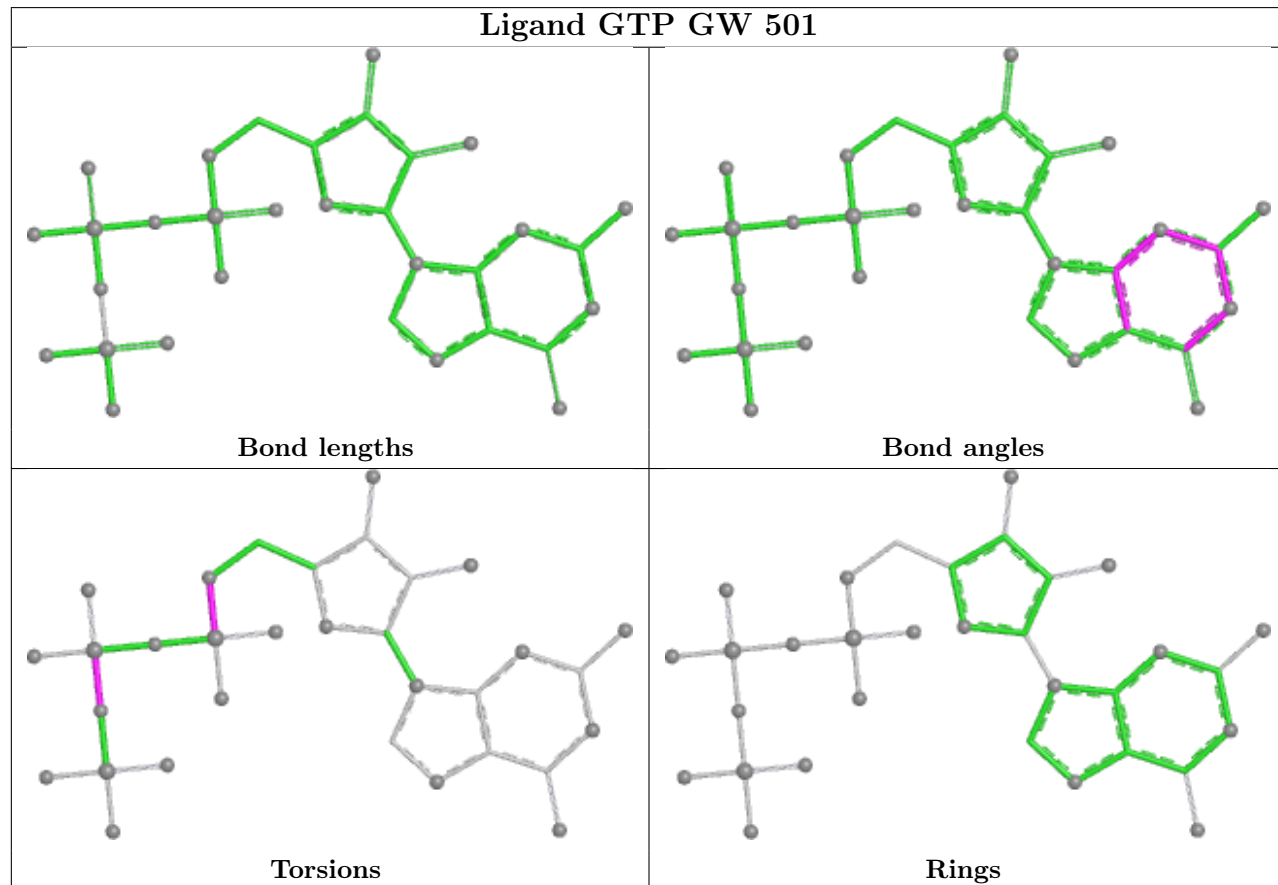




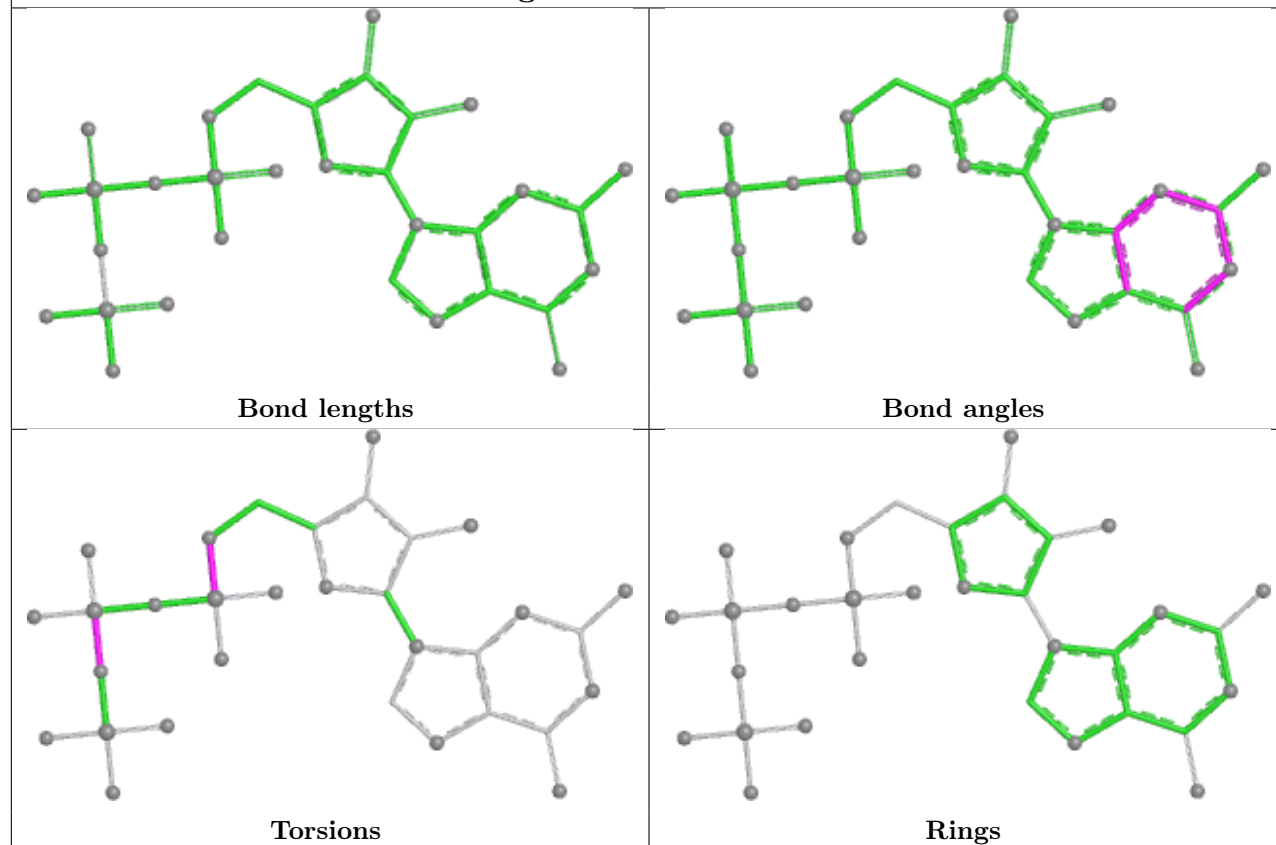
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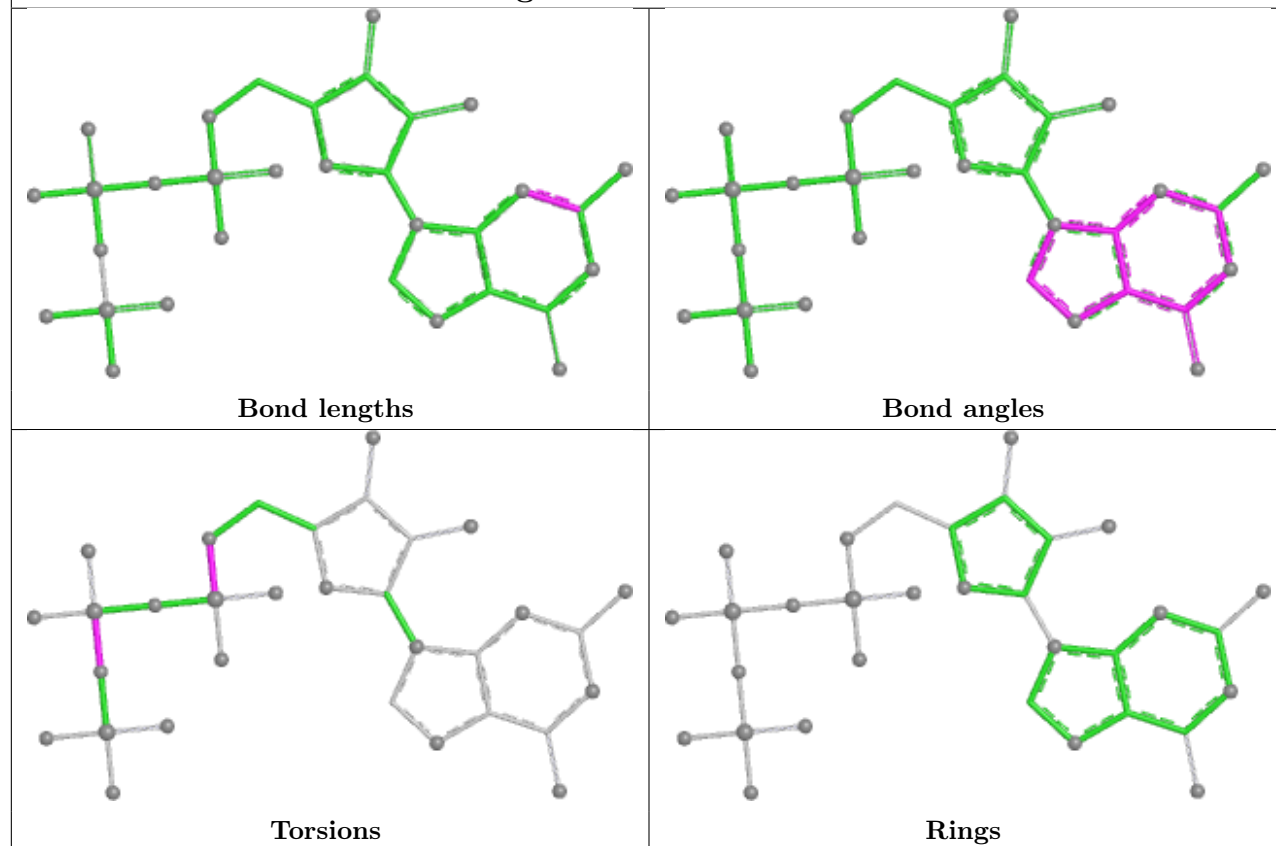
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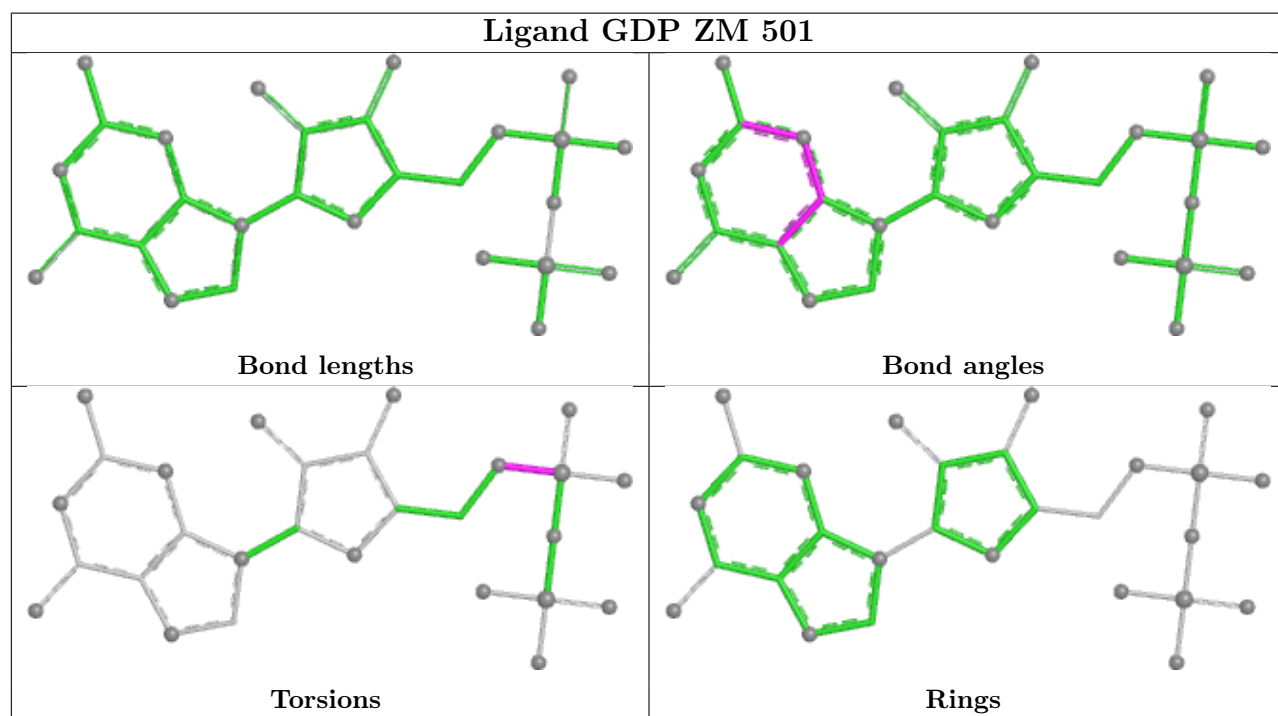
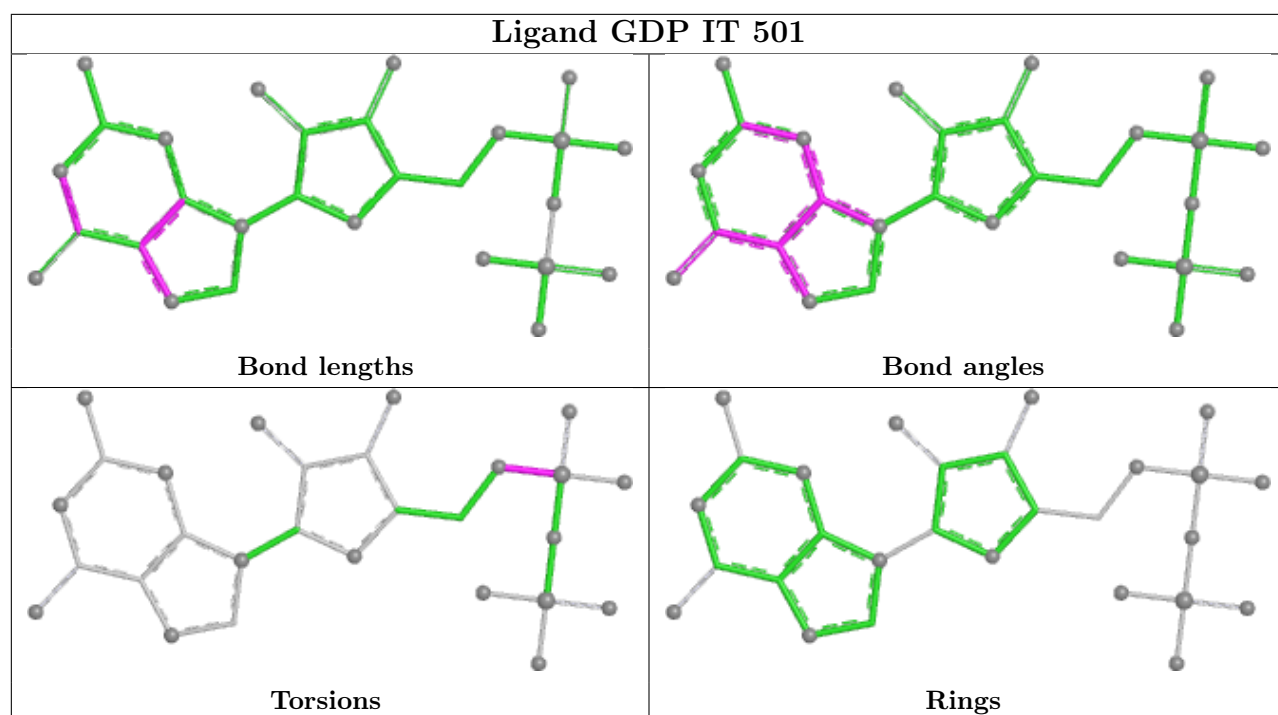


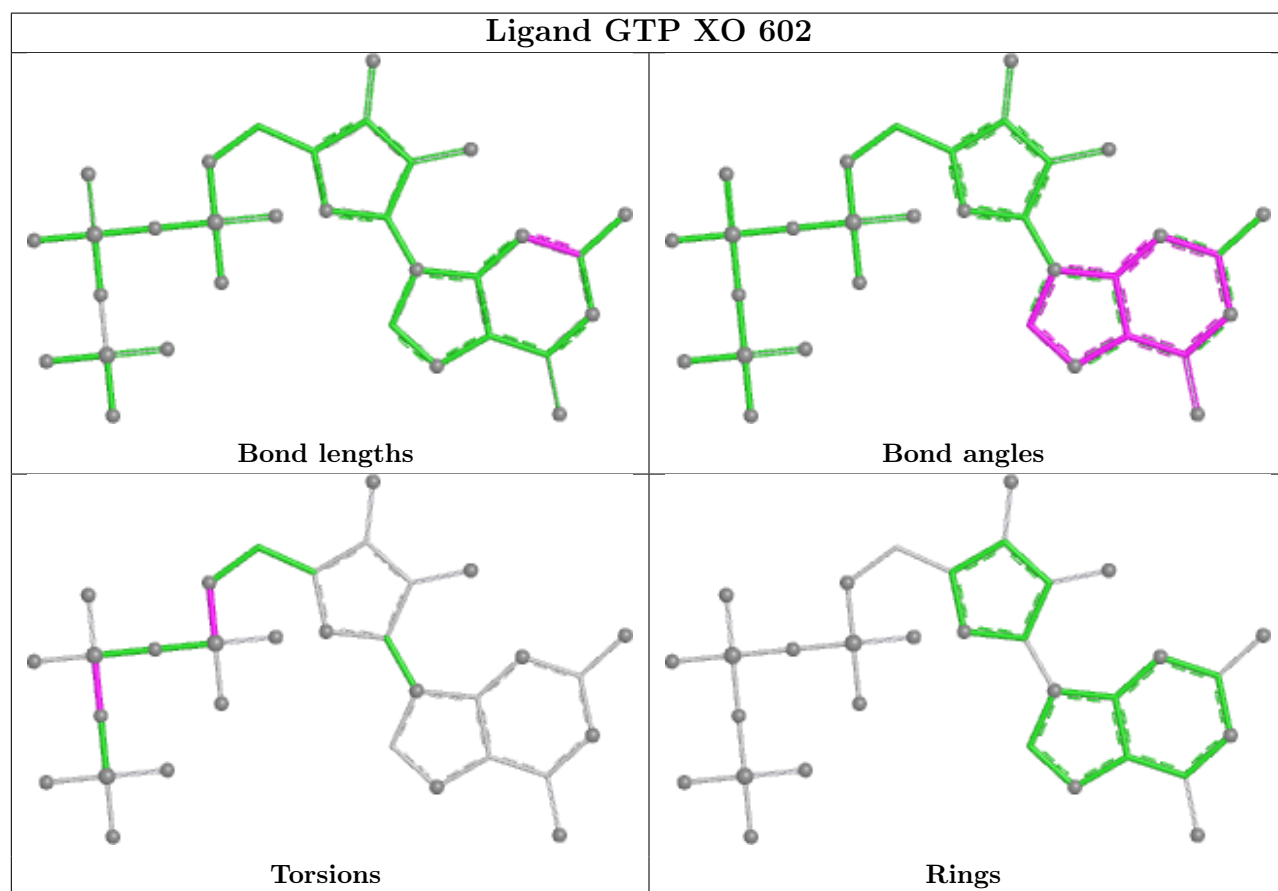
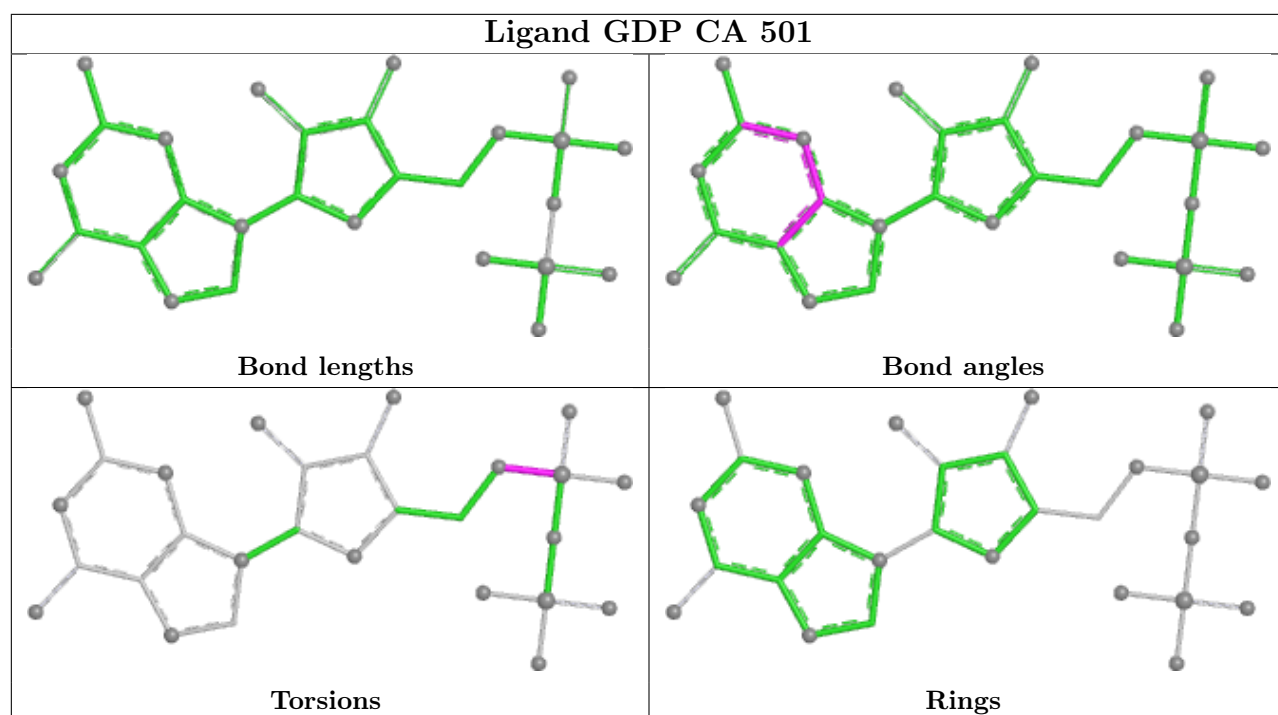
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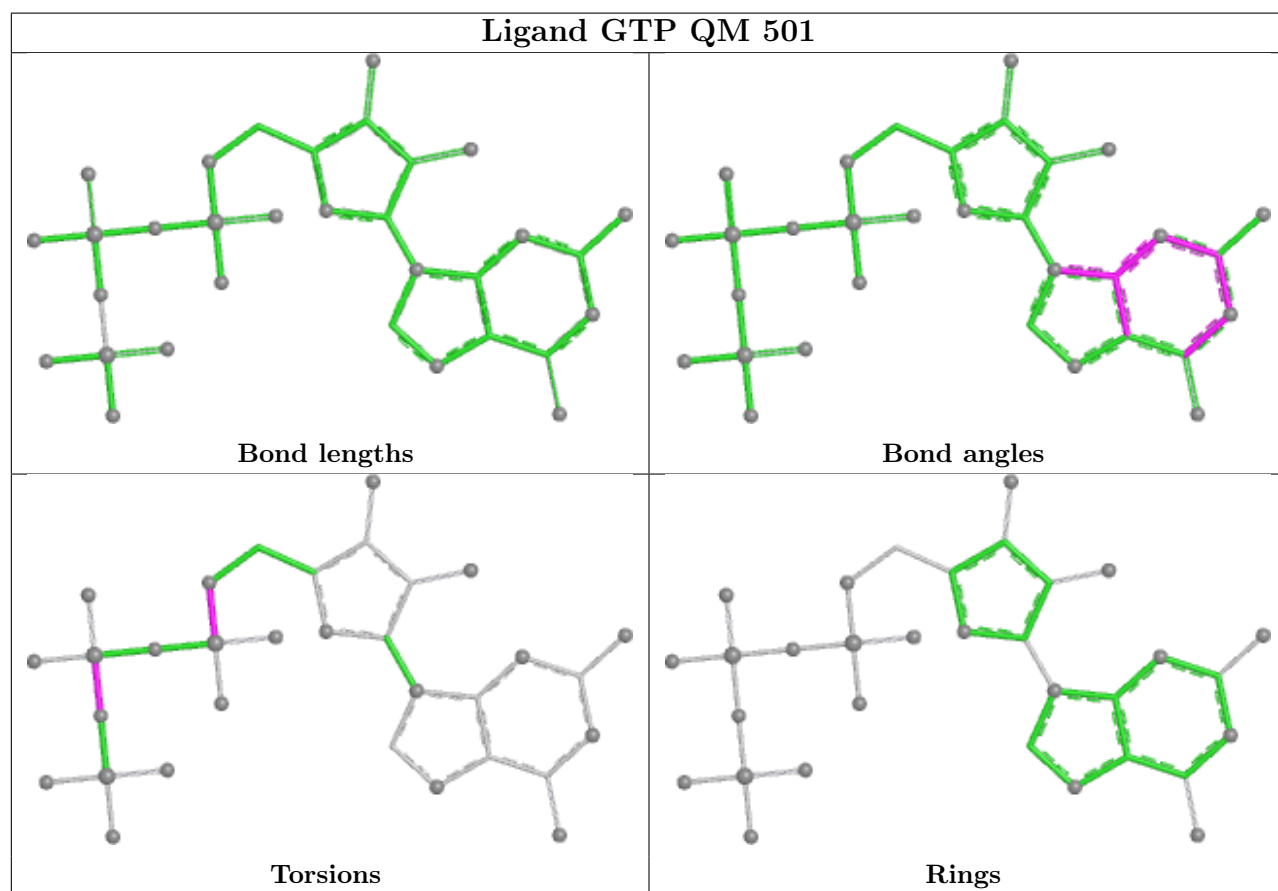
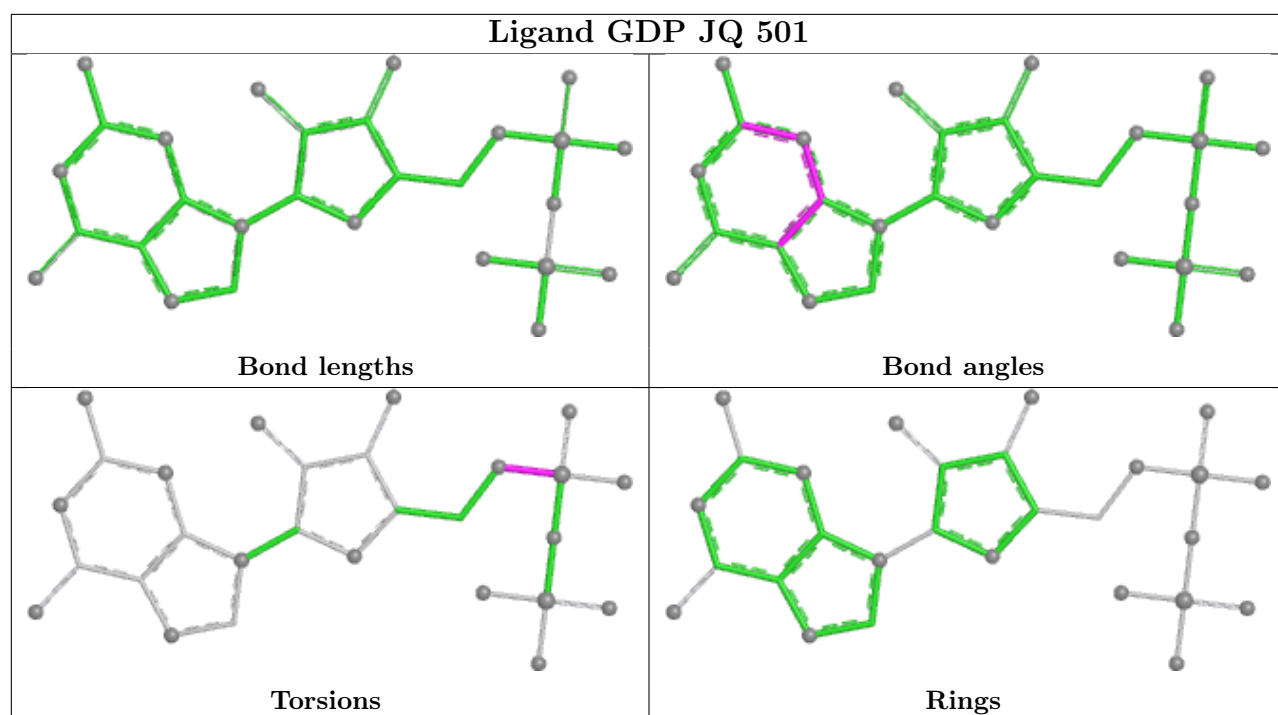


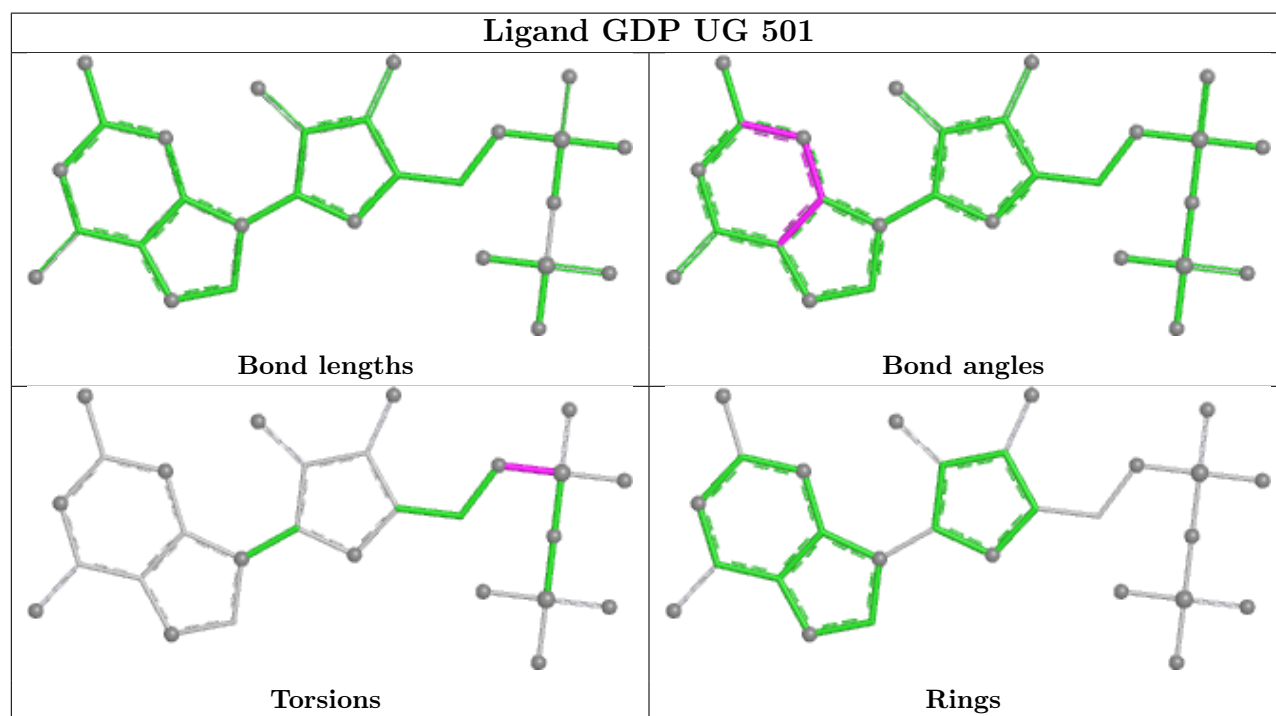
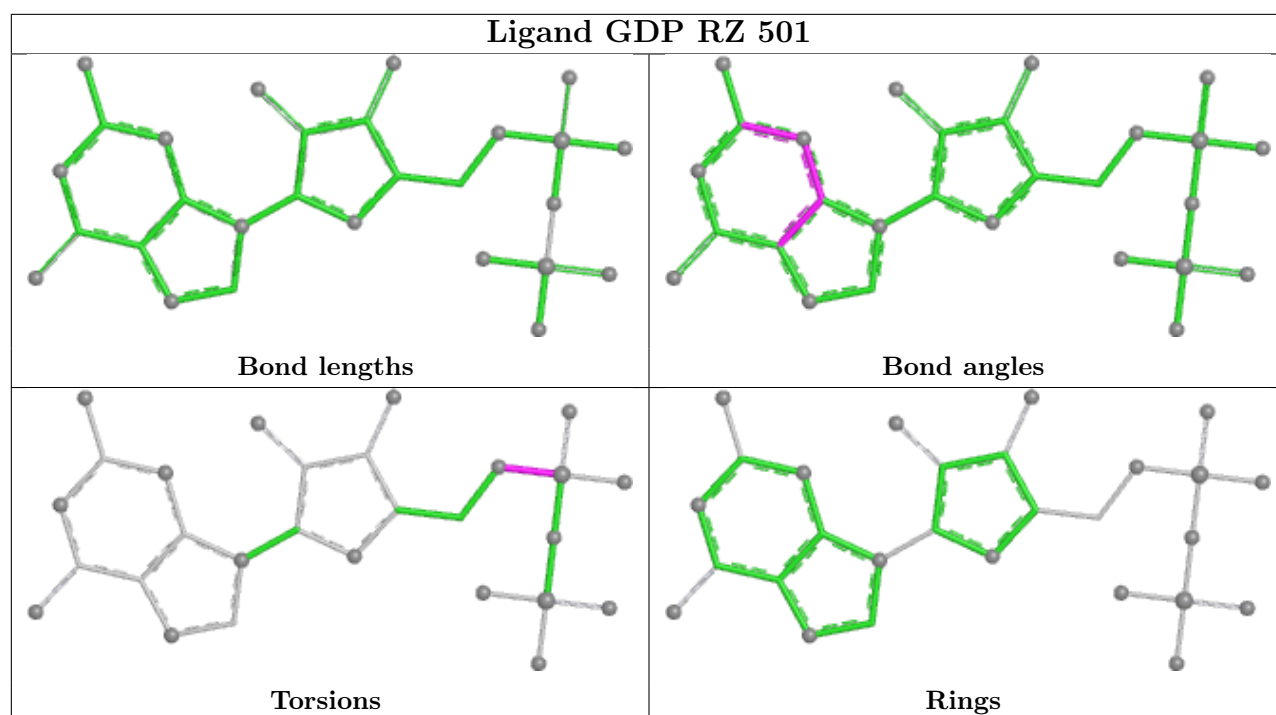
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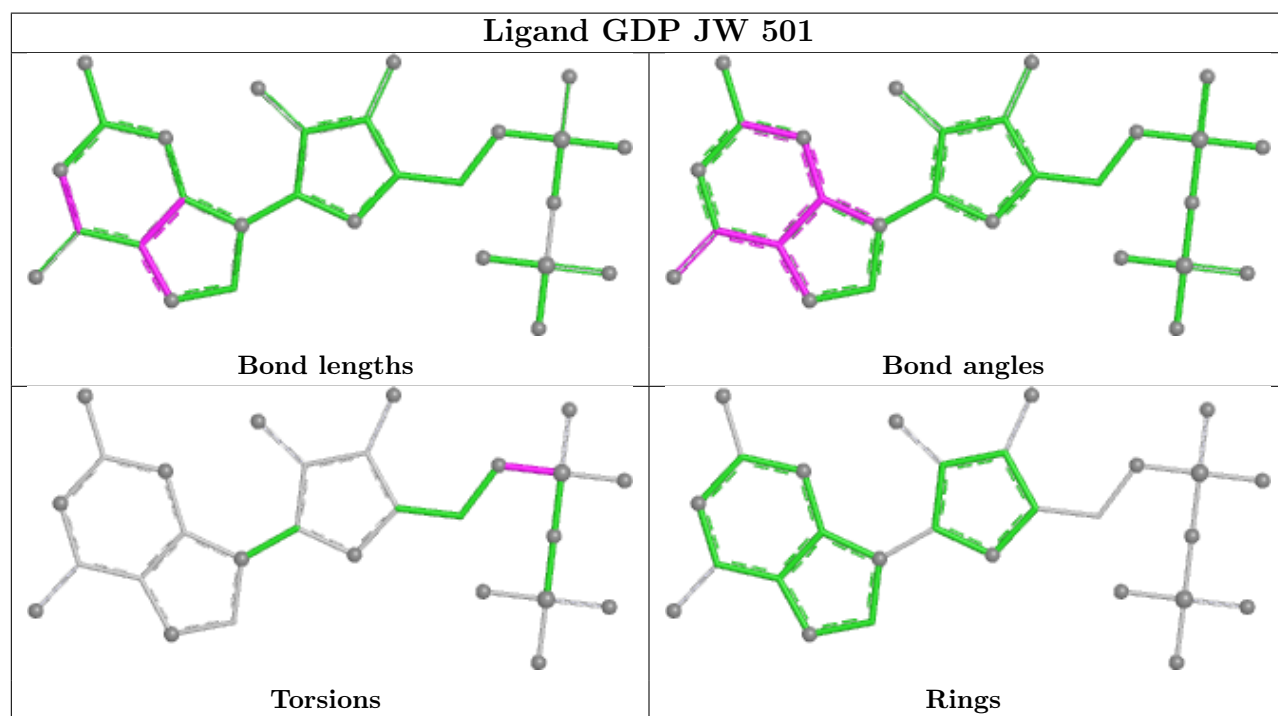
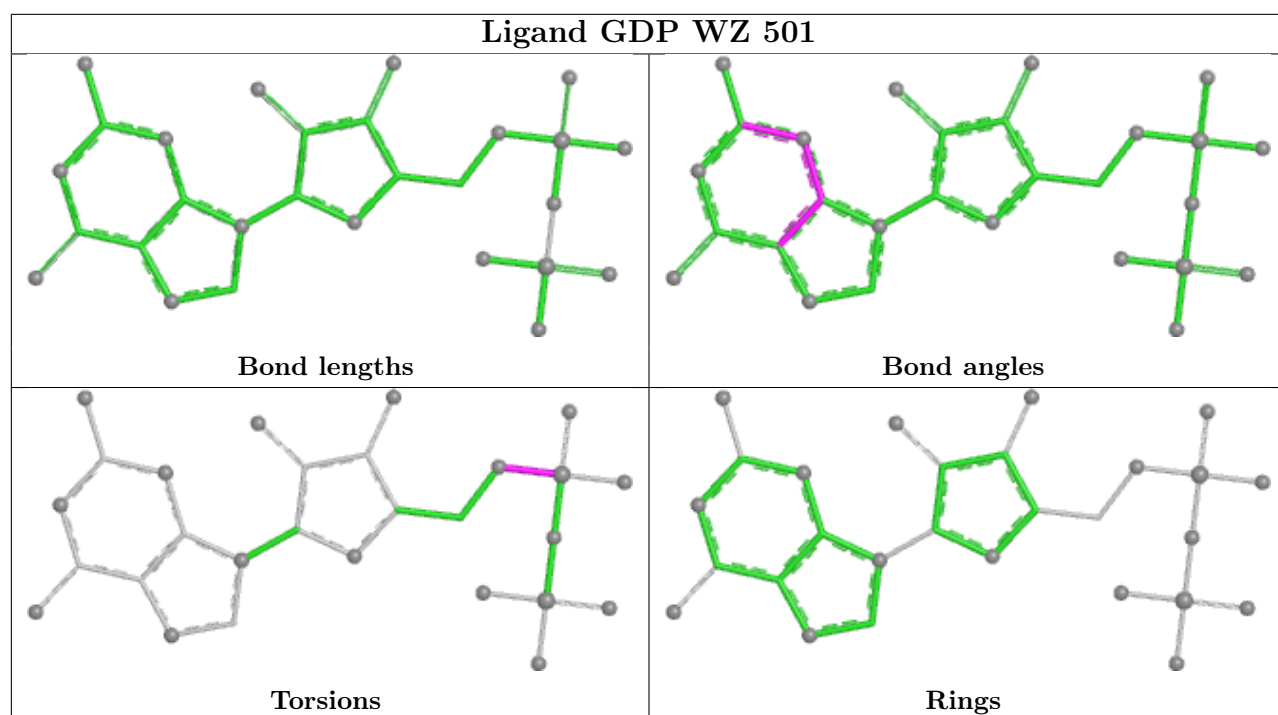


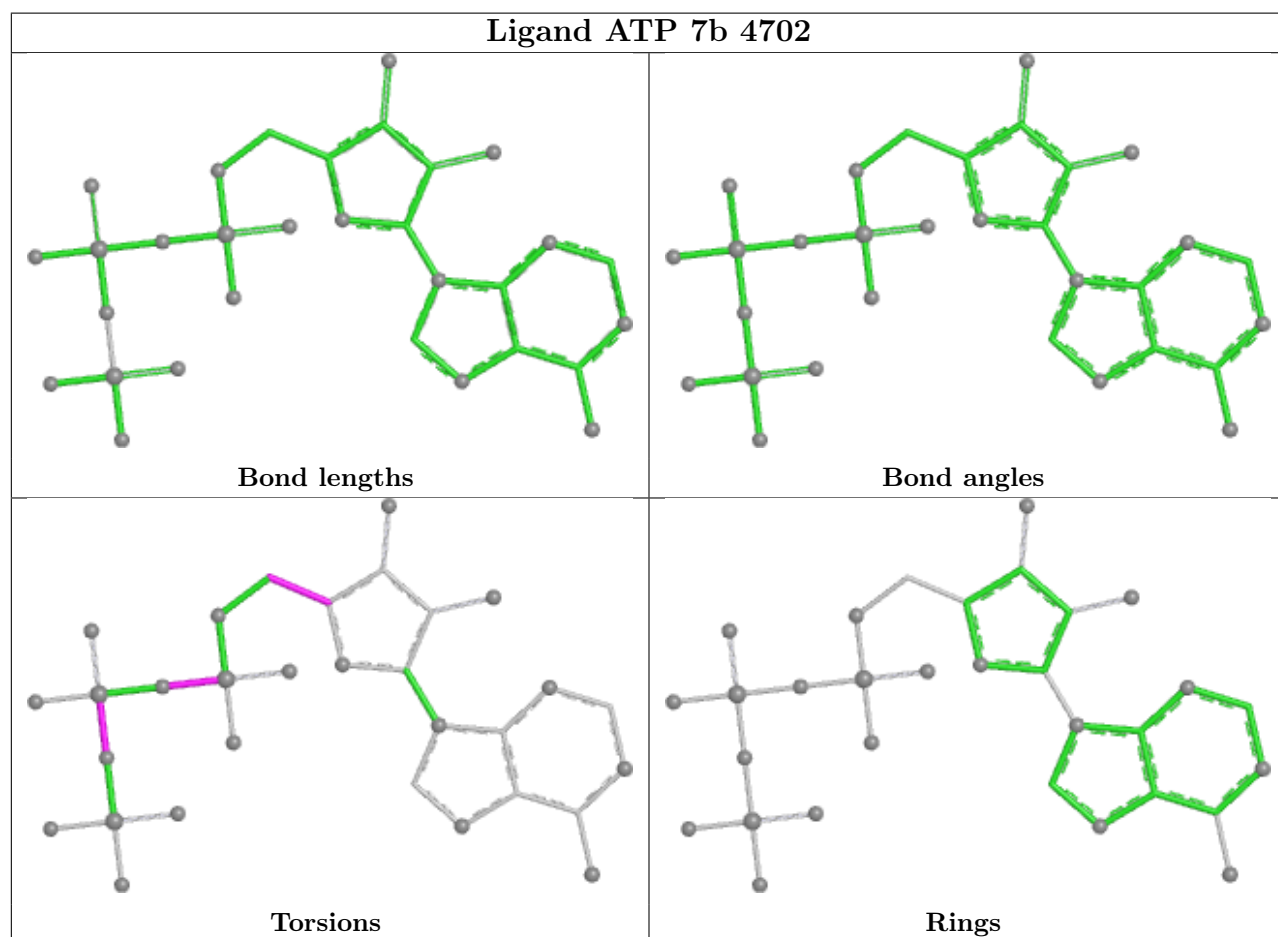
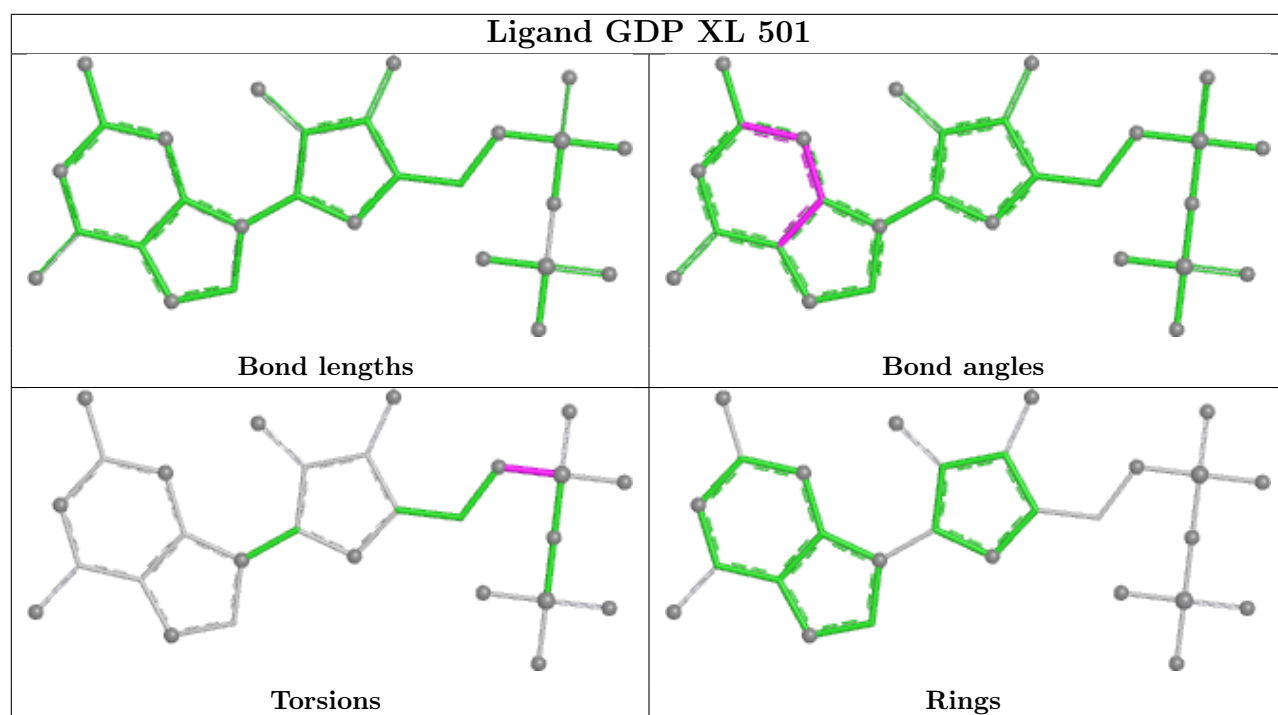


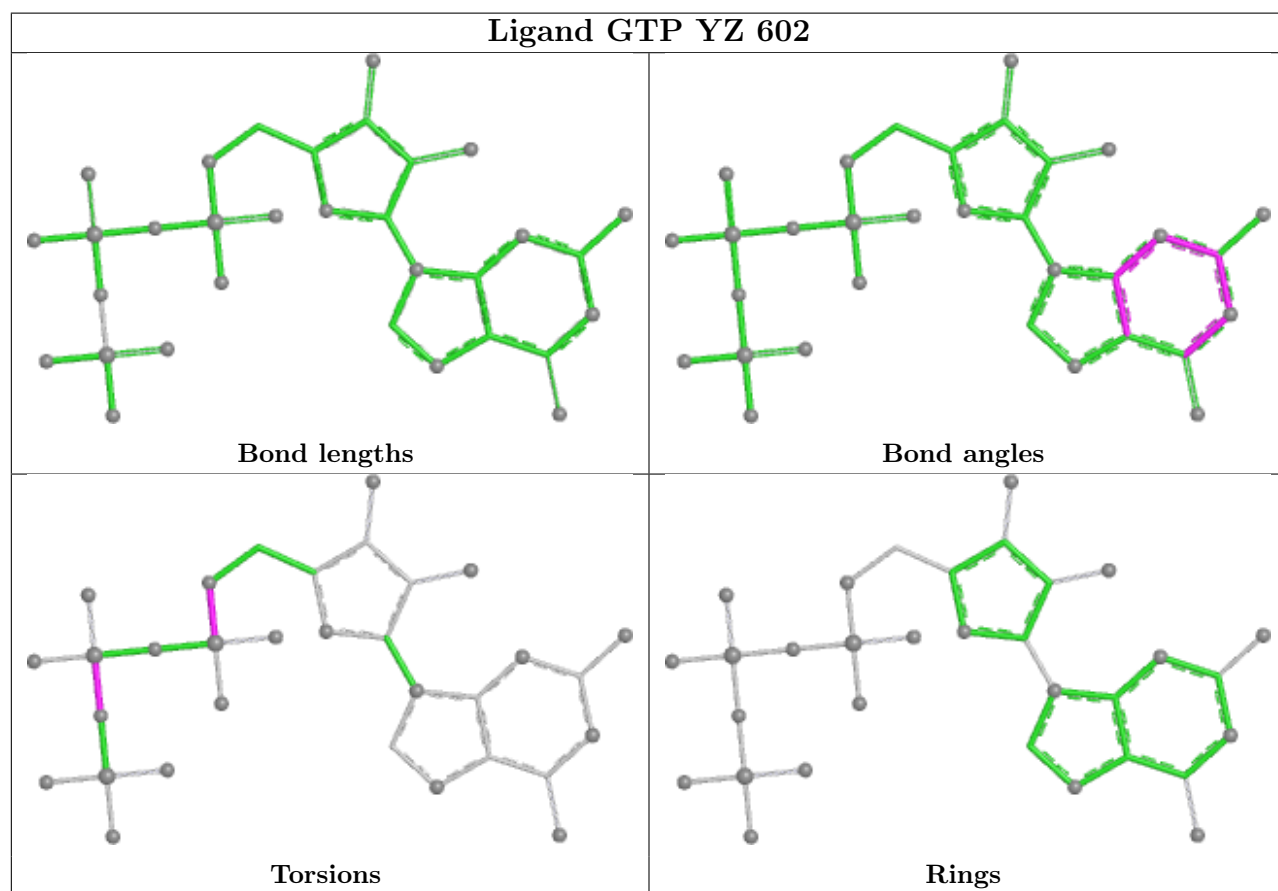
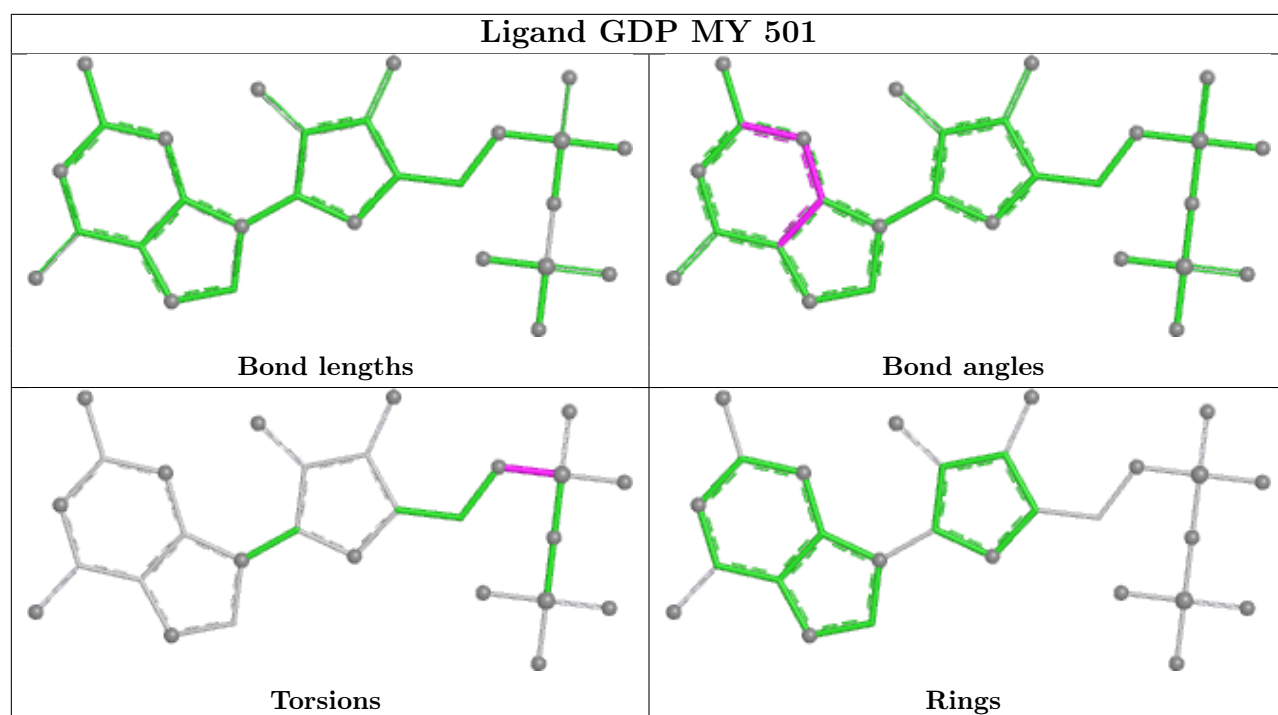


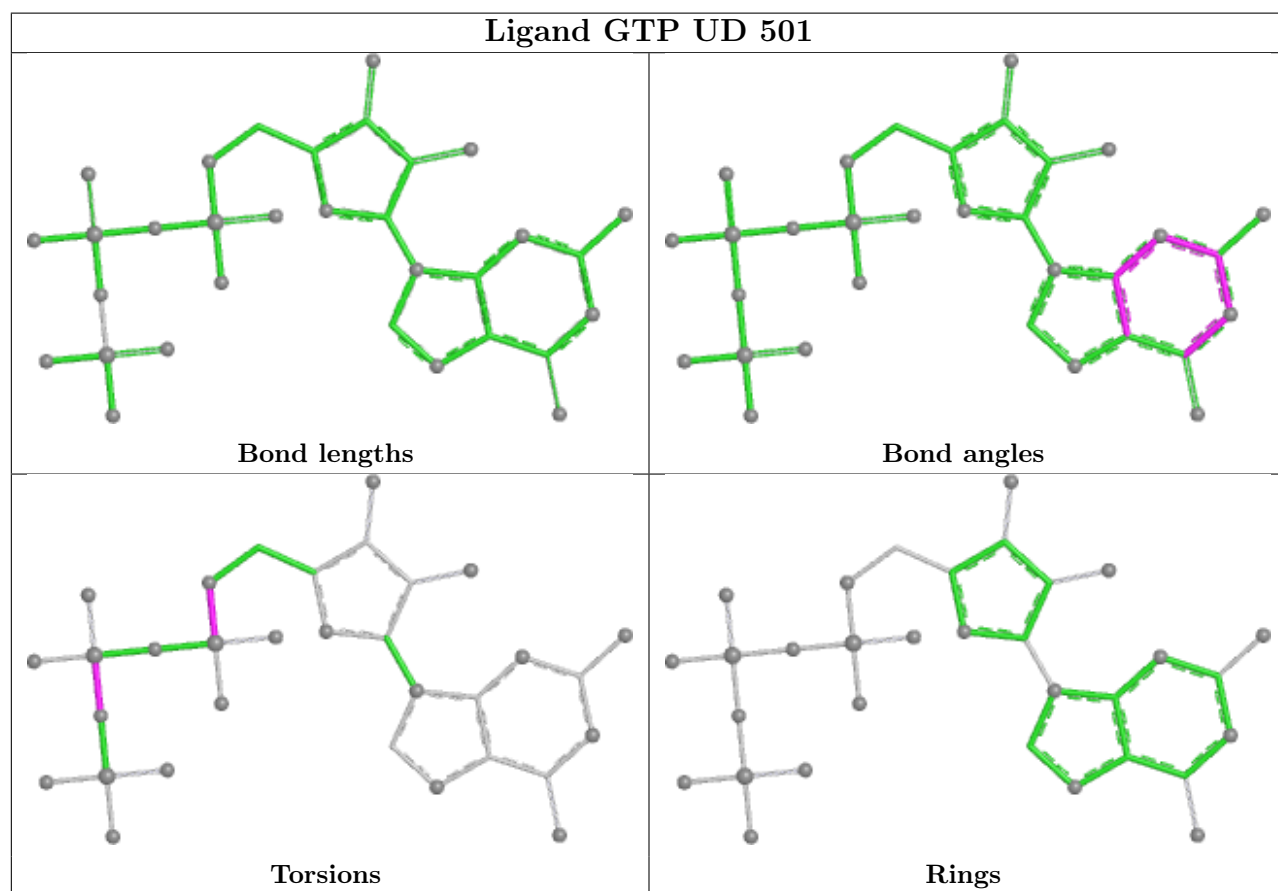
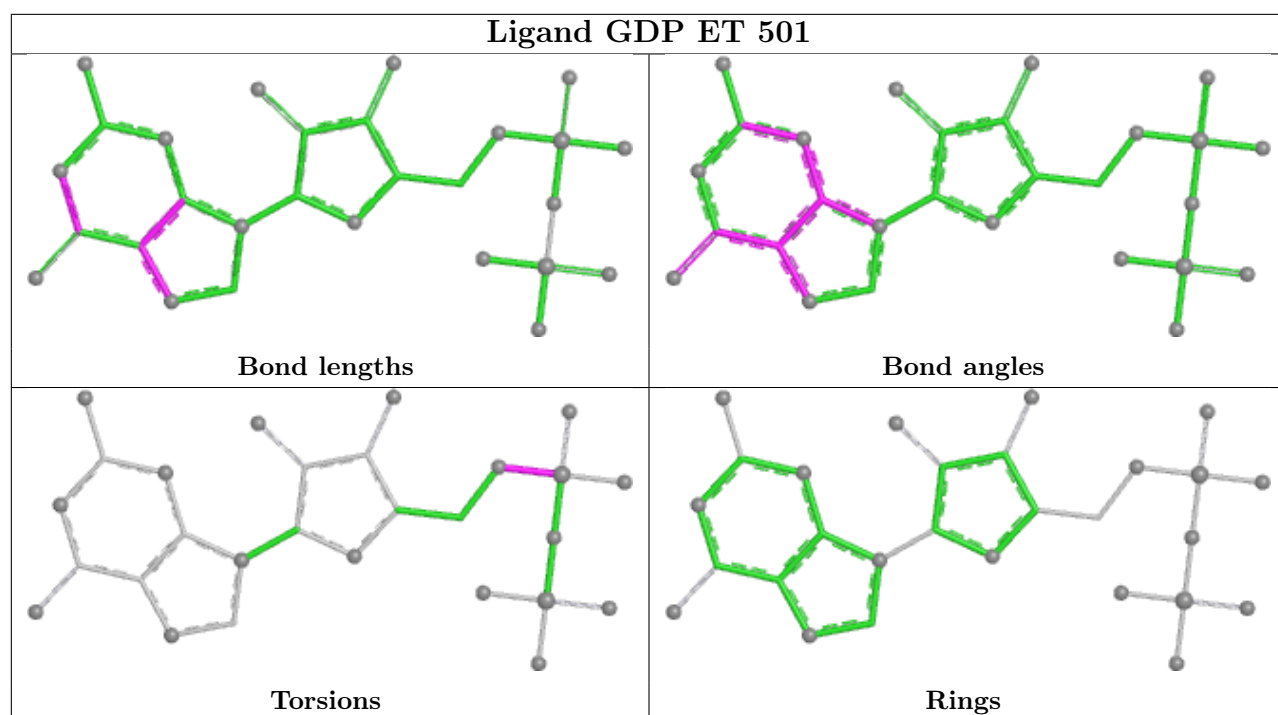




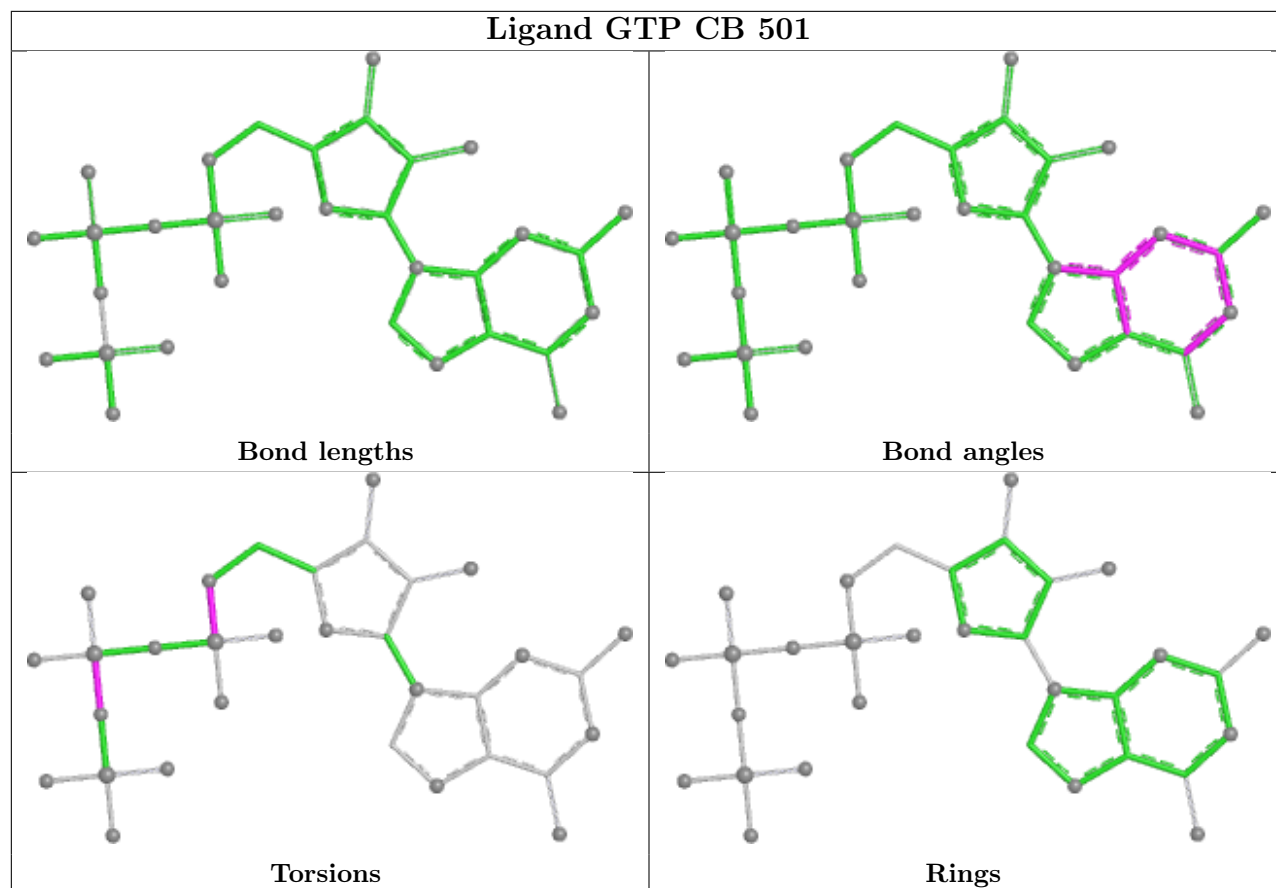




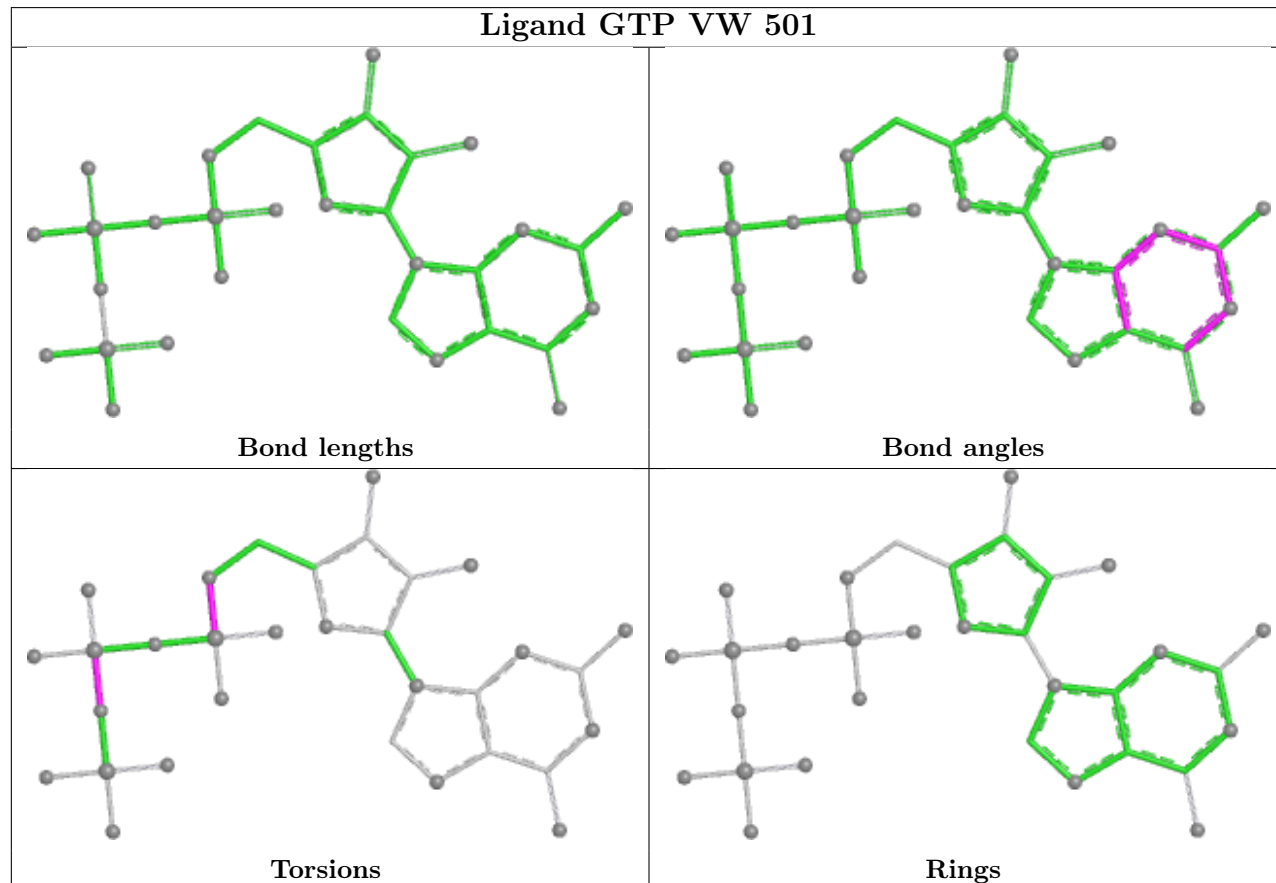


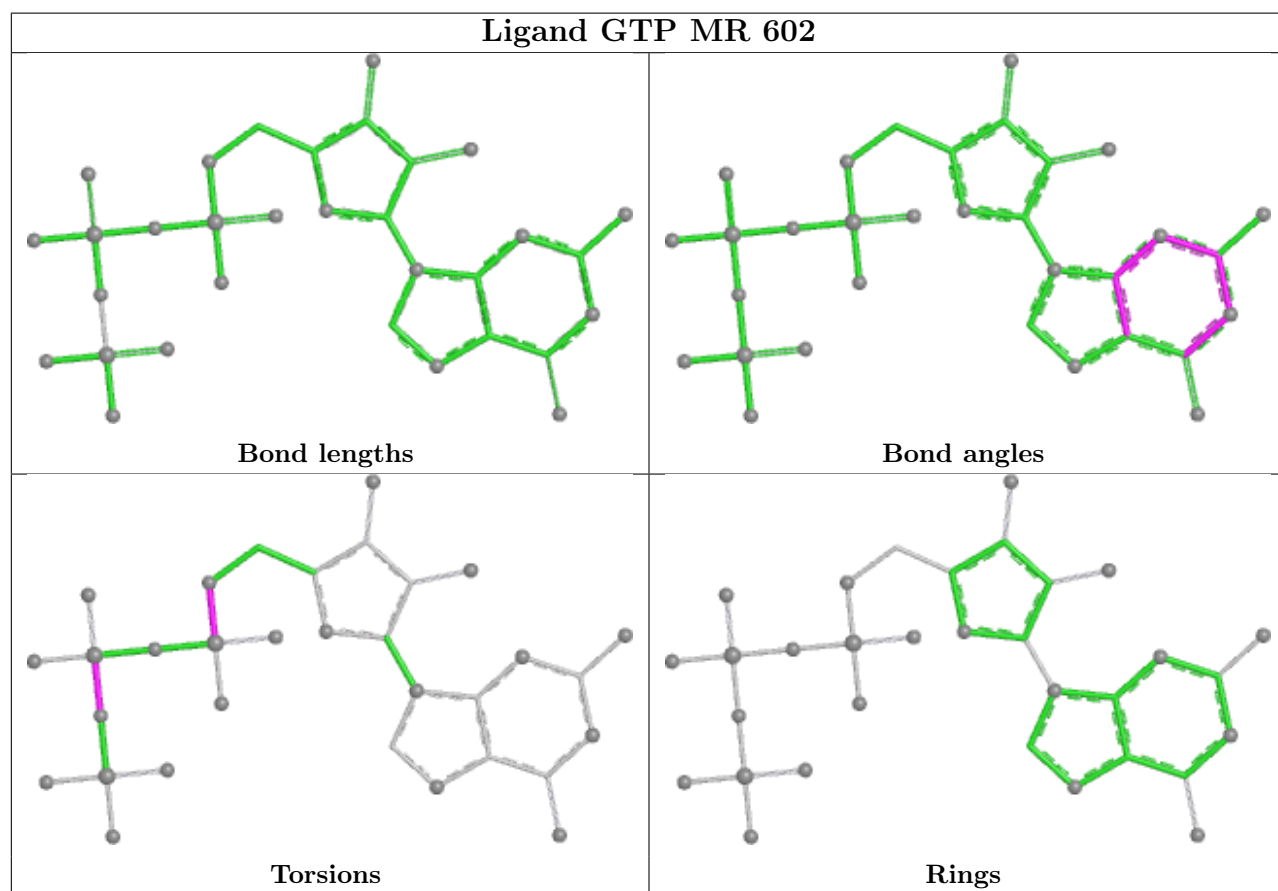
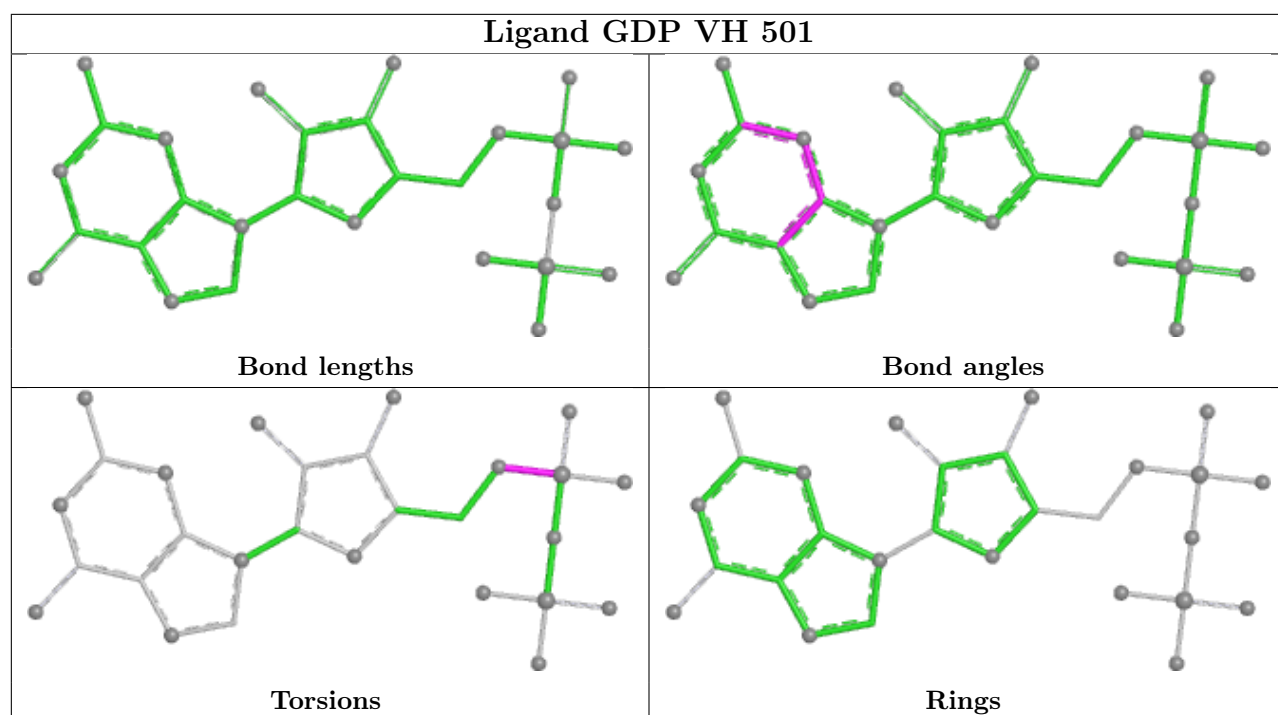


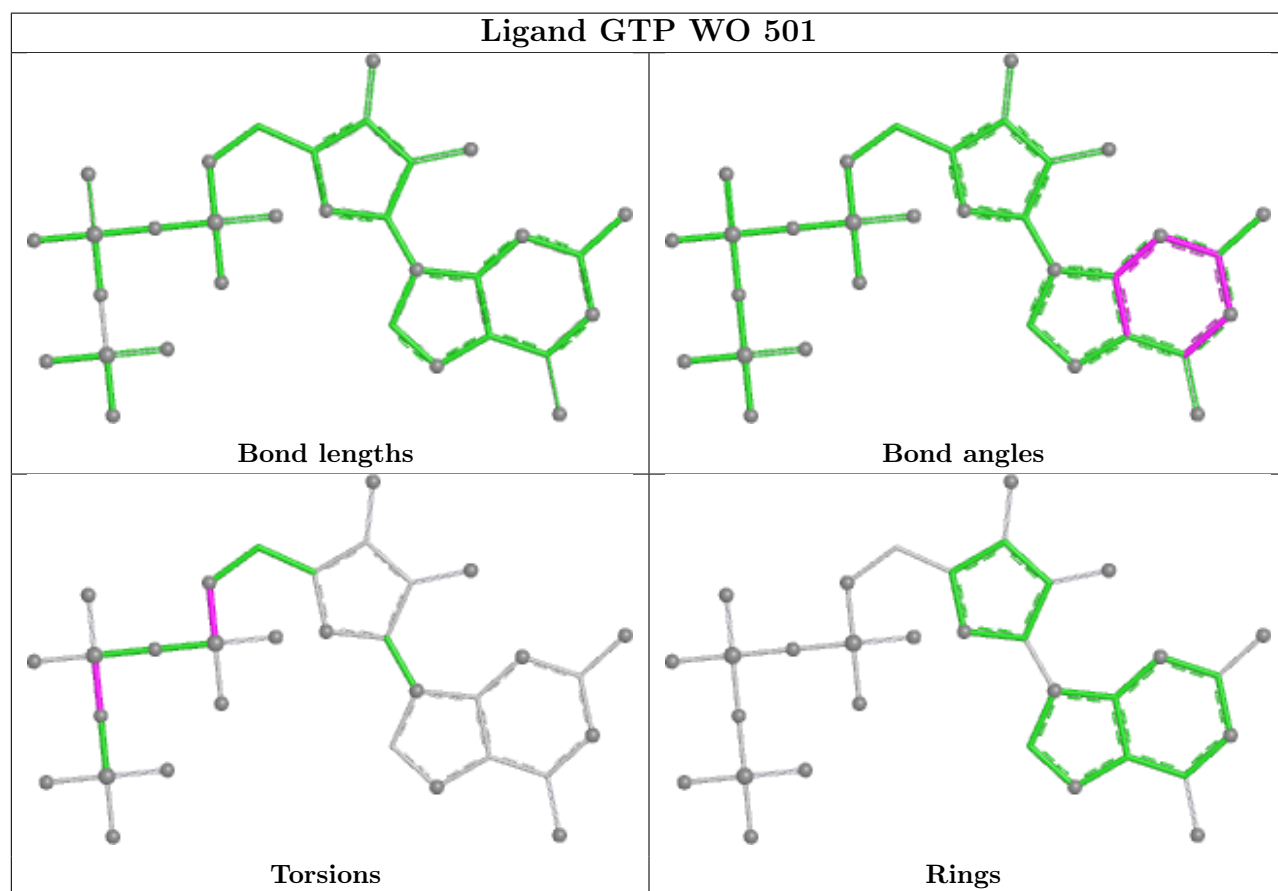
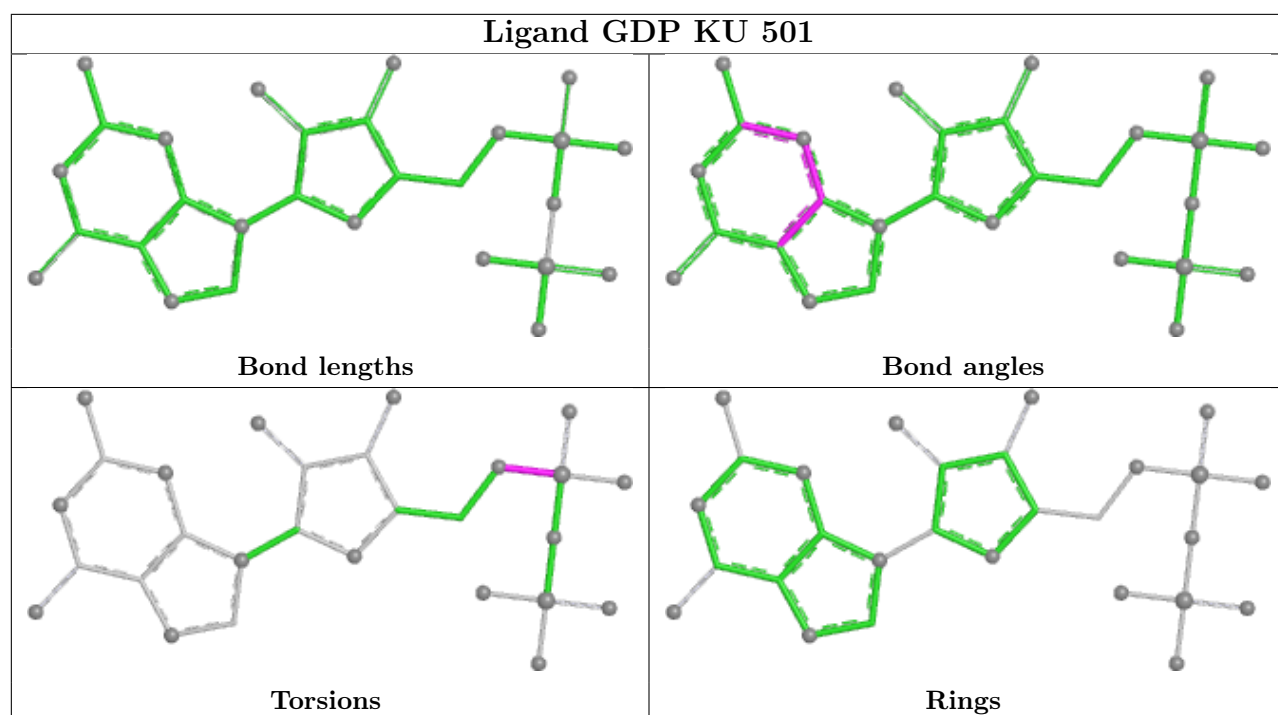
## Ligand GTP CB 501

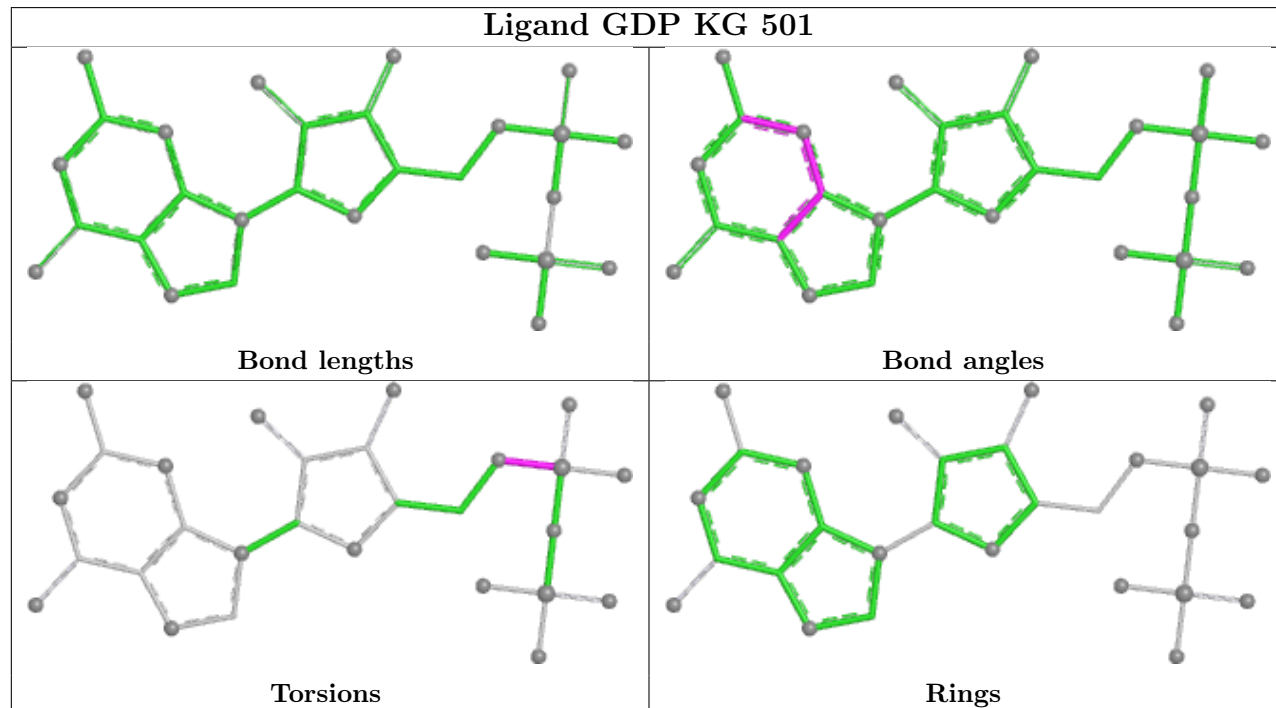
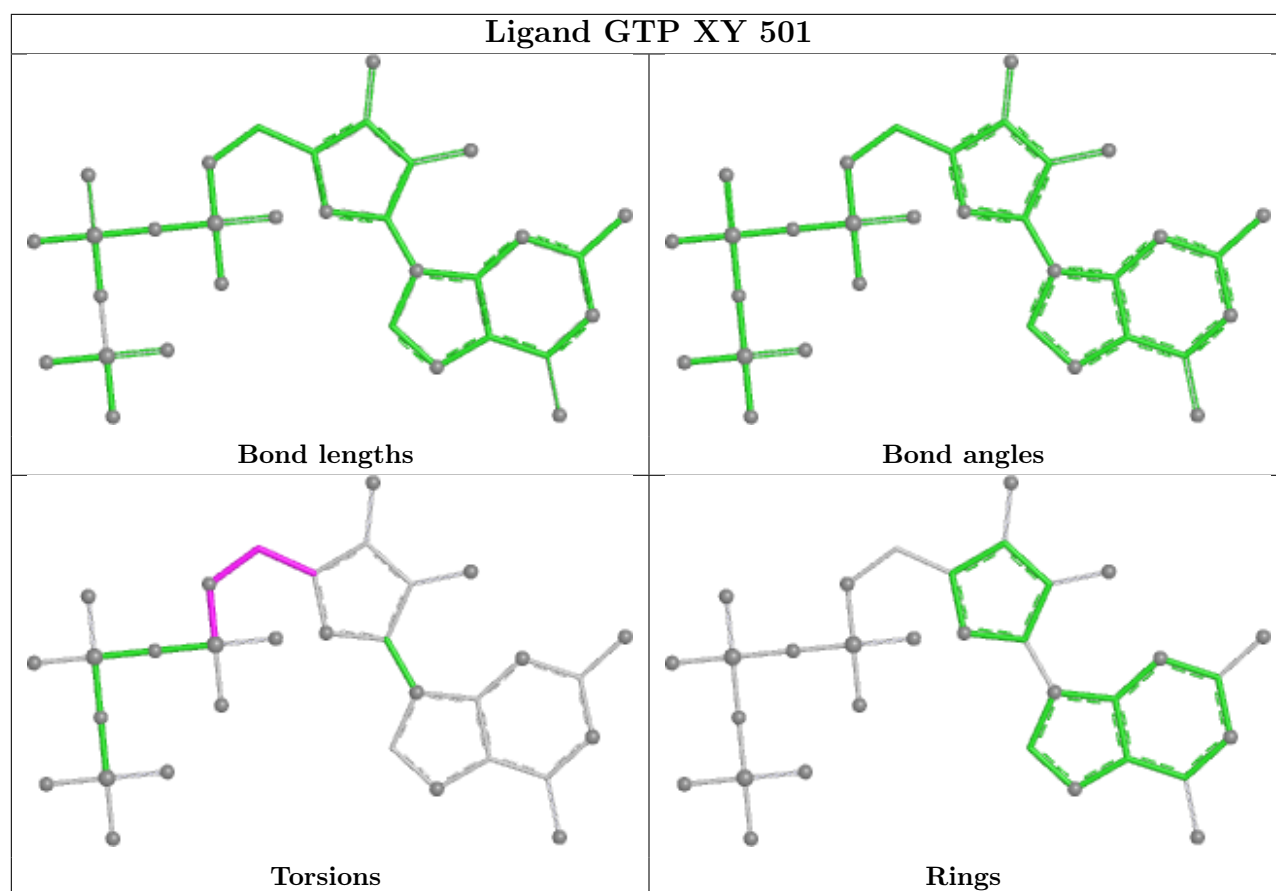


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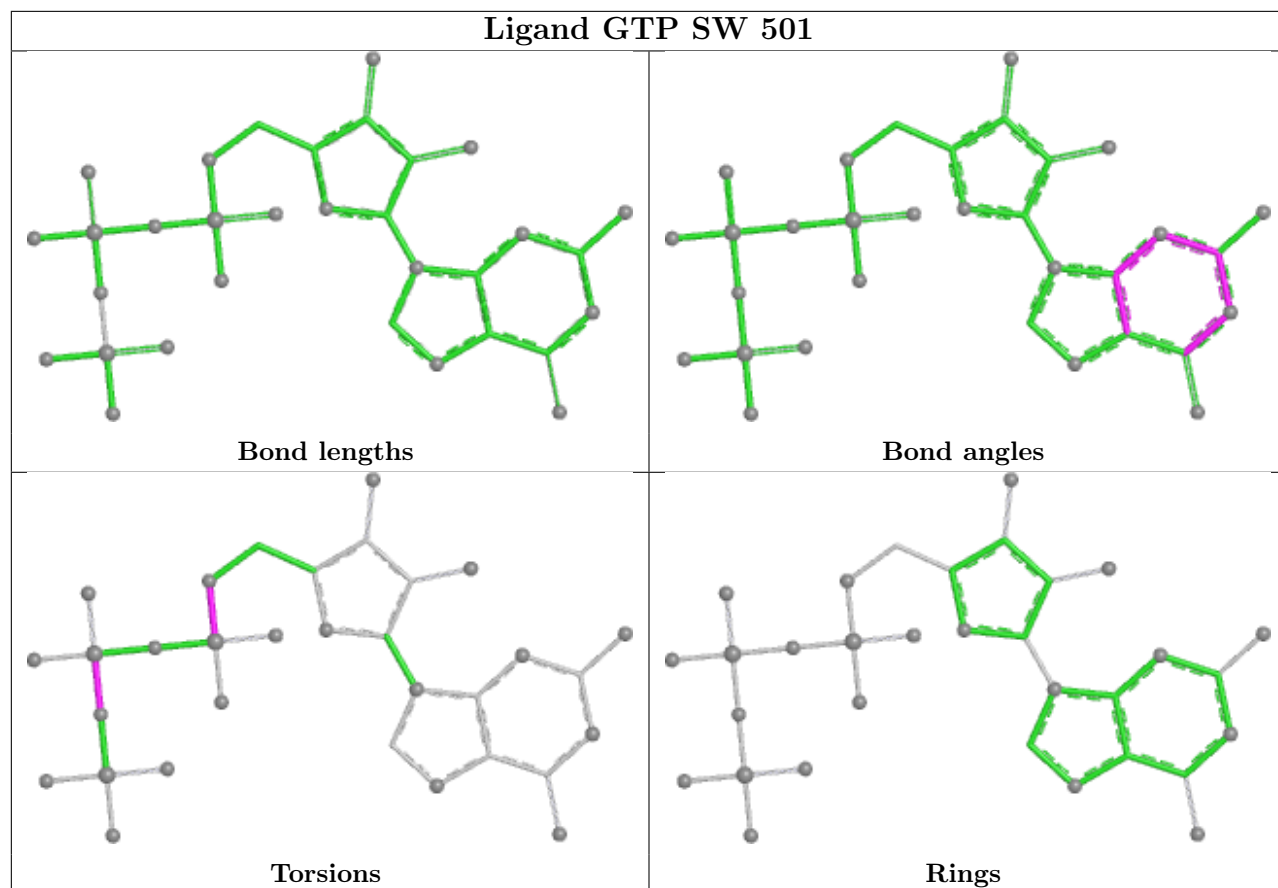




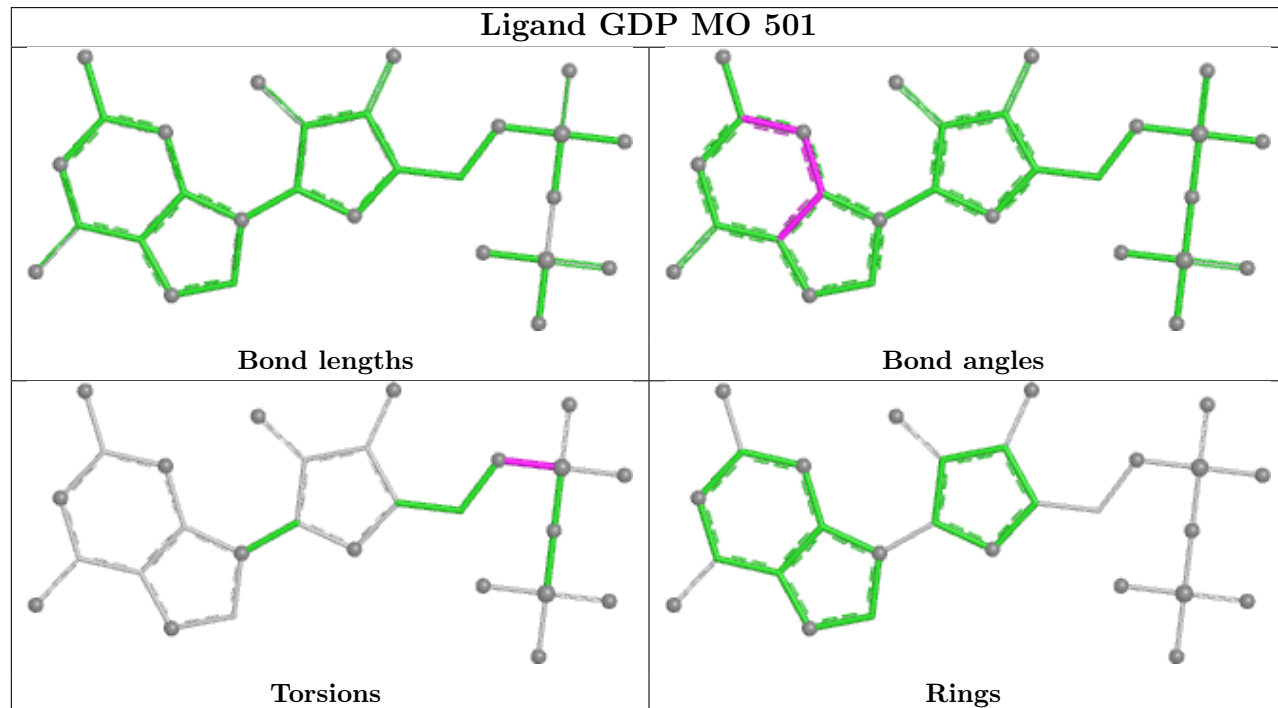




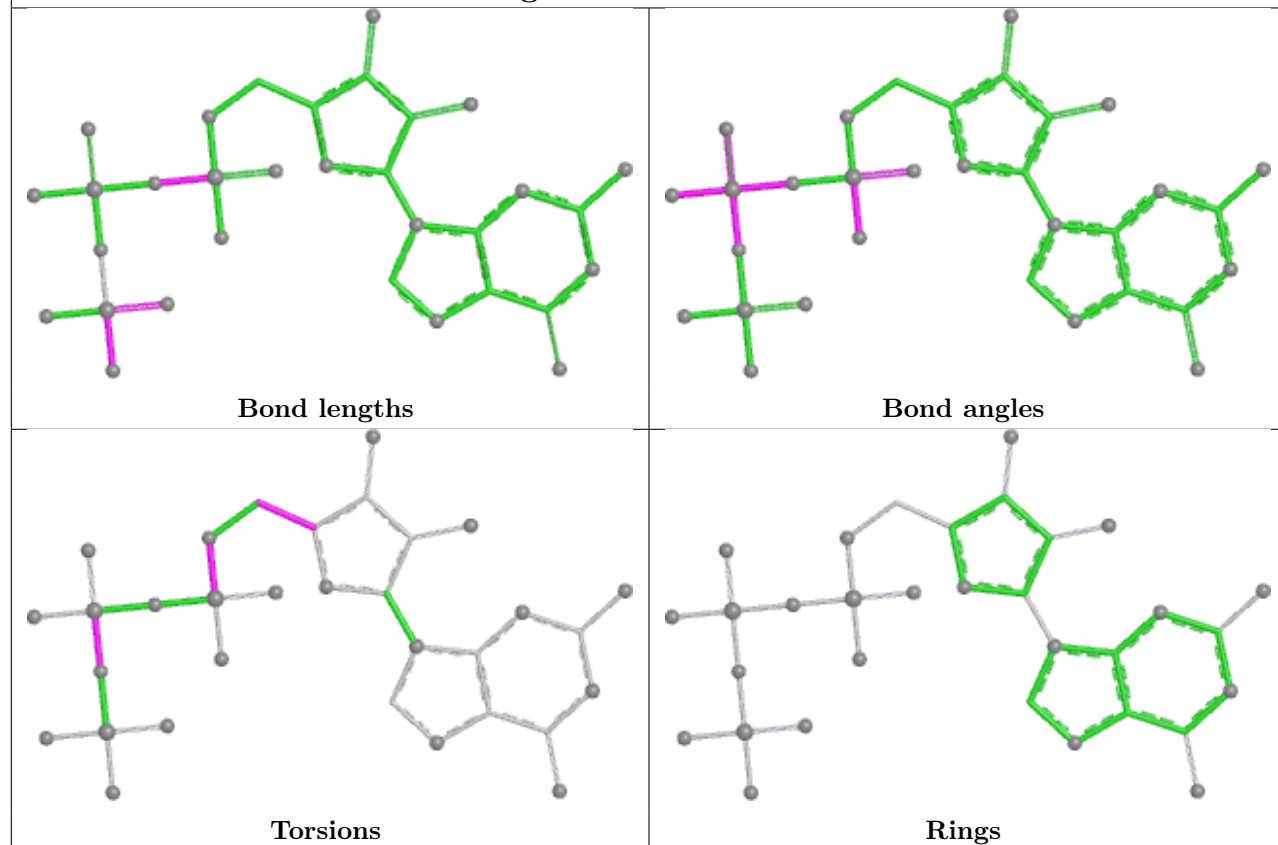
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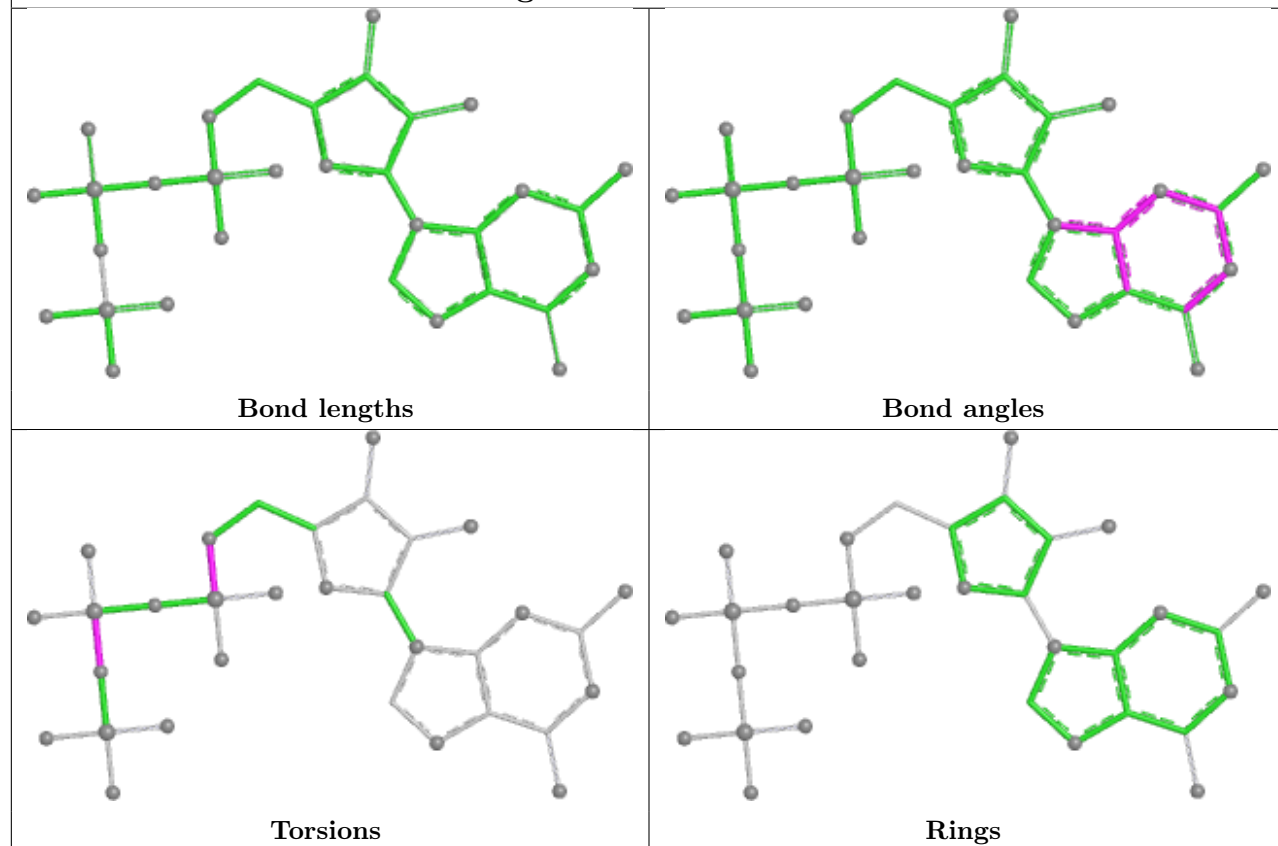
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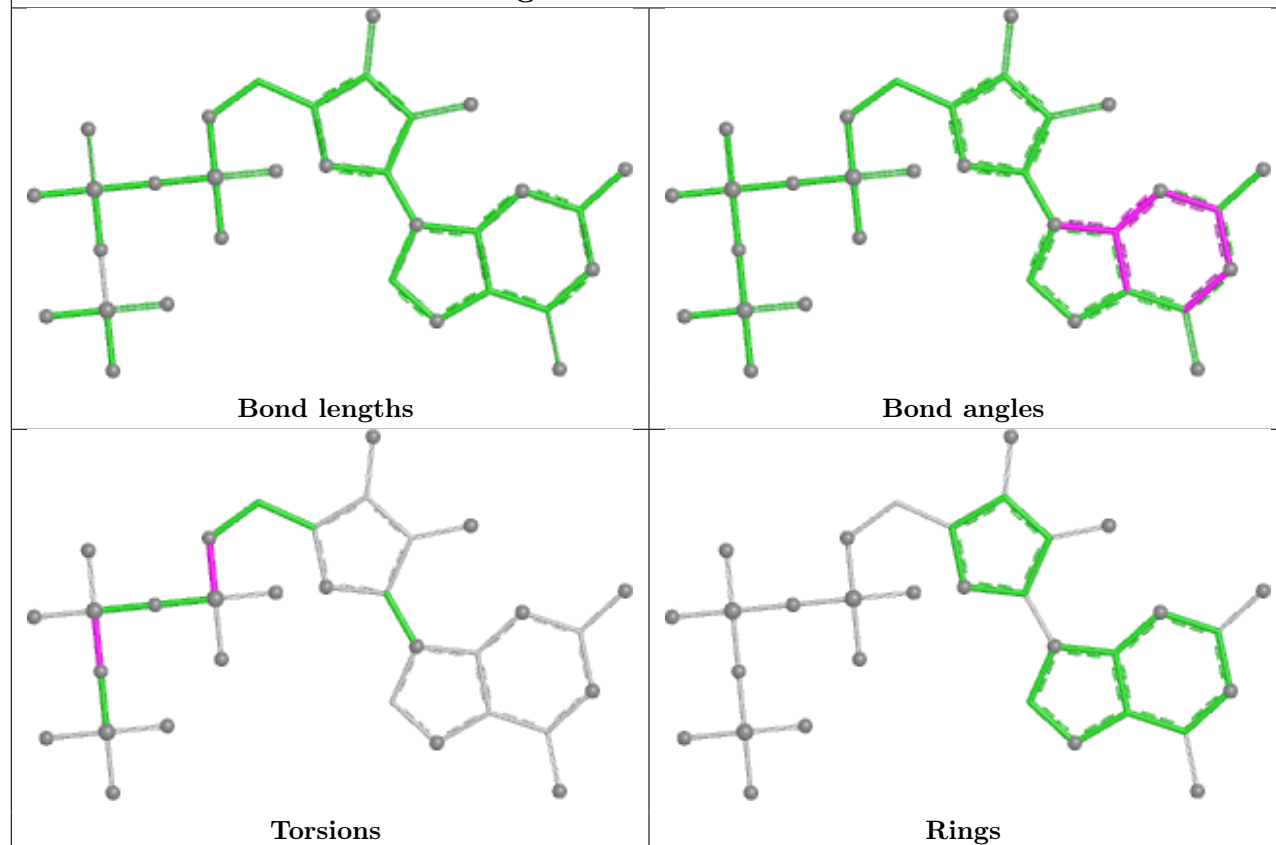
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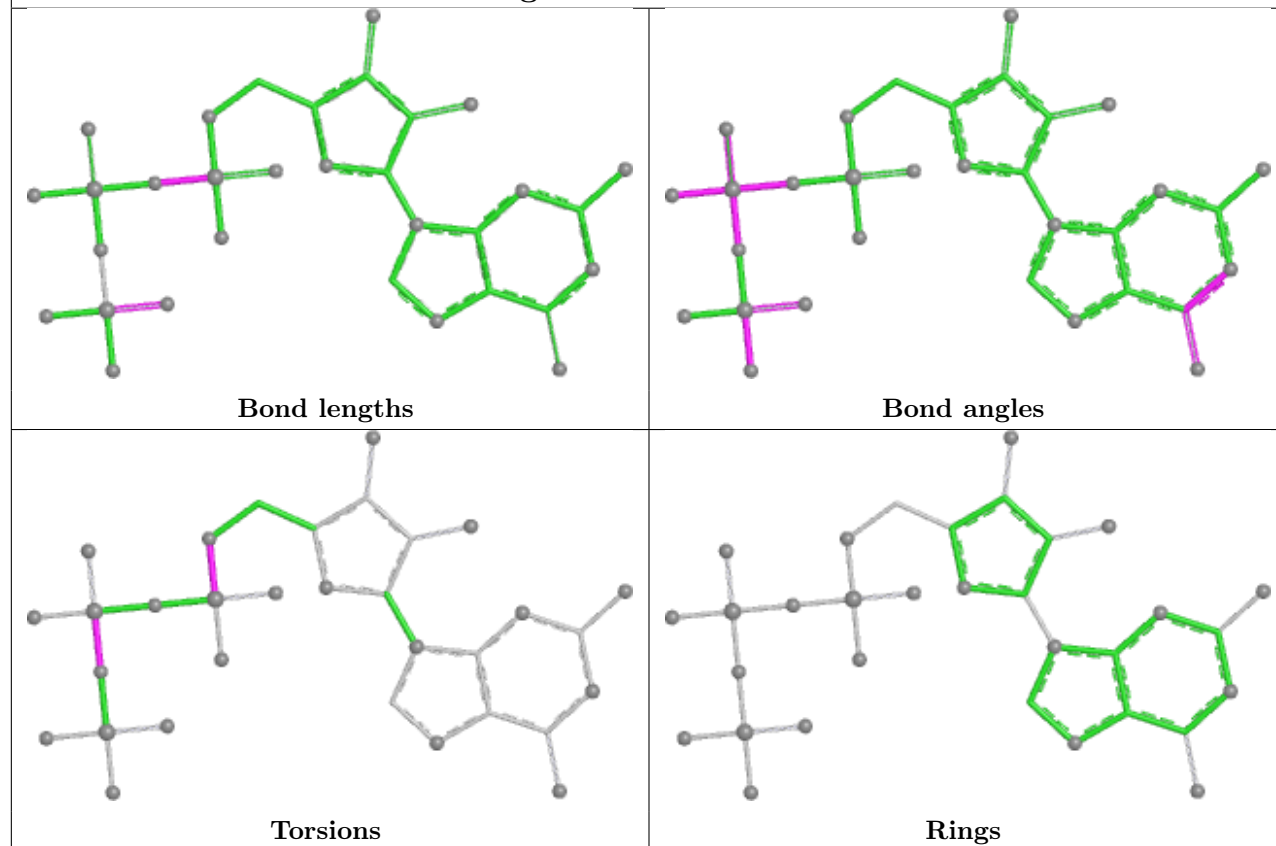
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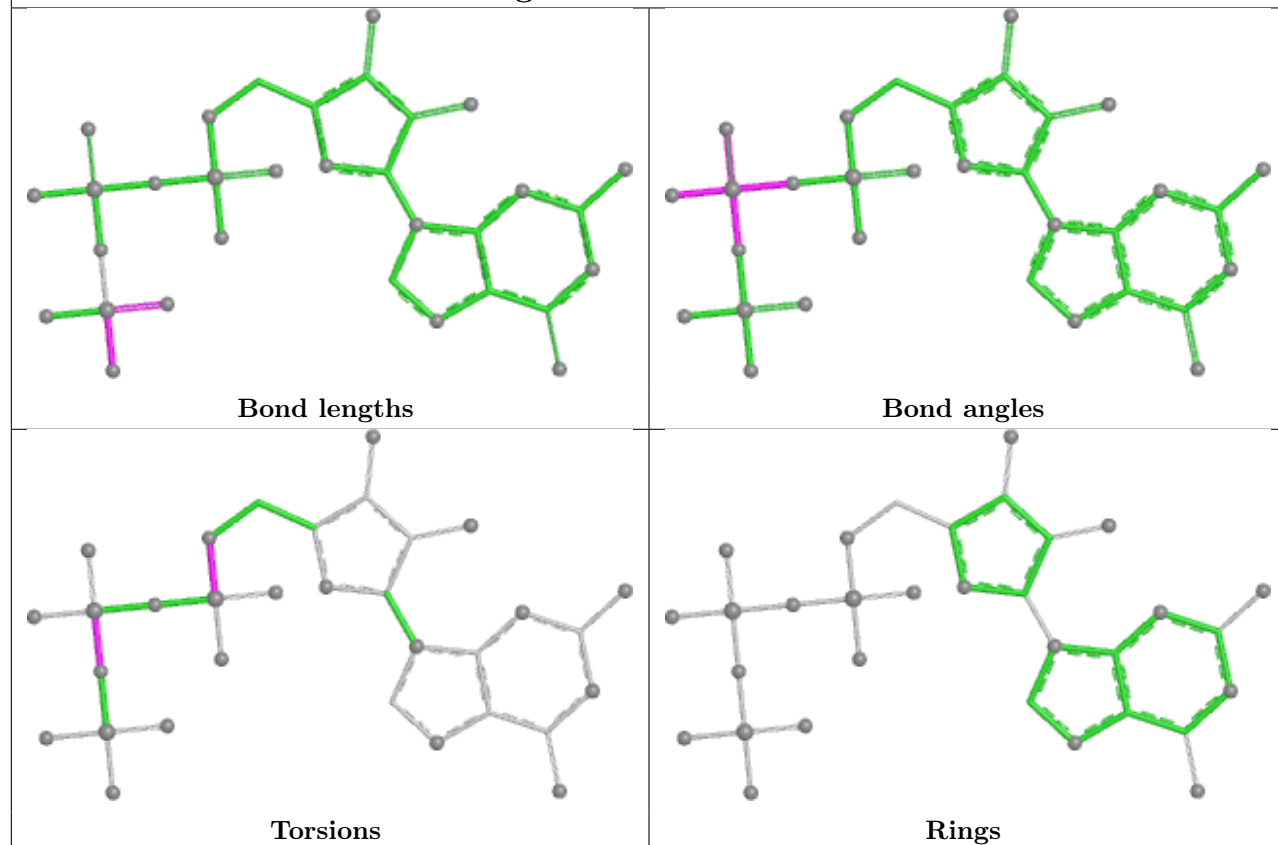
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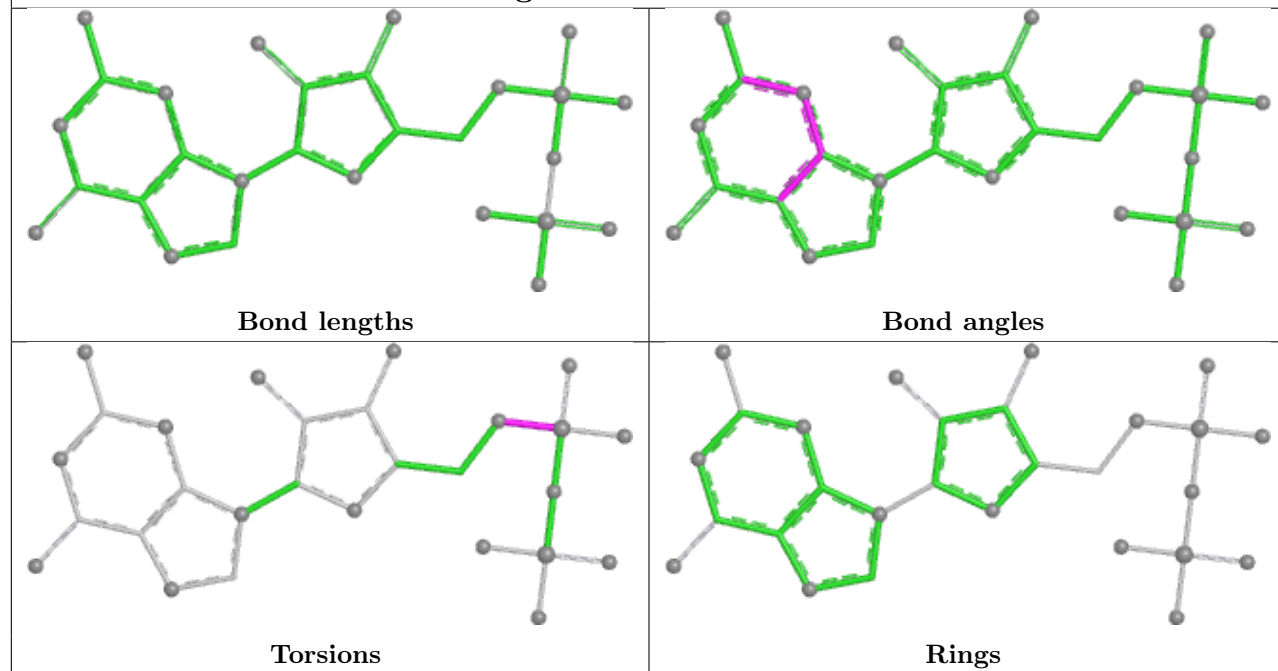
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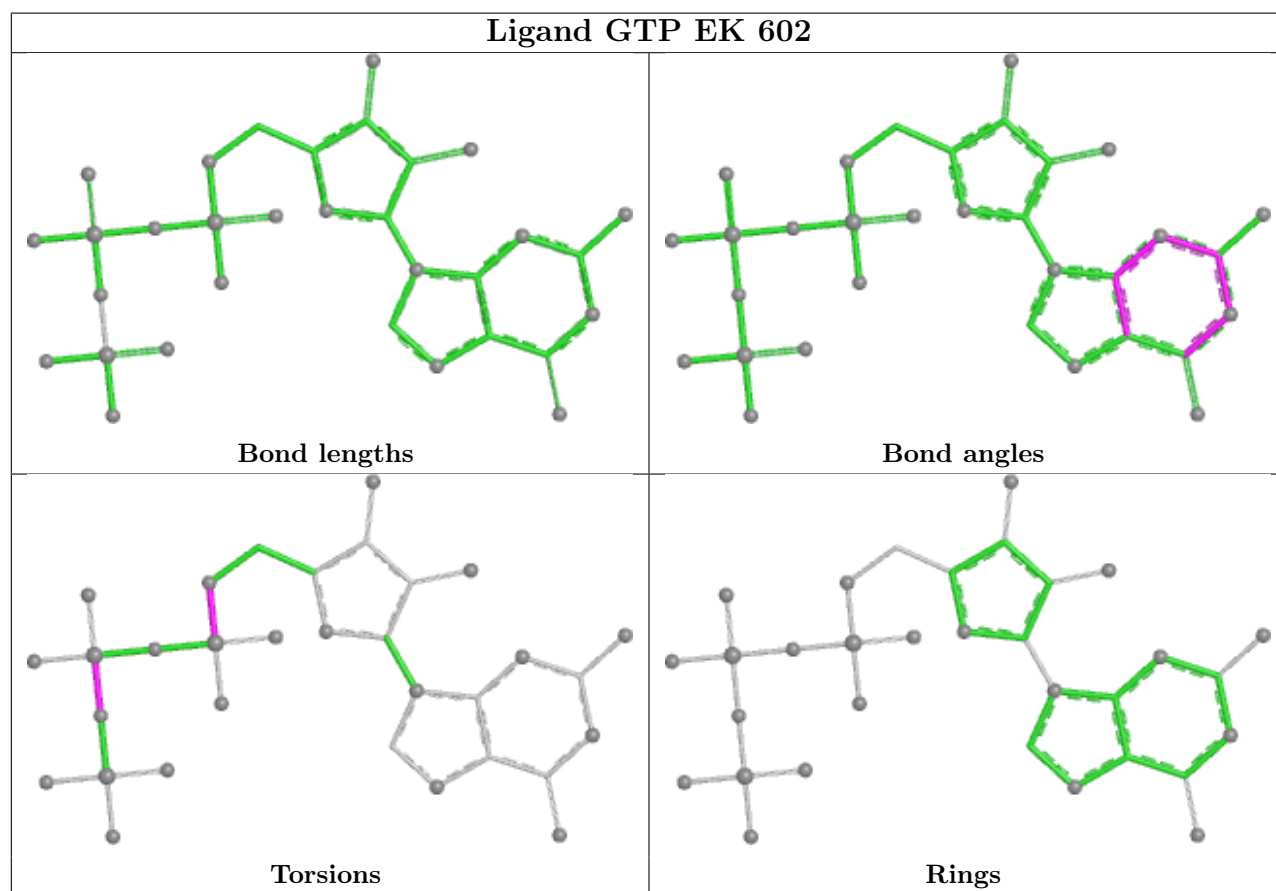
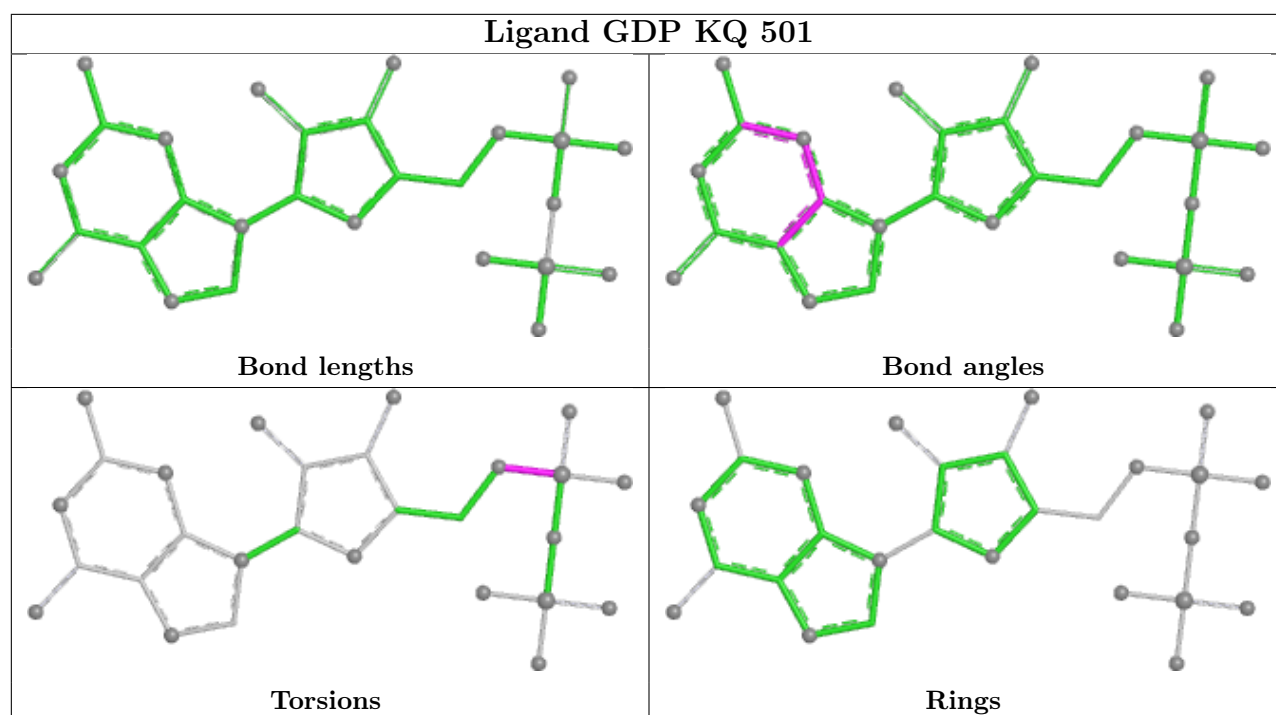


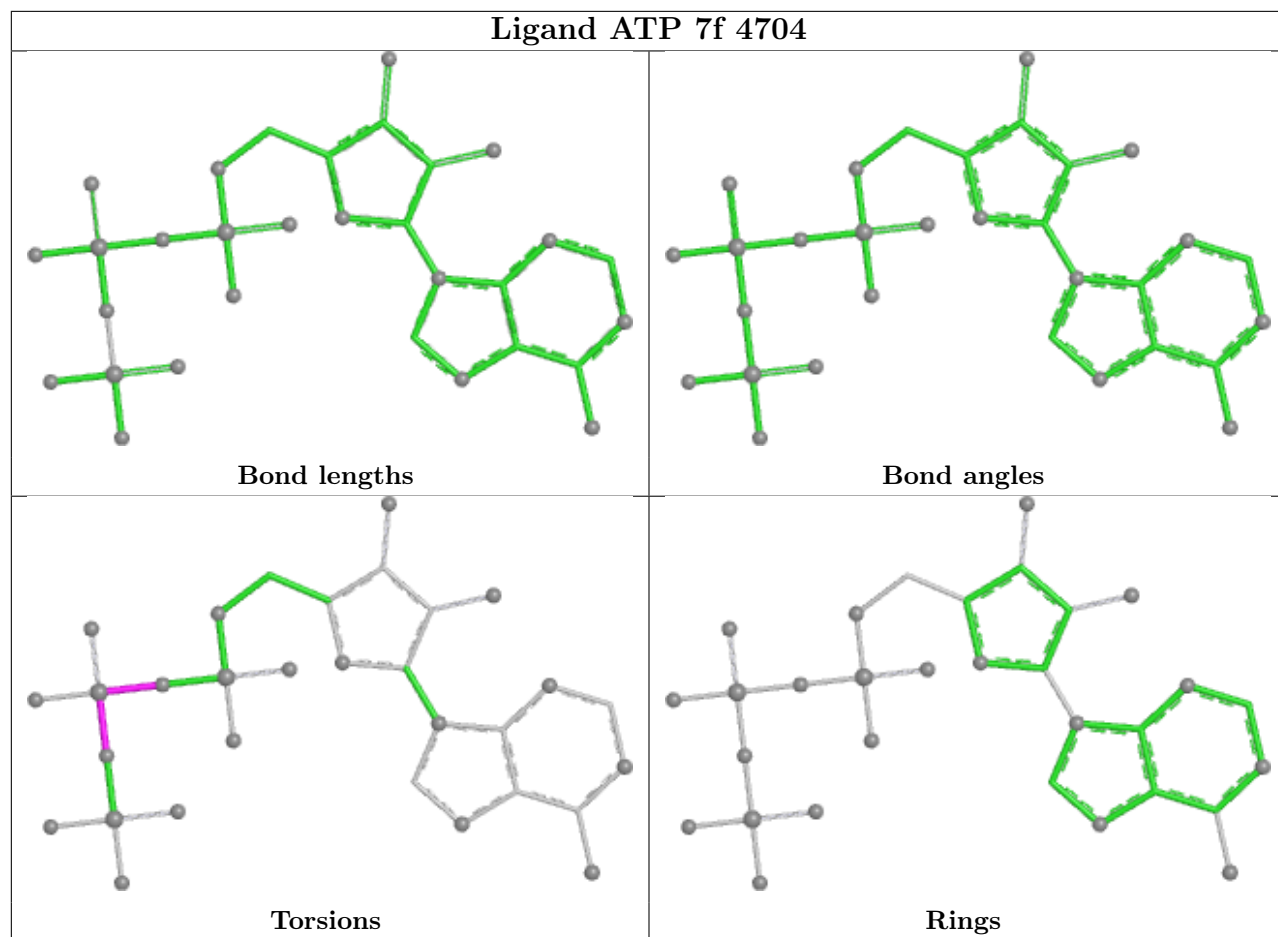
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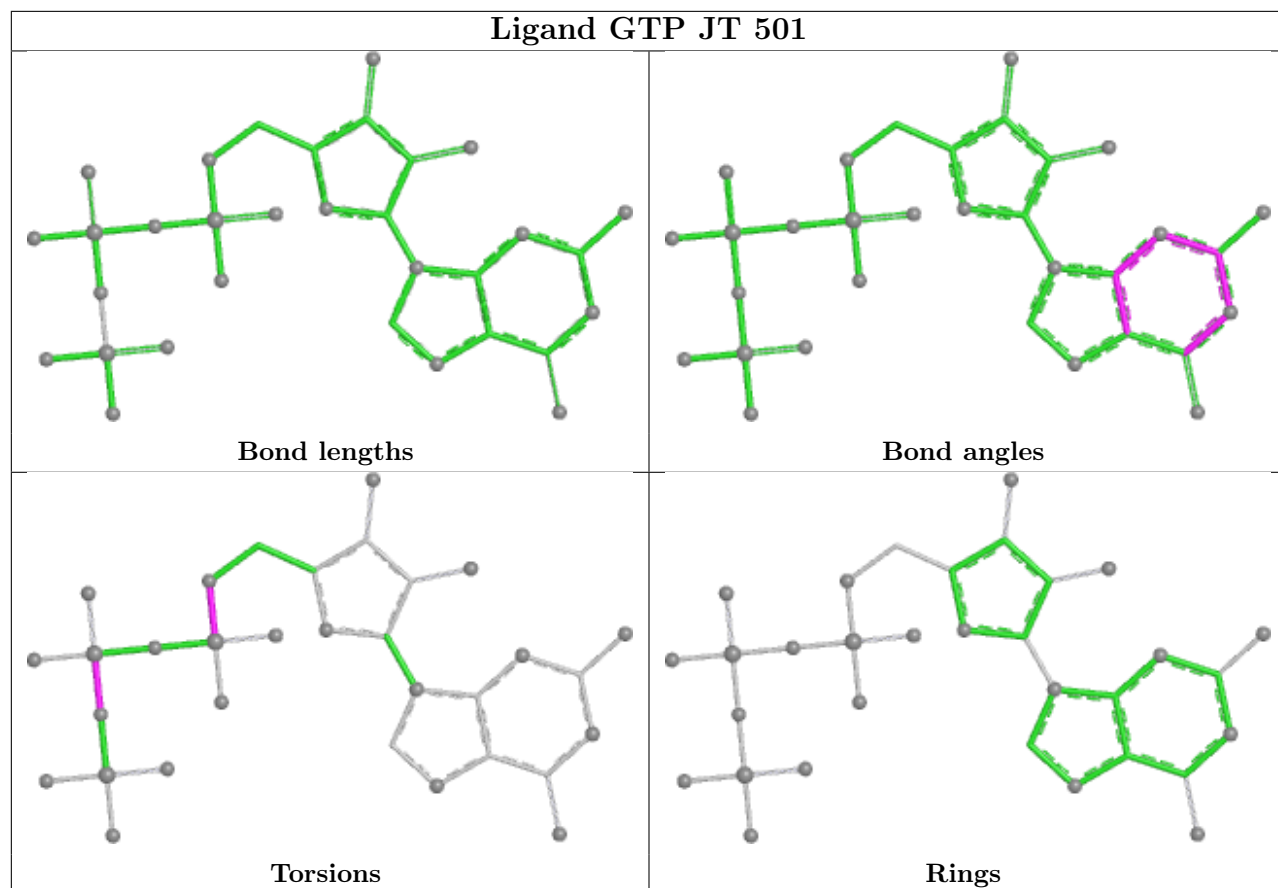
## Ligand GDP OO 501



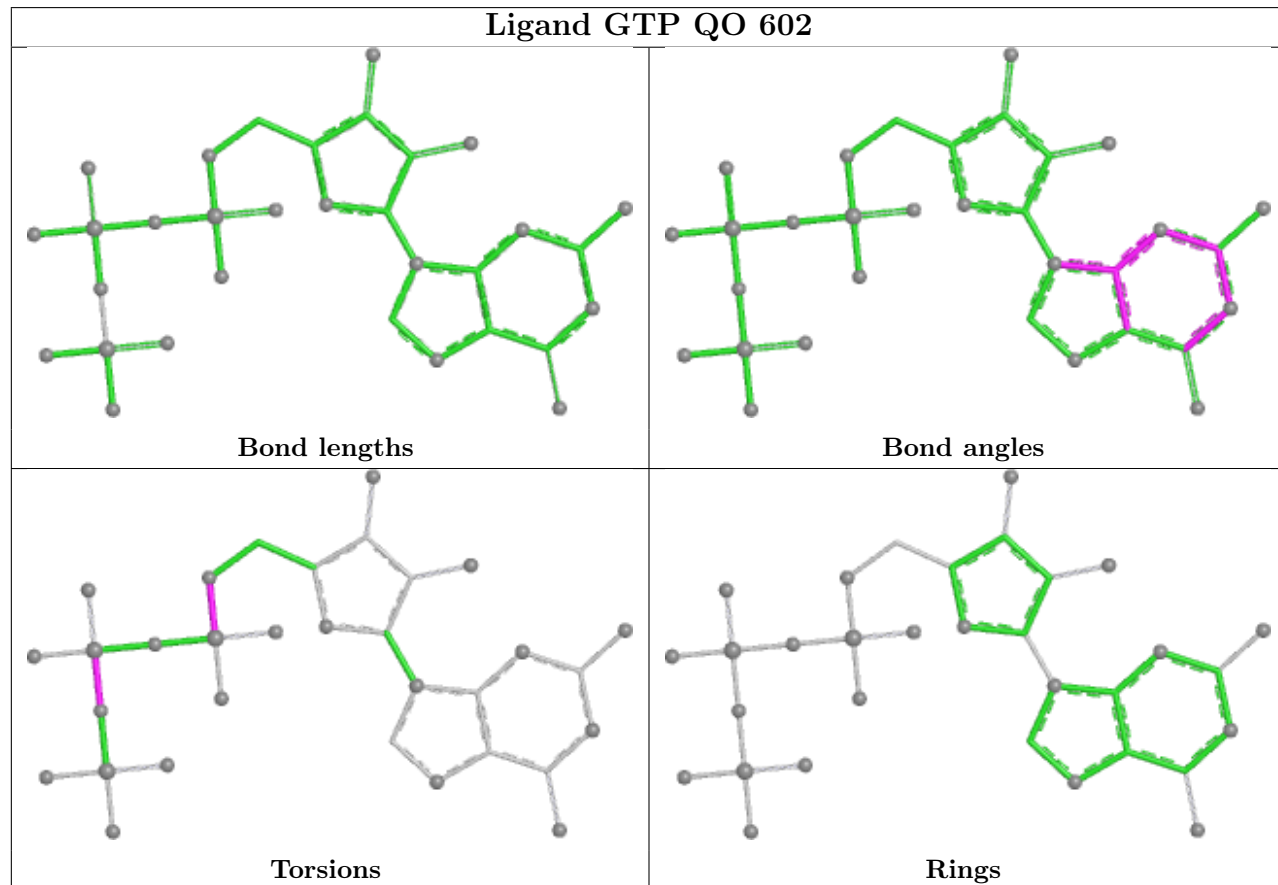


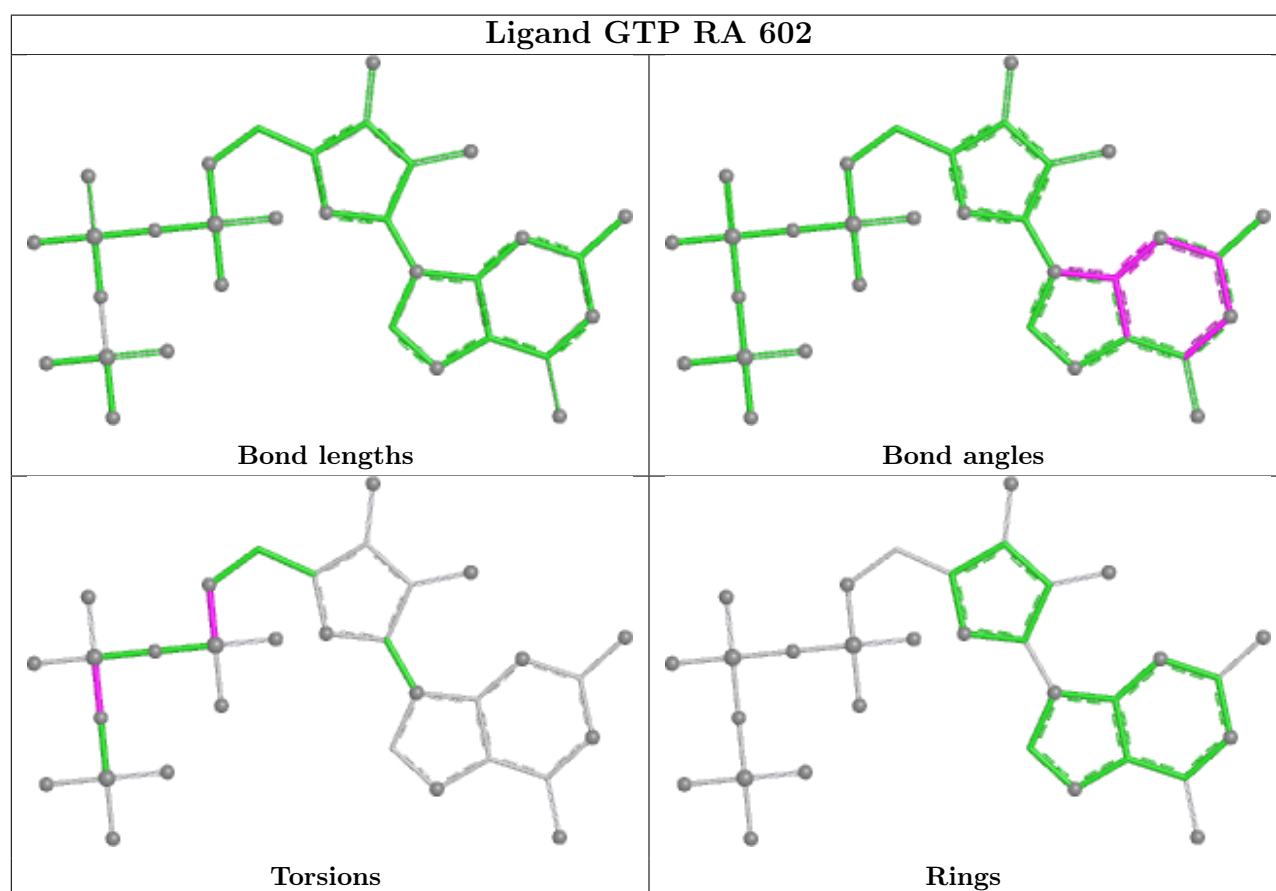
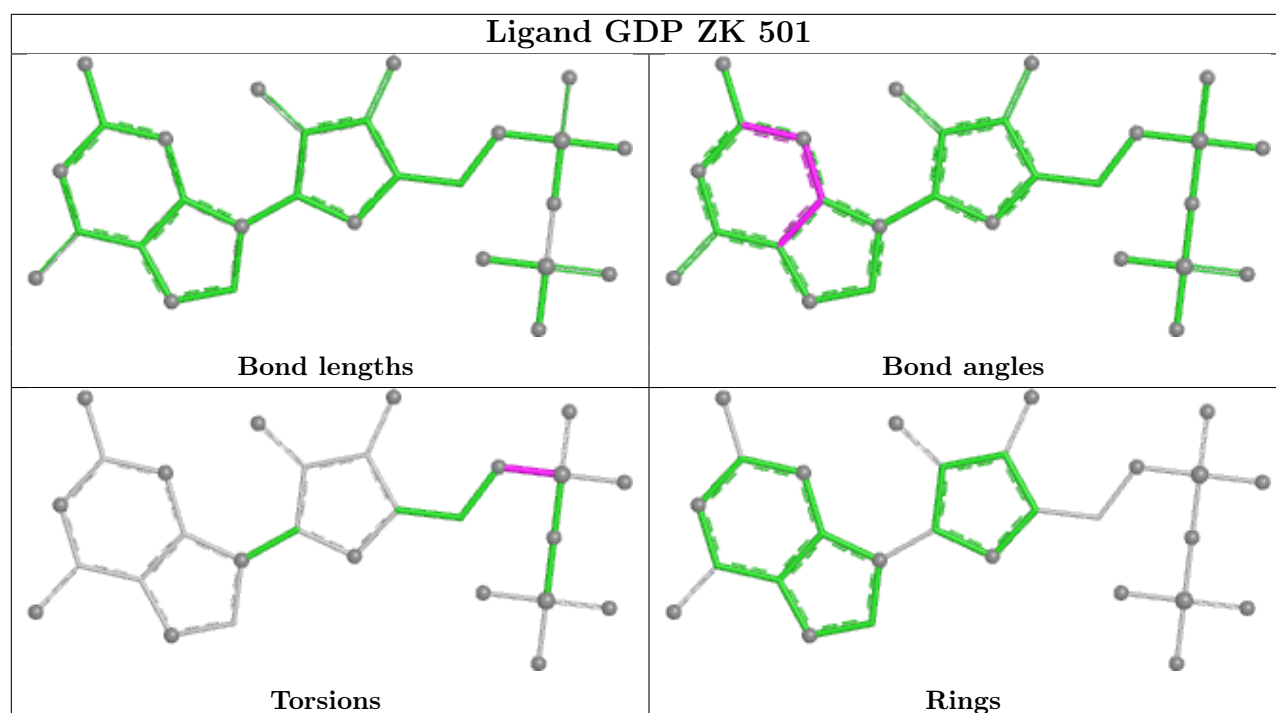


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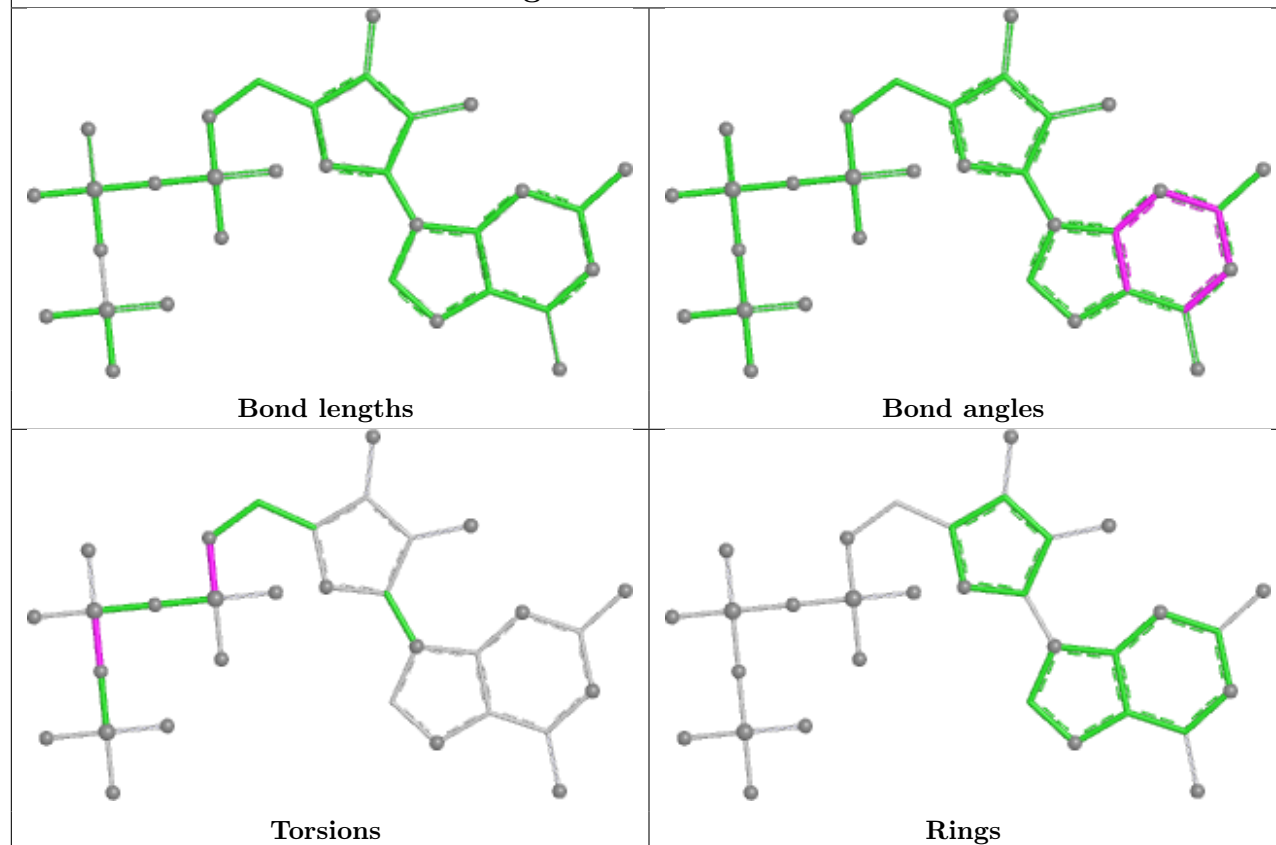
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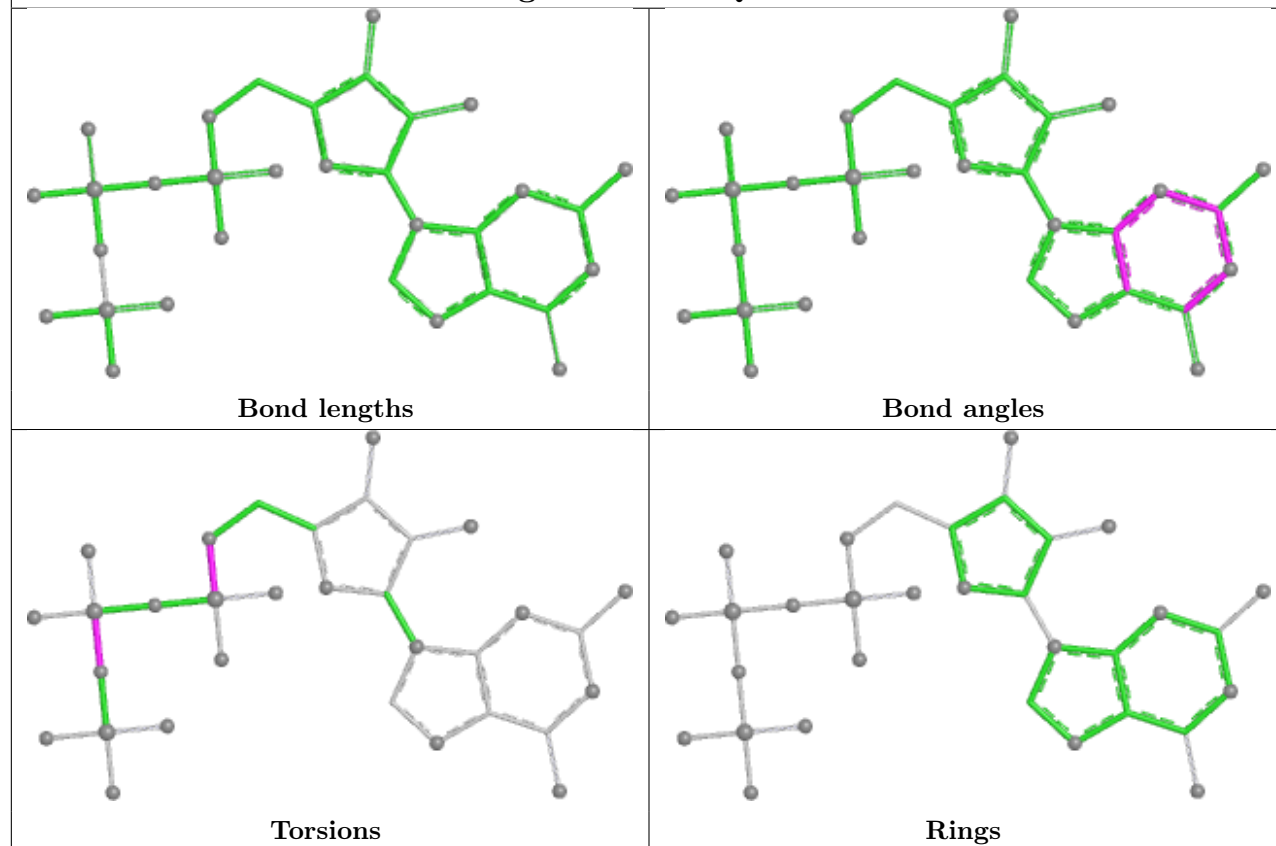




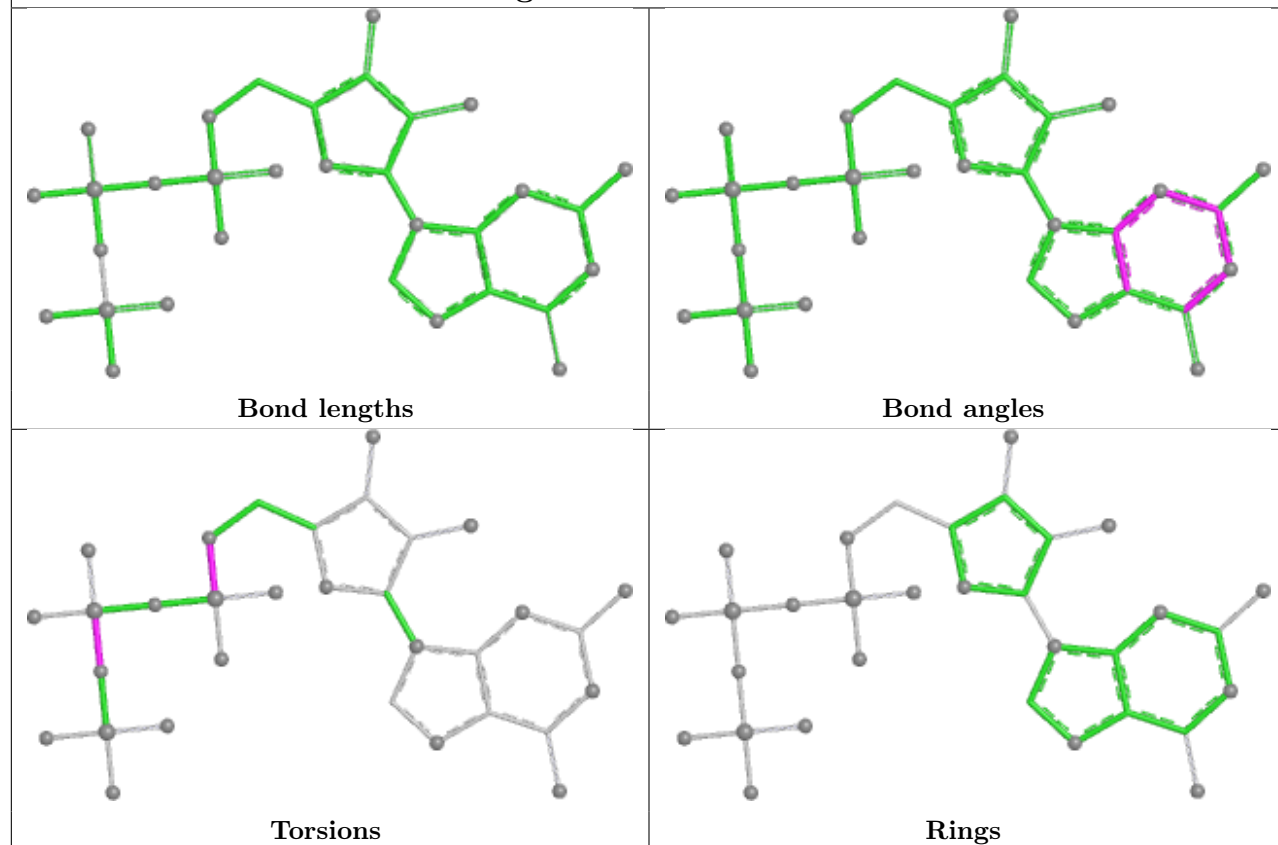
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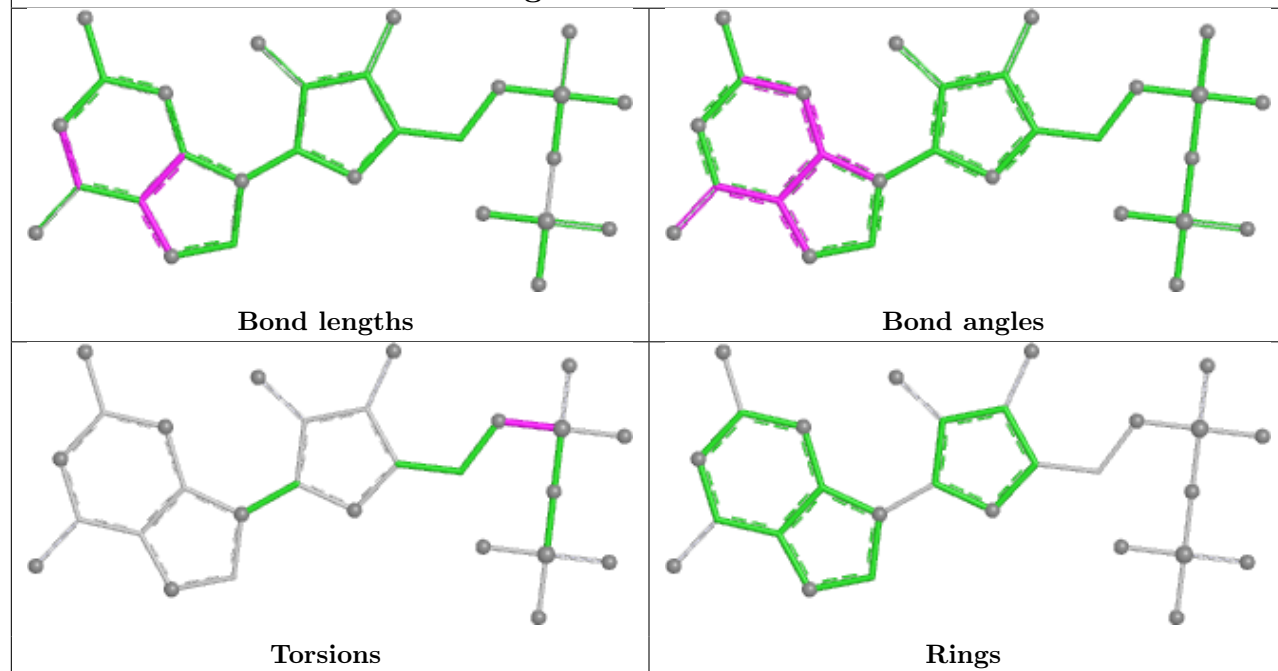
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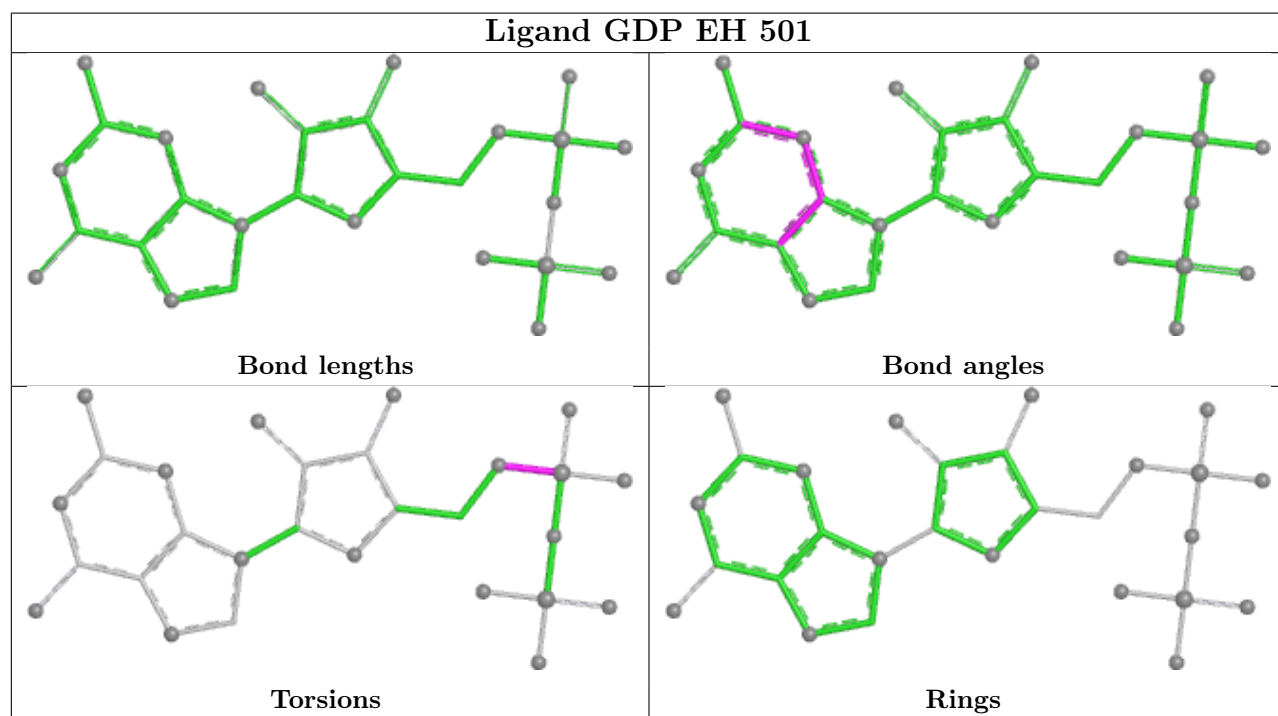
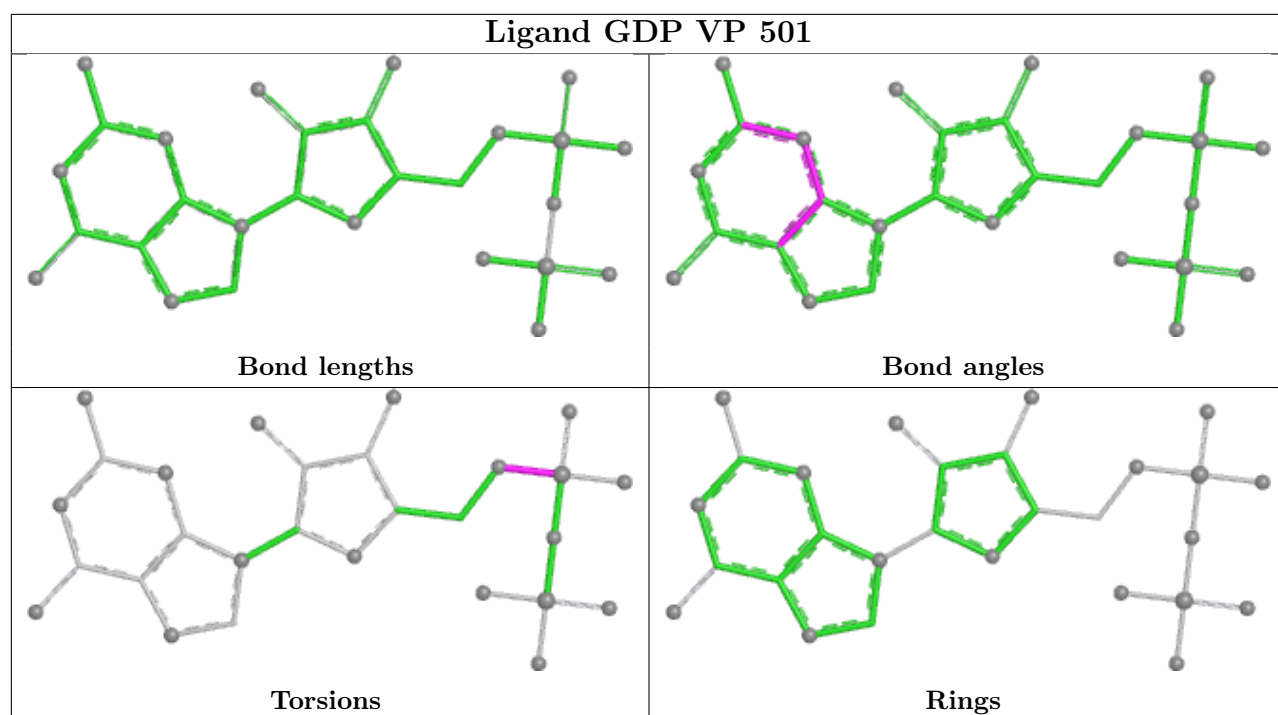


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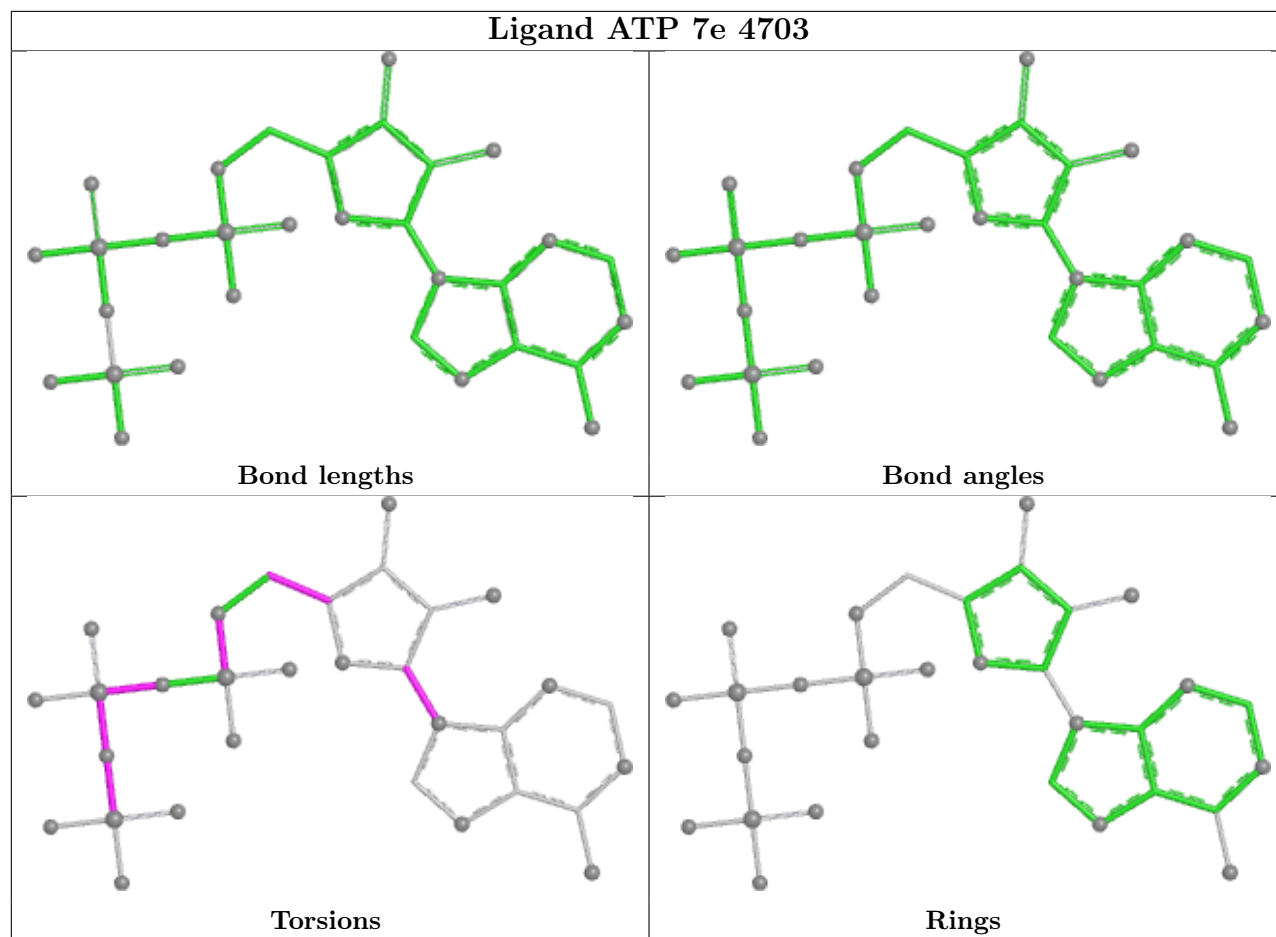


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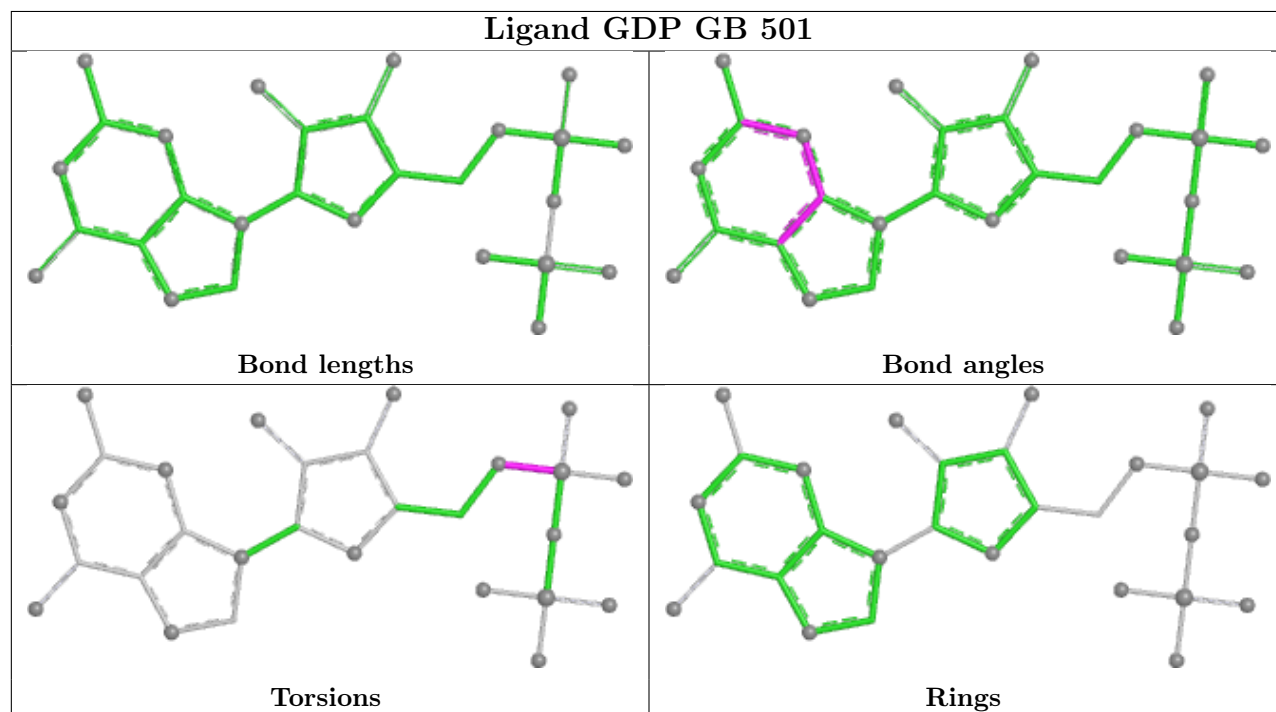


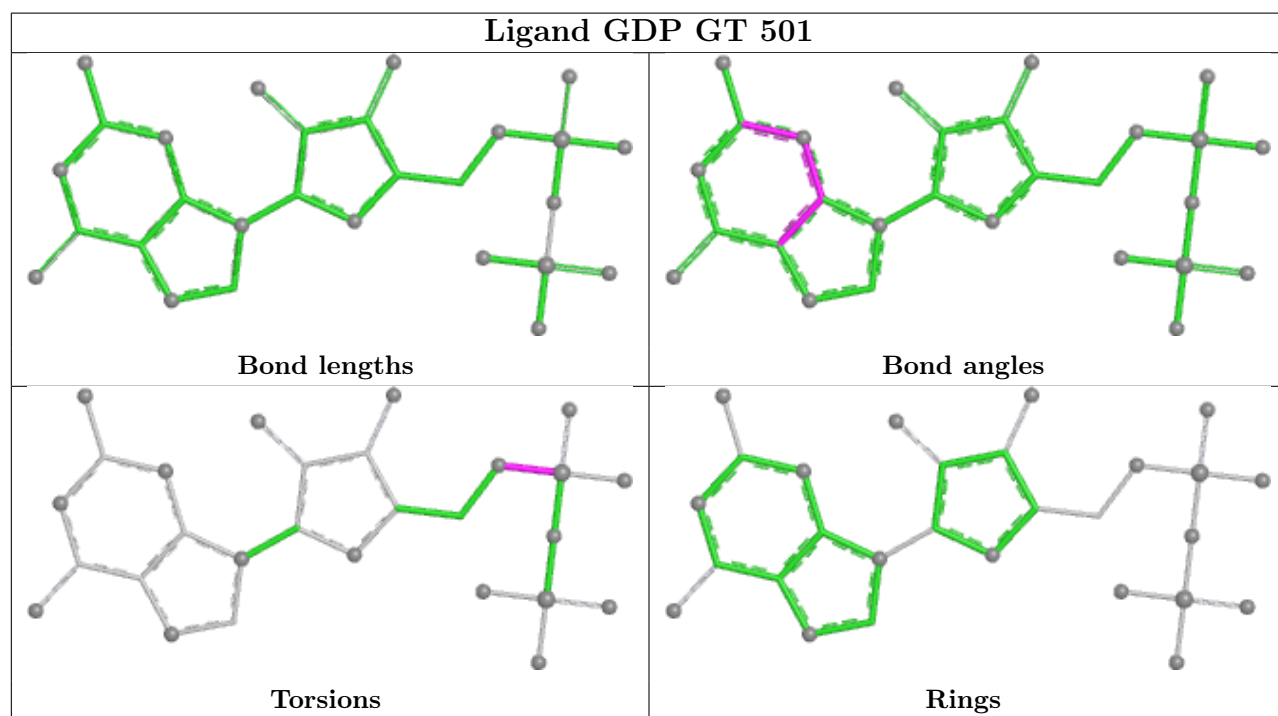
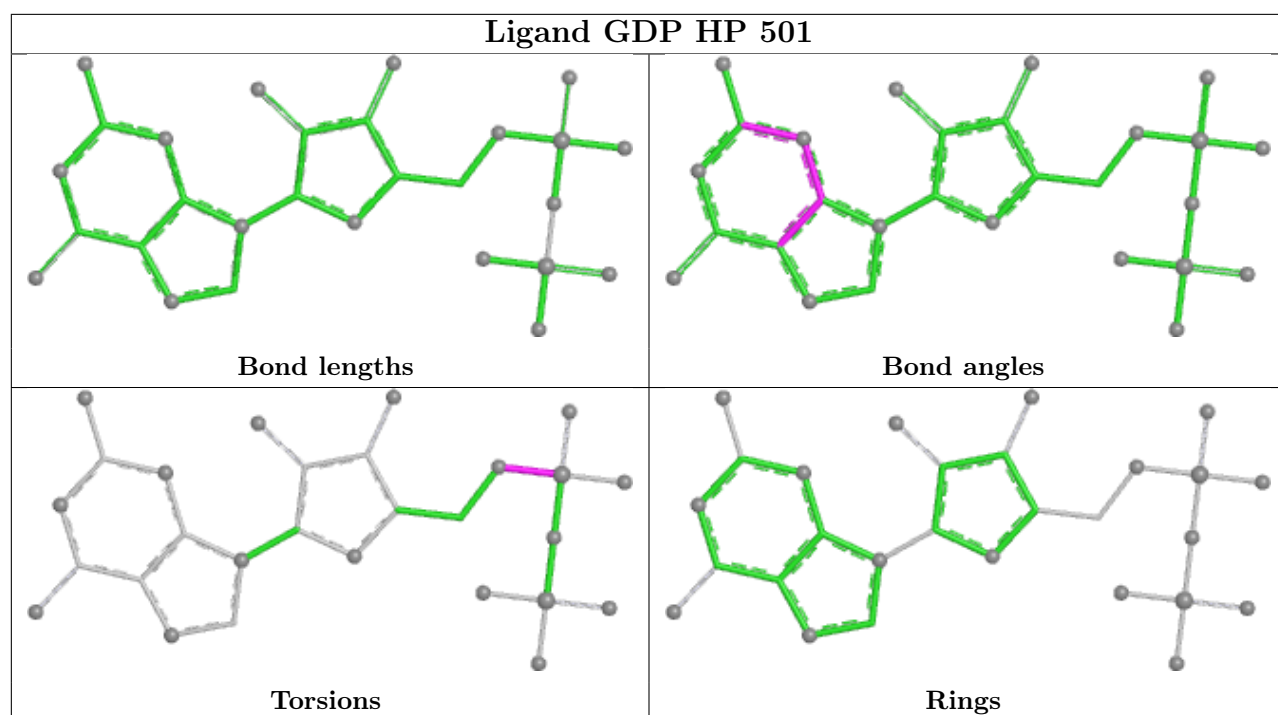


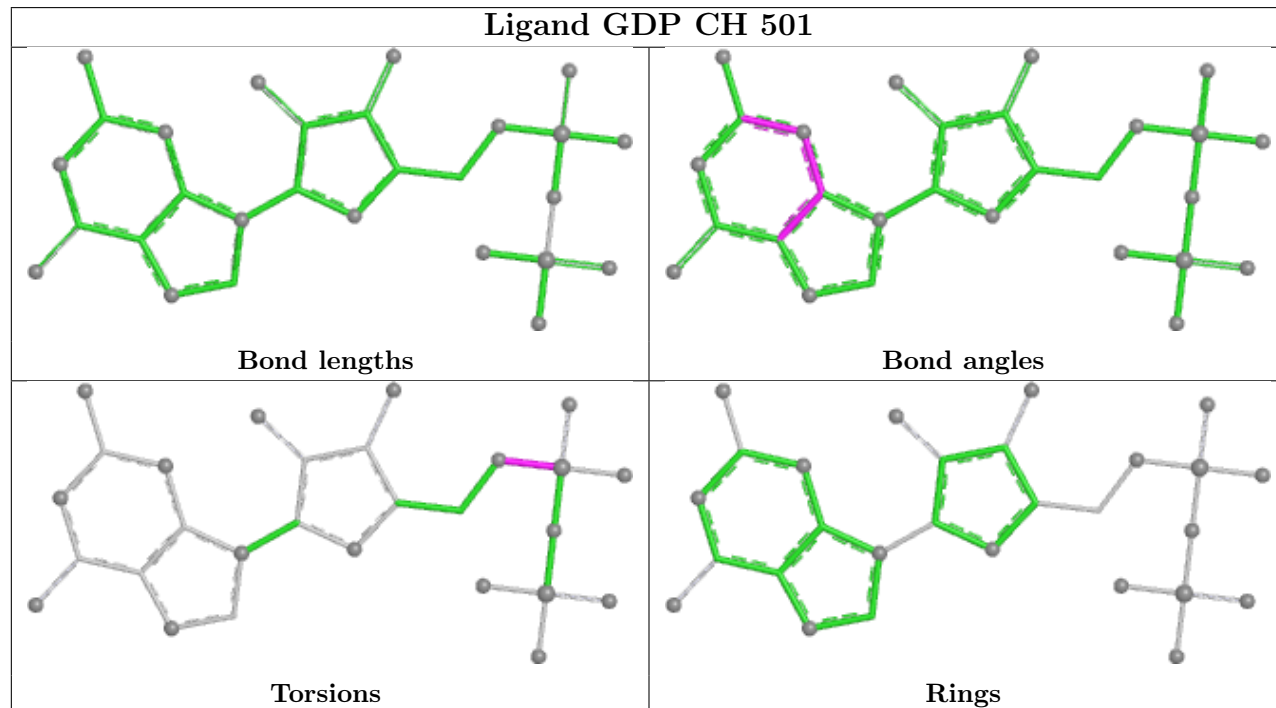
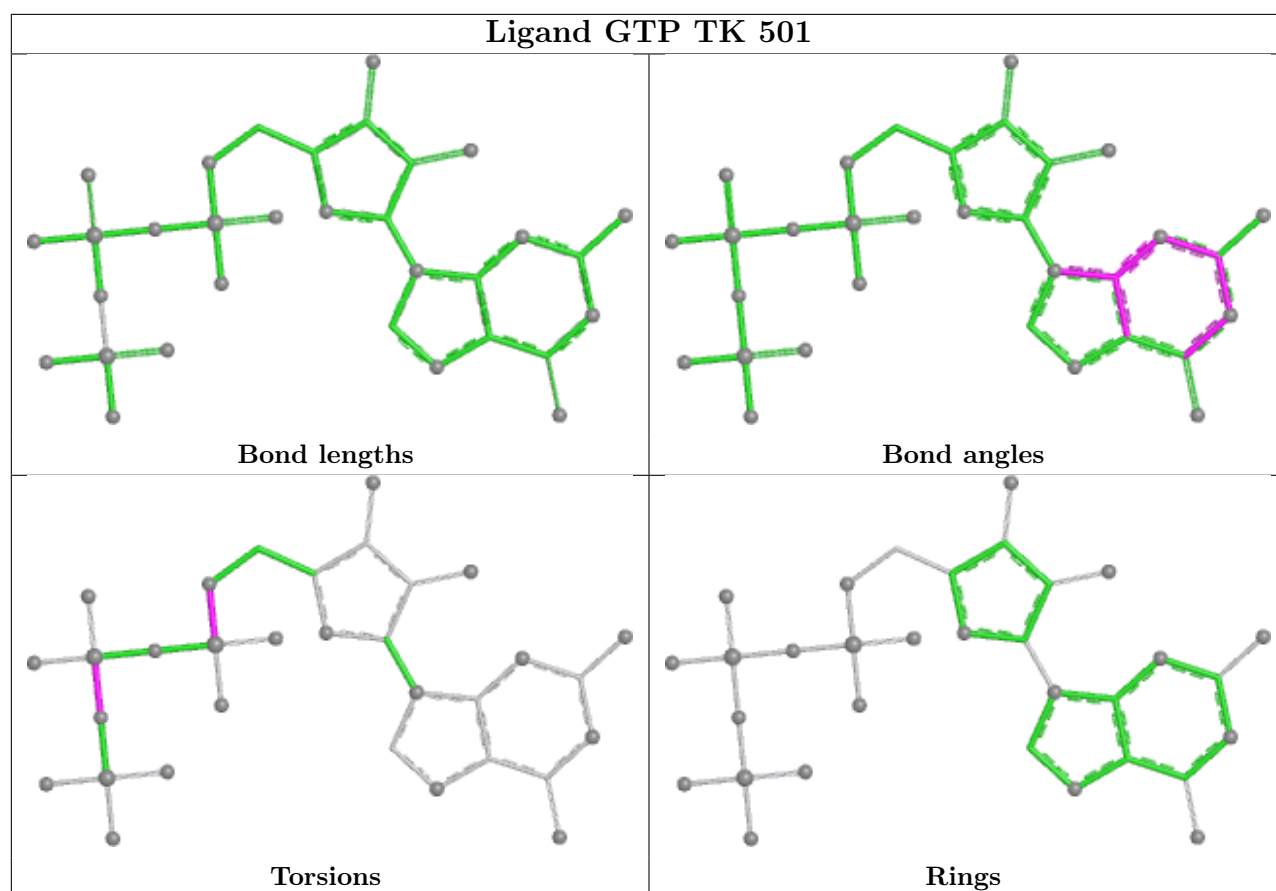
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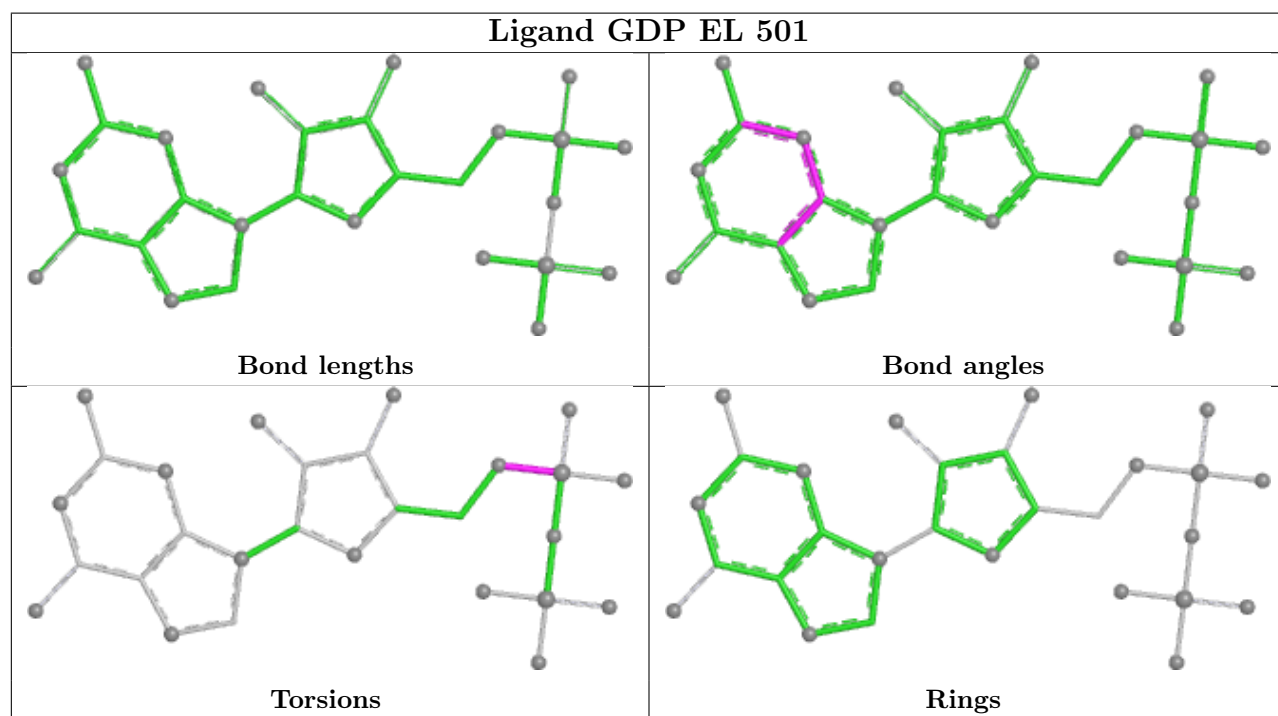
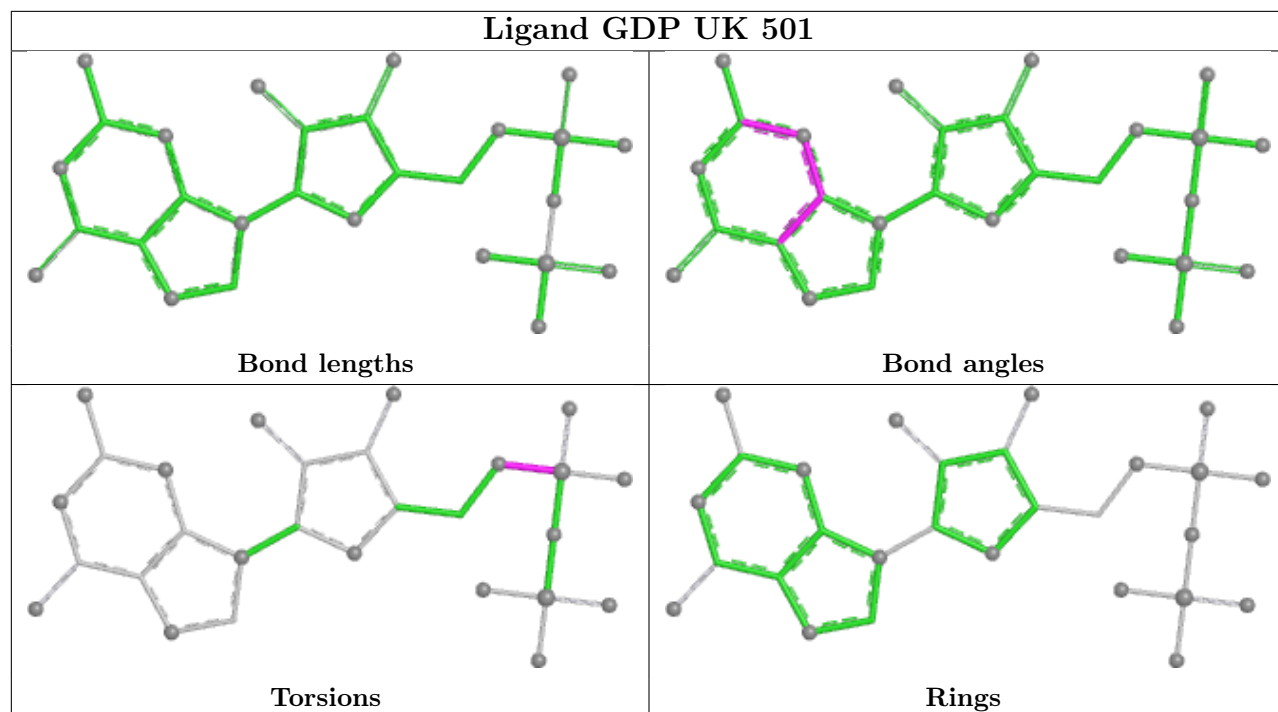


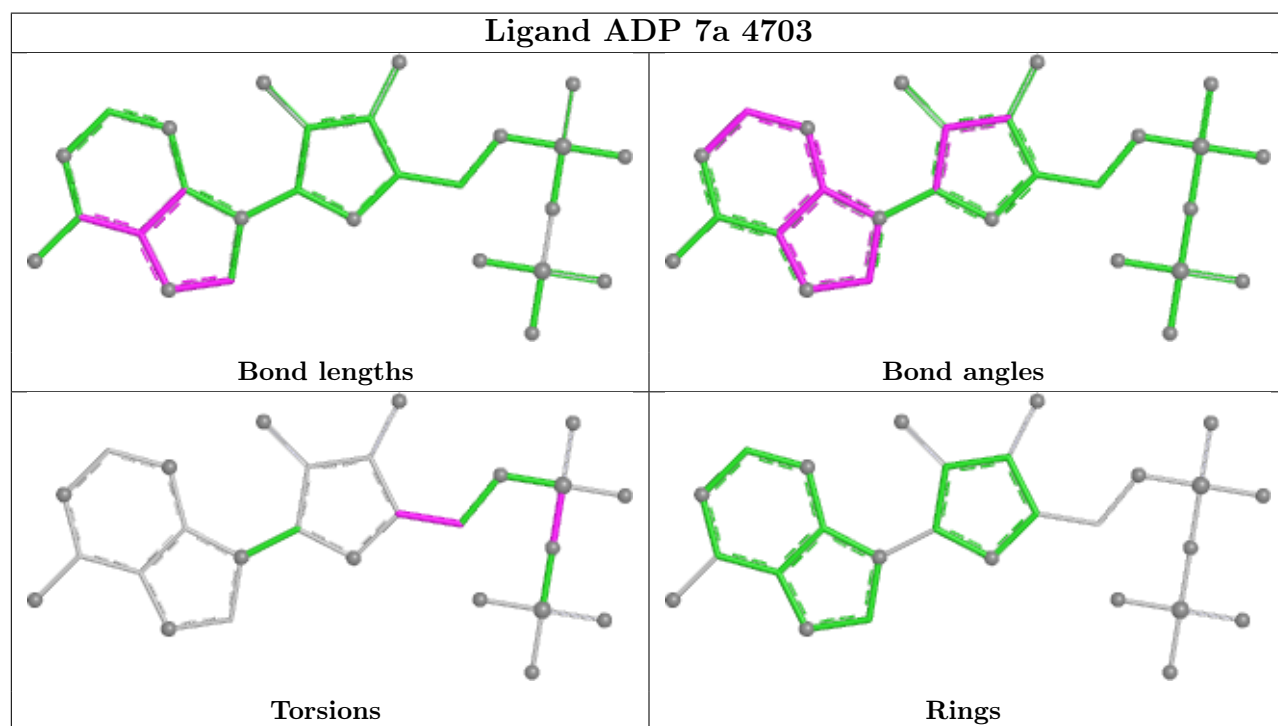
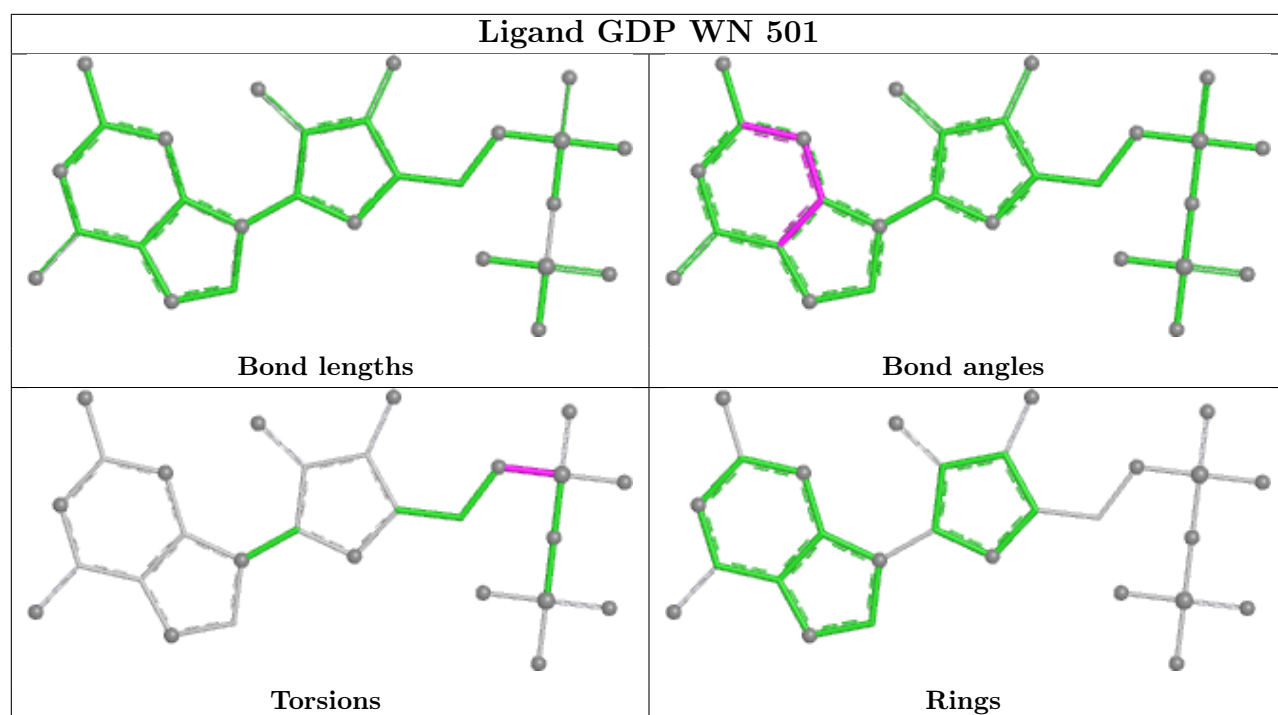
## Ligand GDP GB 501





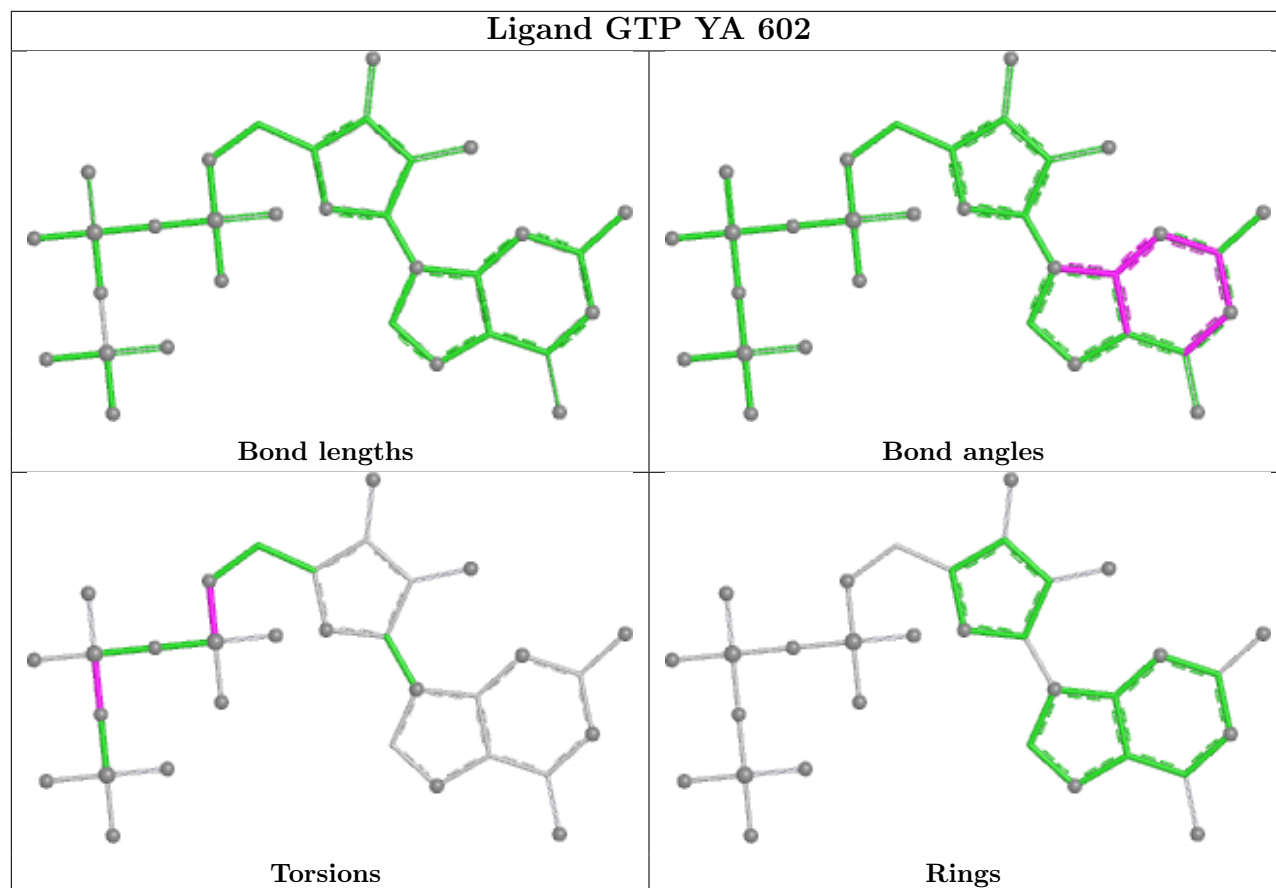




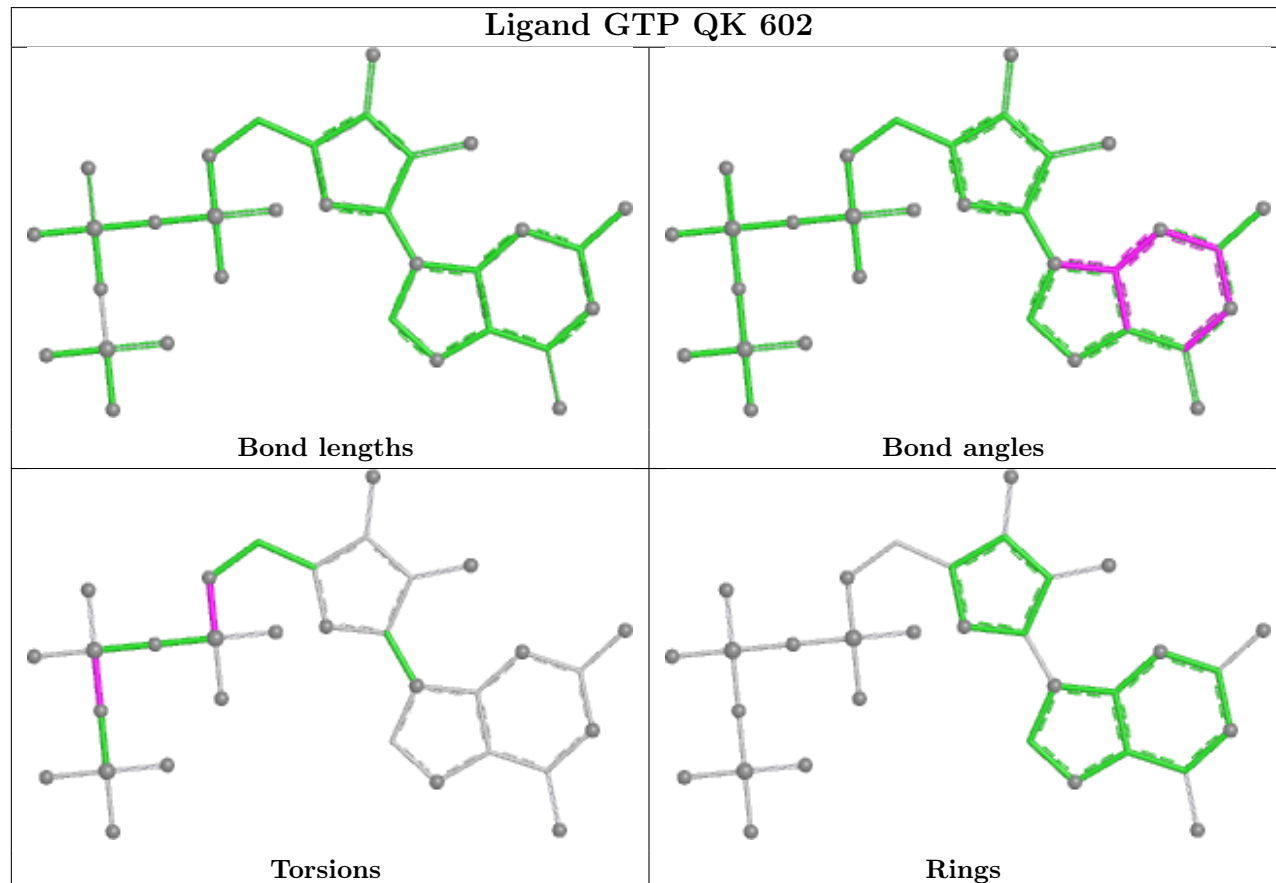




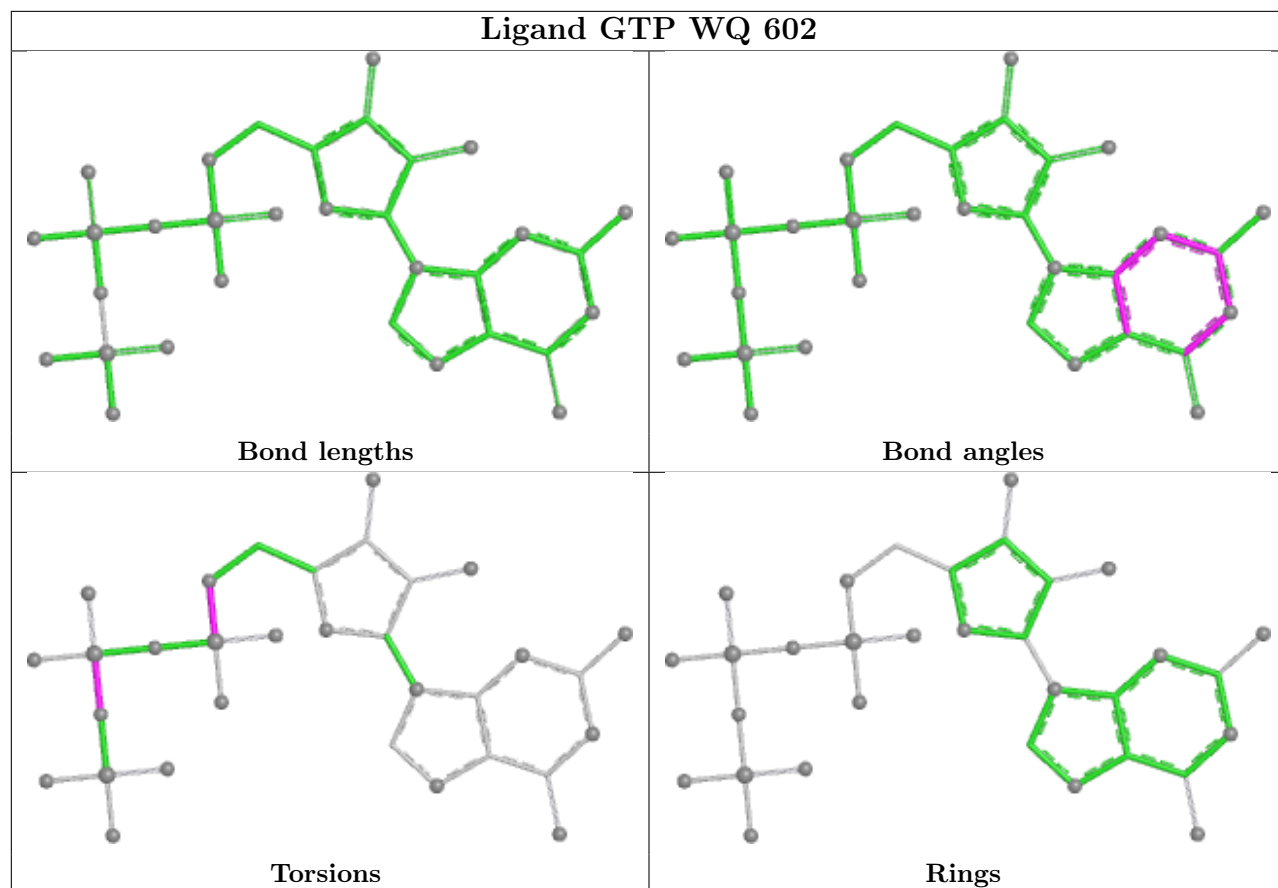
## Ligand GTP YA 602



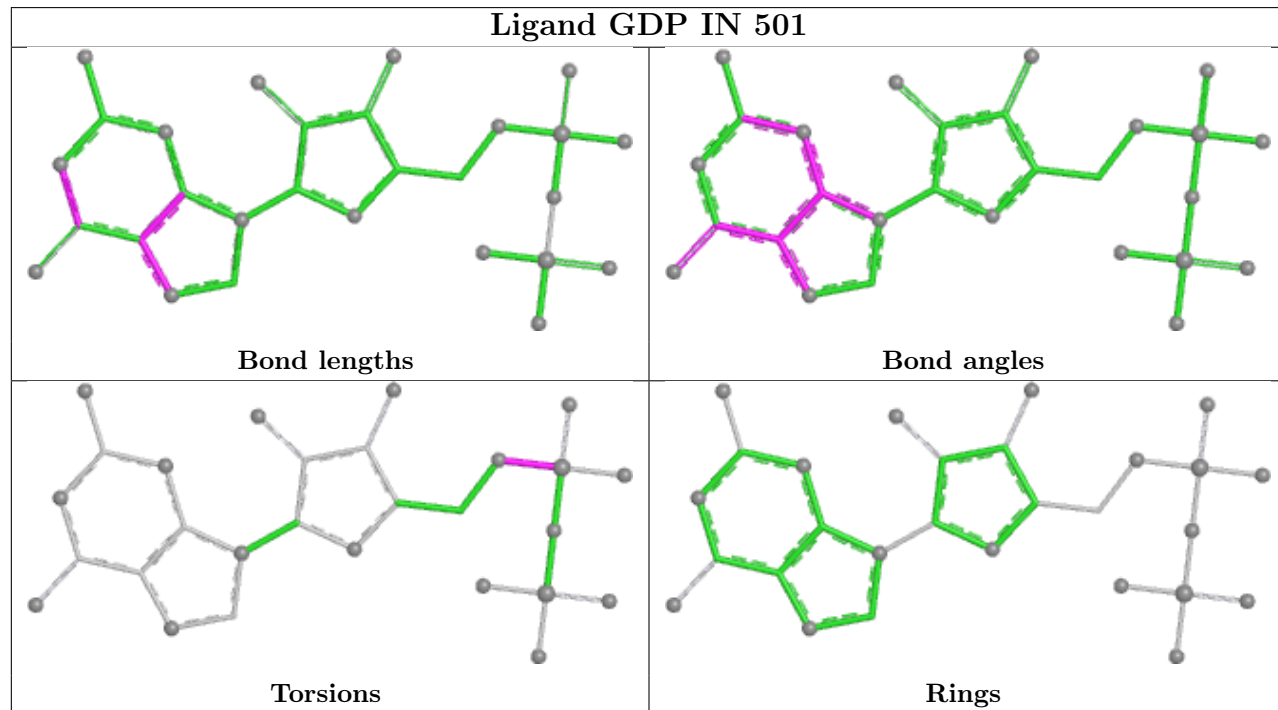
## Ligand GTP QK 602

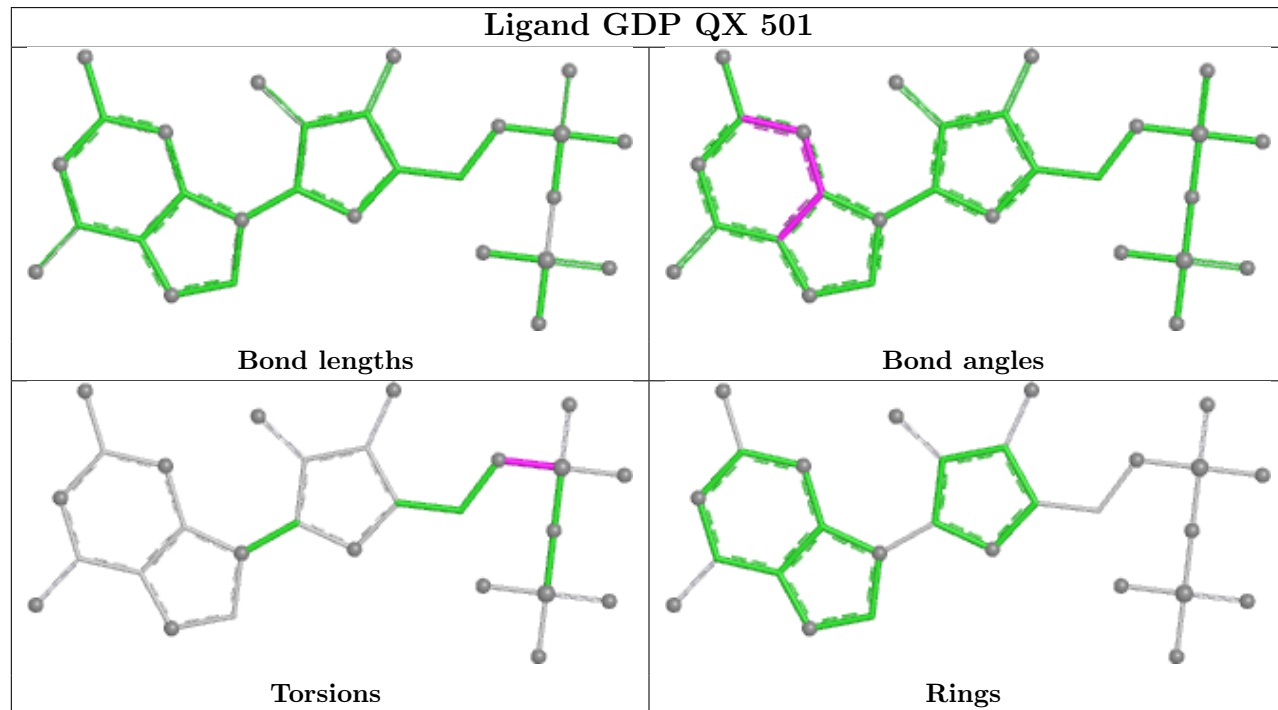
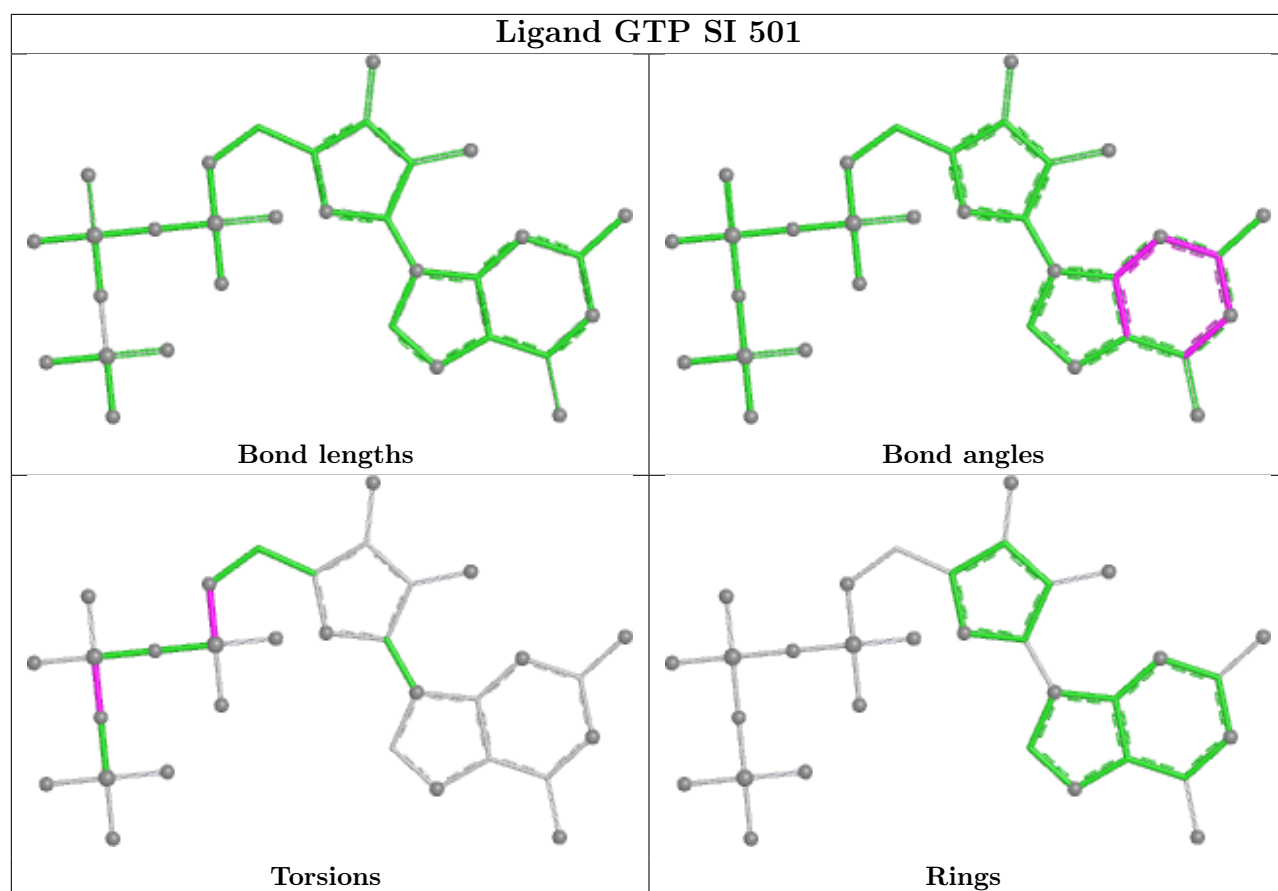


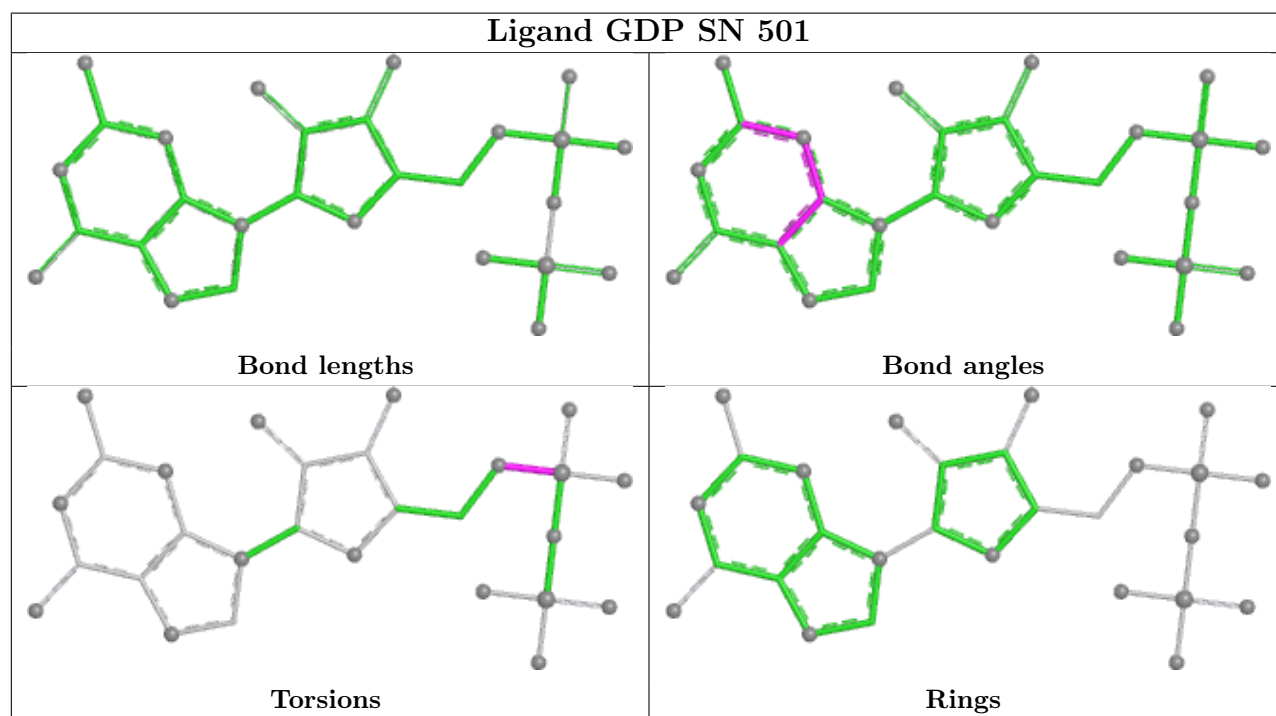
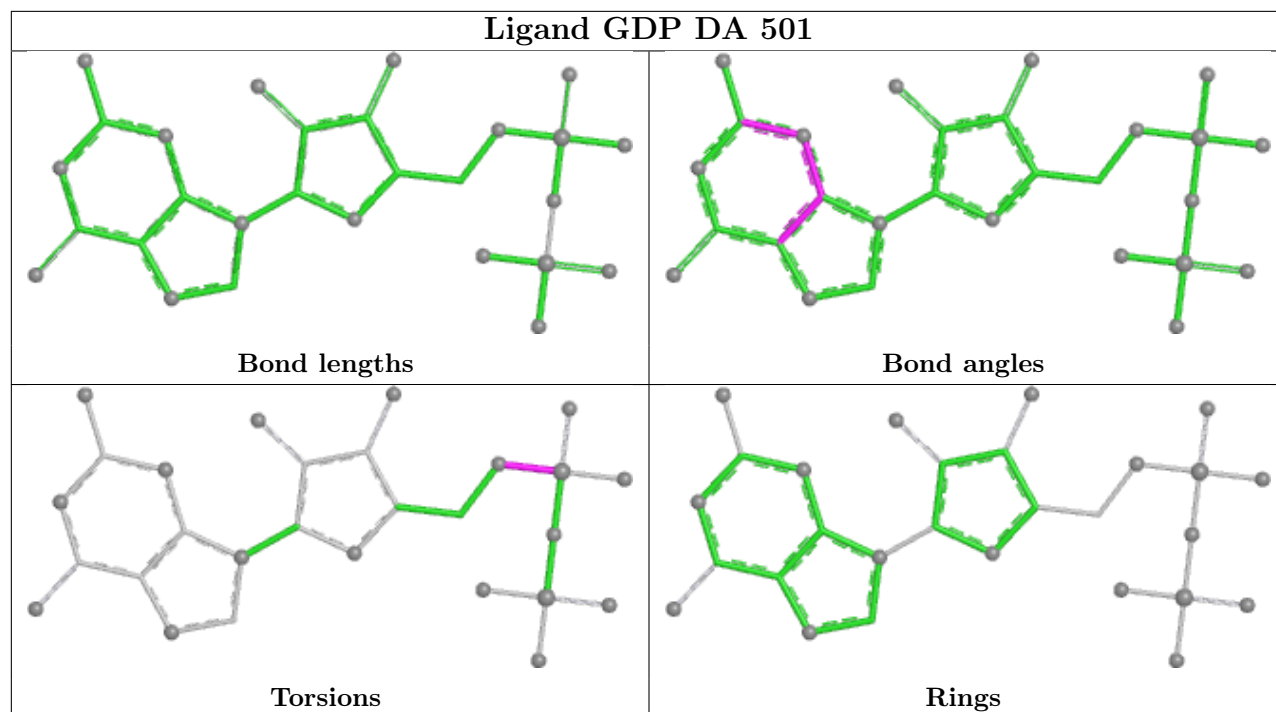
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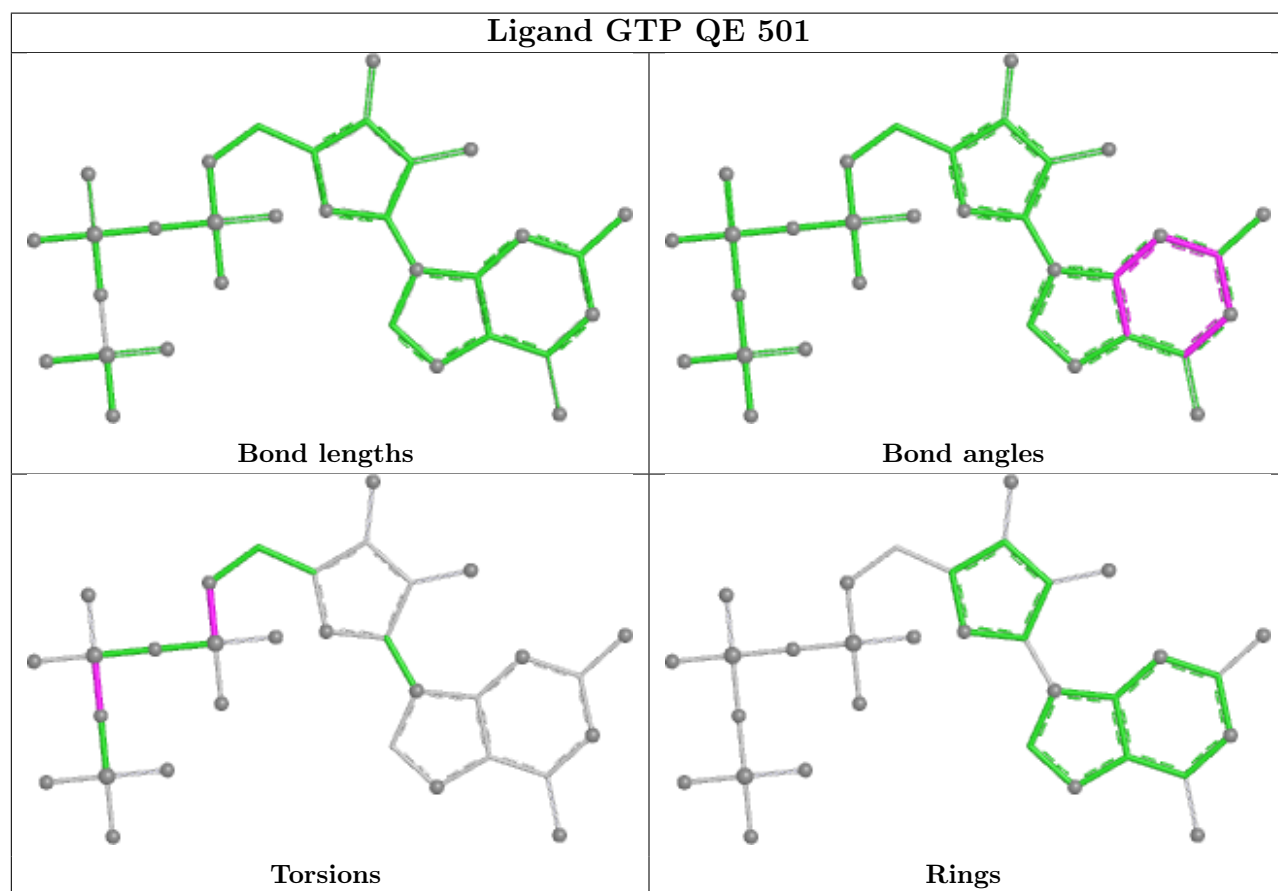
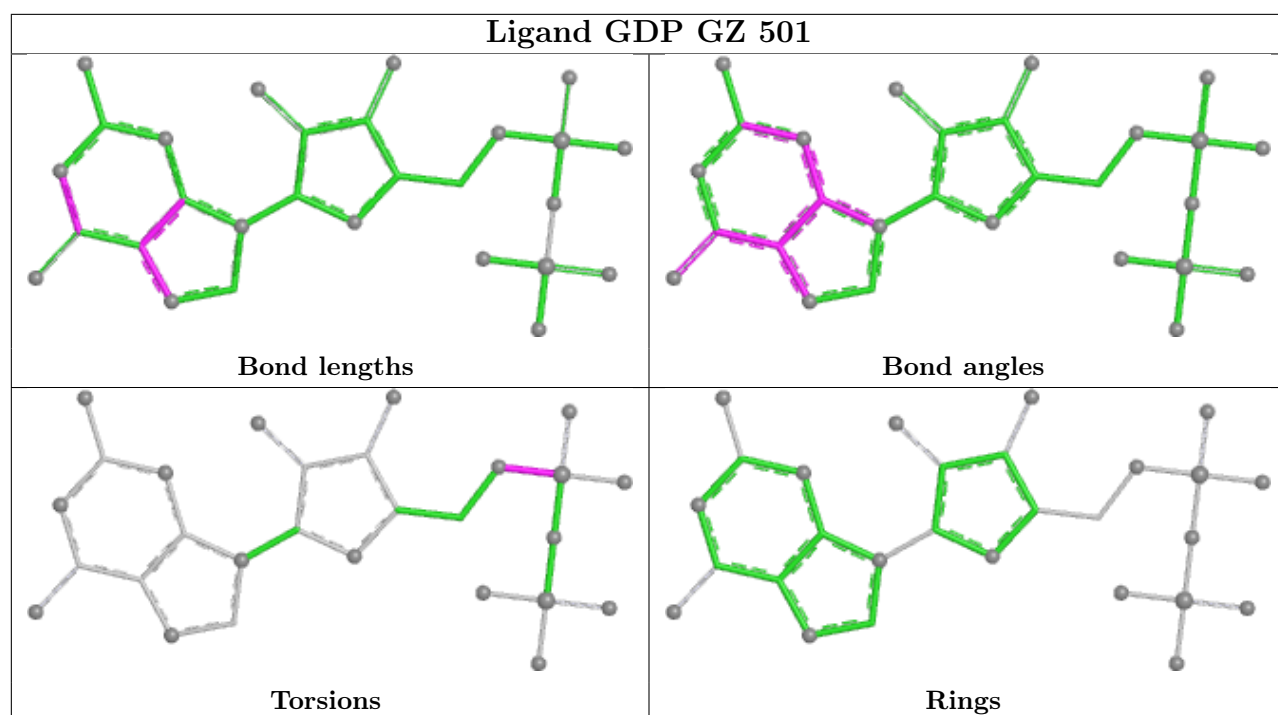


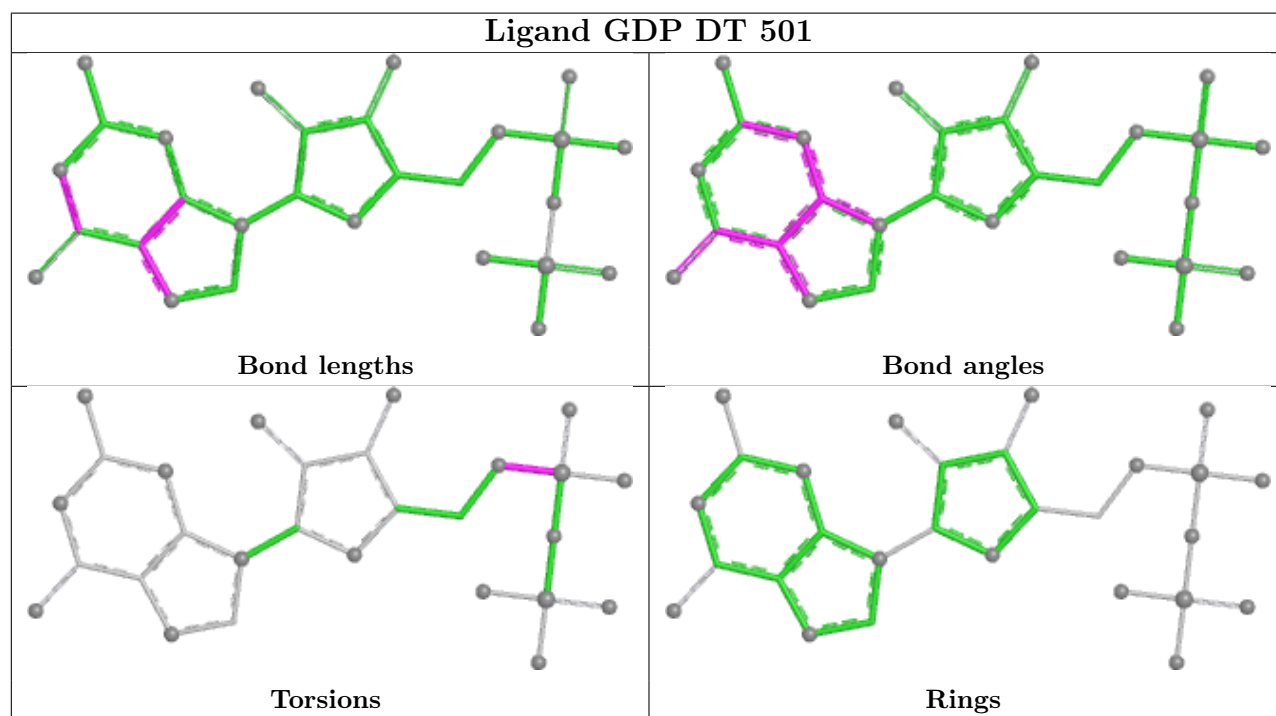
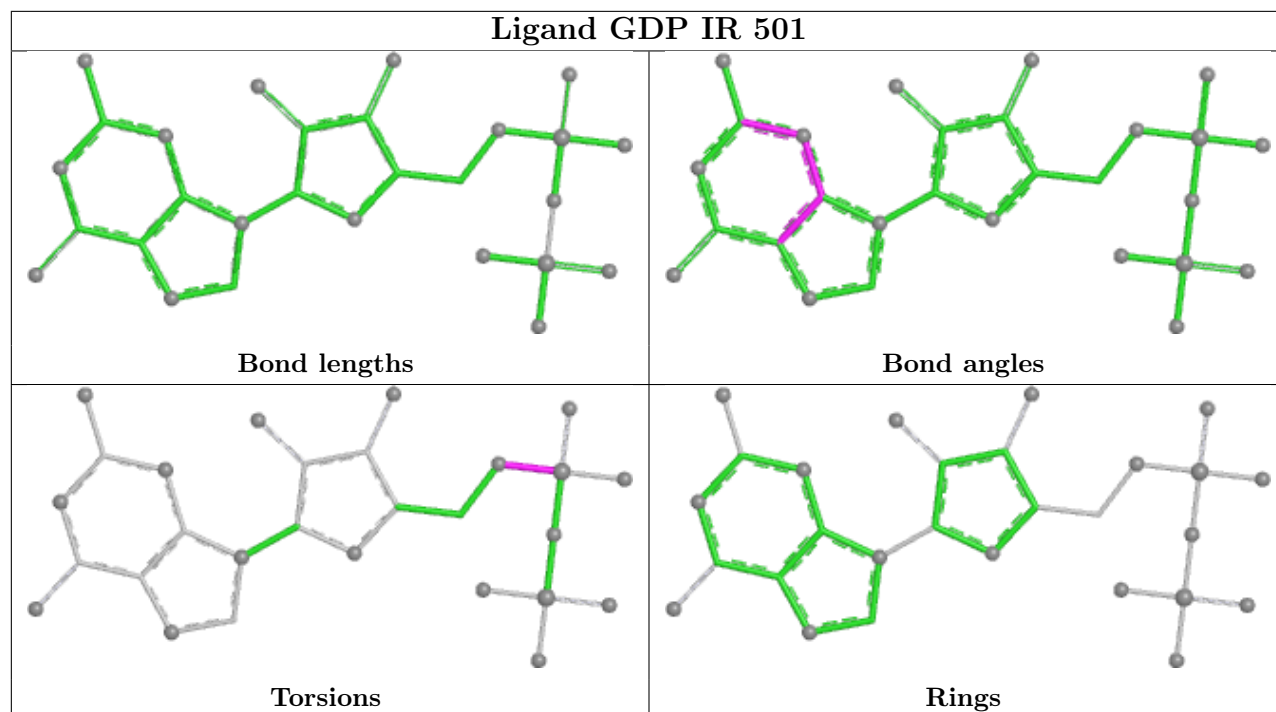
## Ligand GDP IN 501



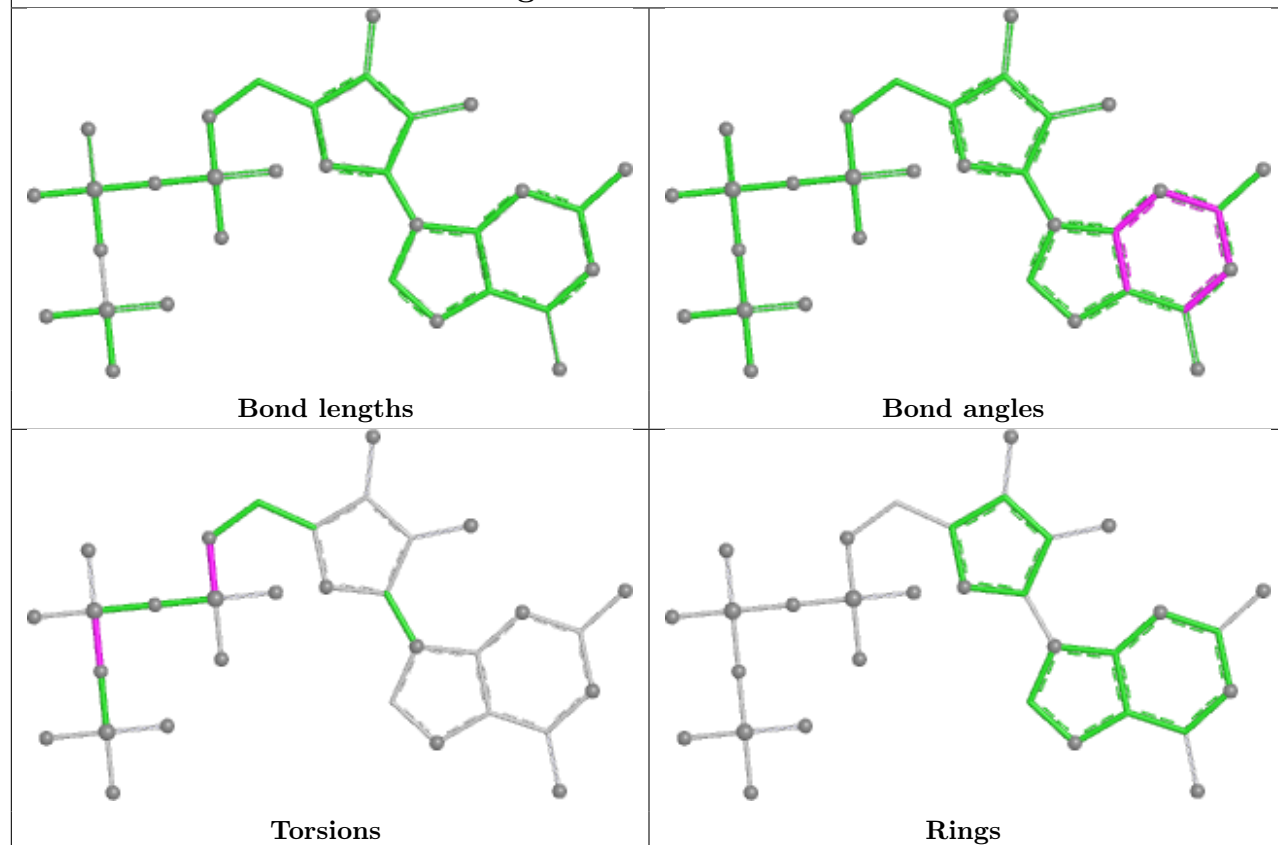




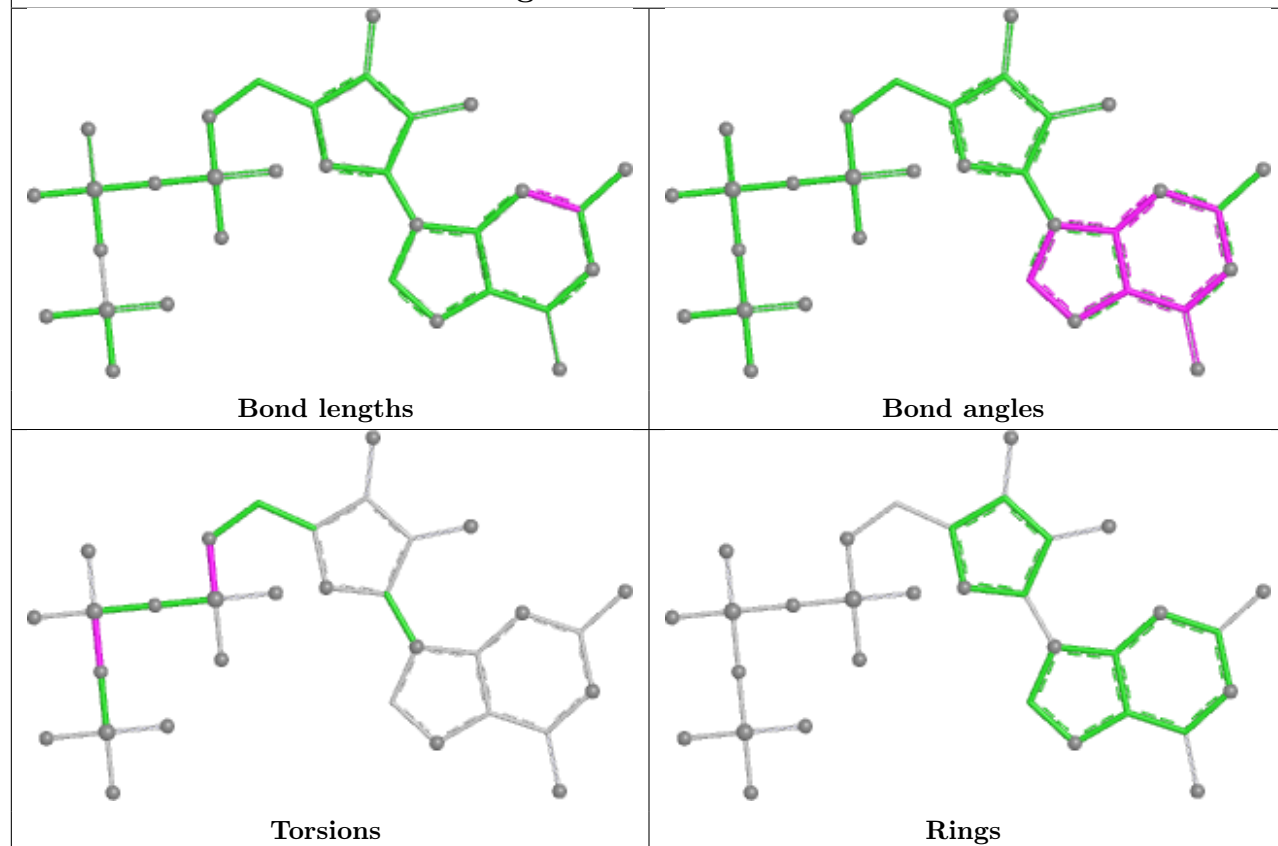


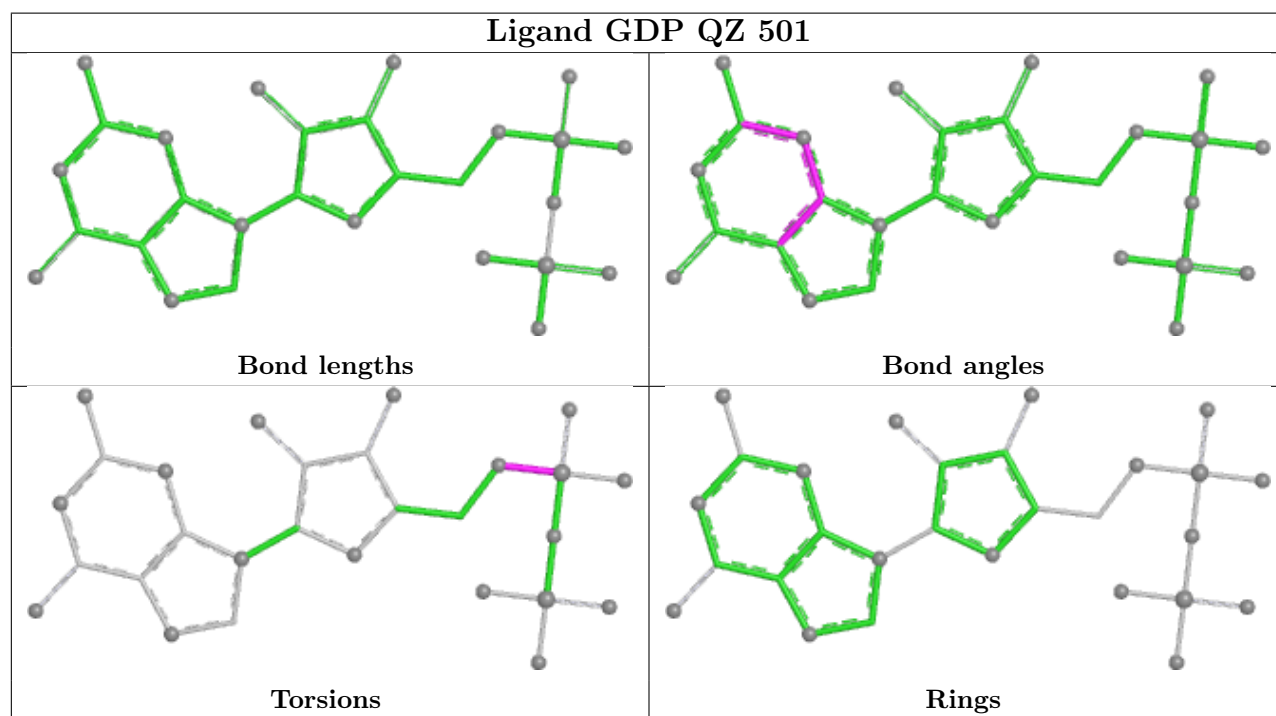
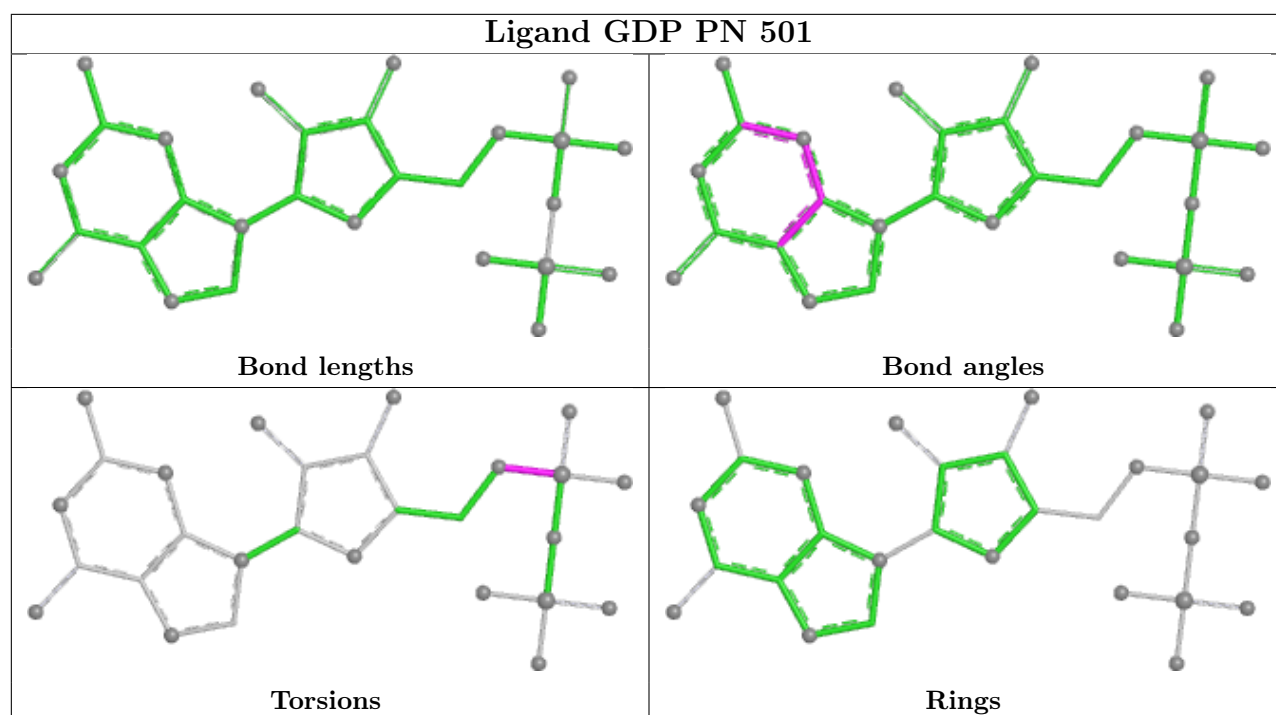


## Ligand GTP OB 501

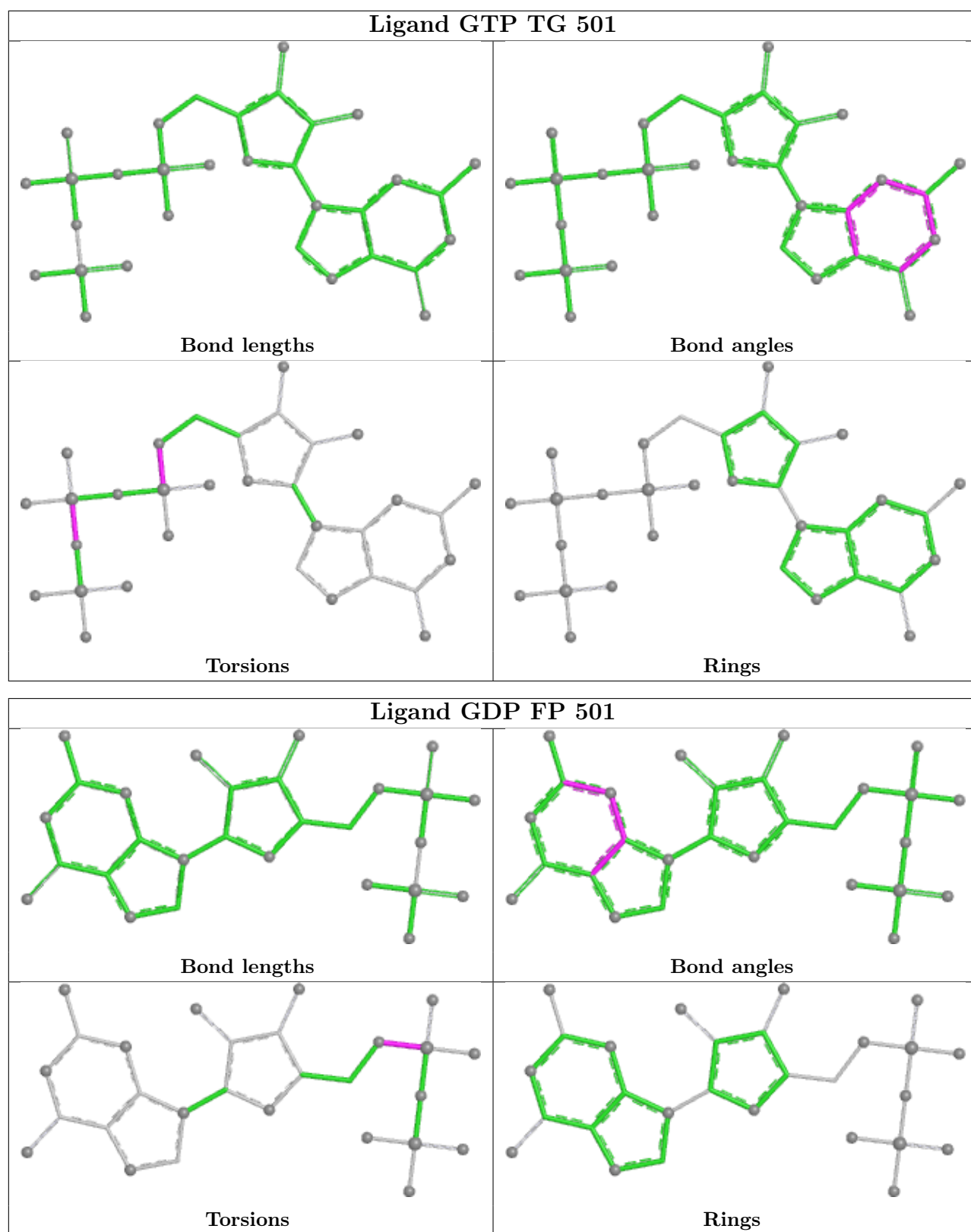


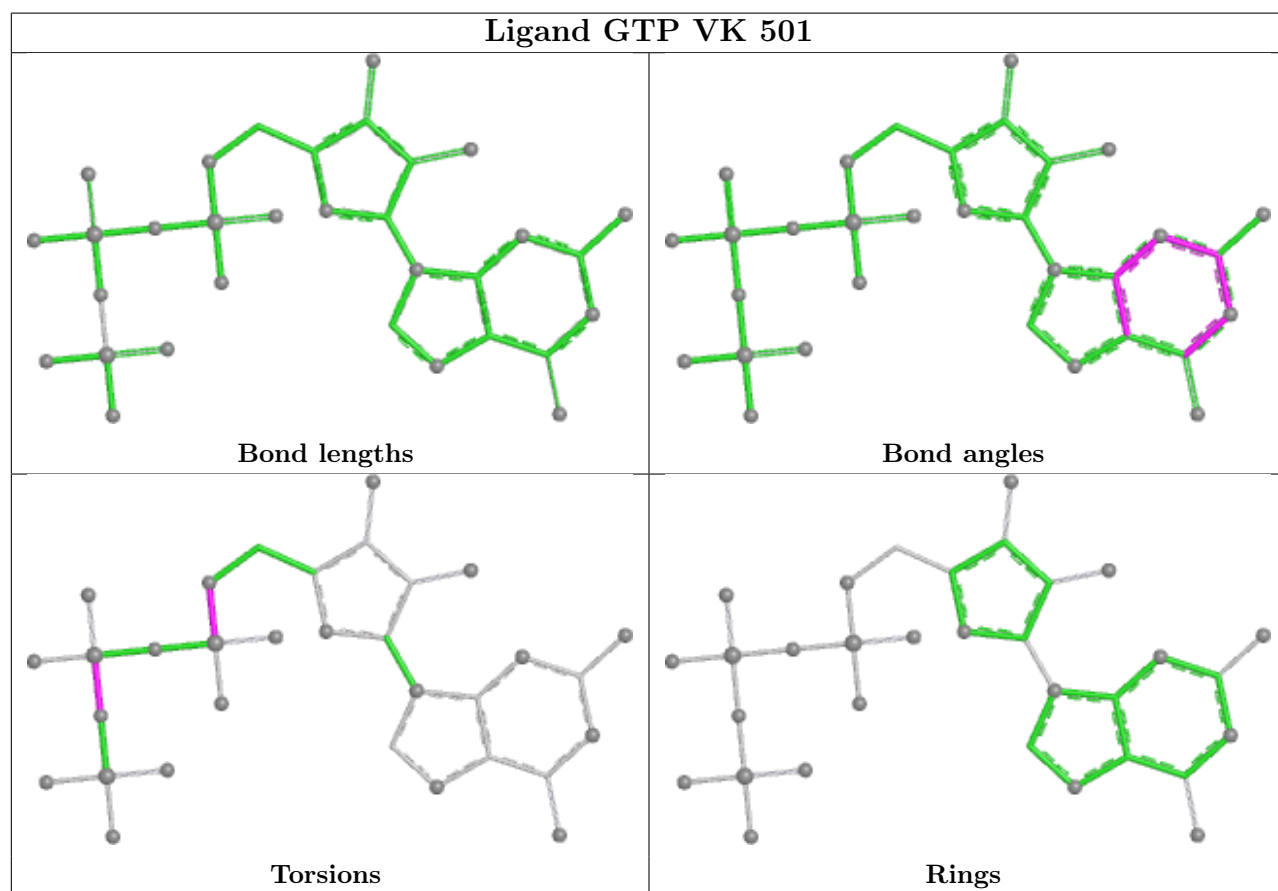
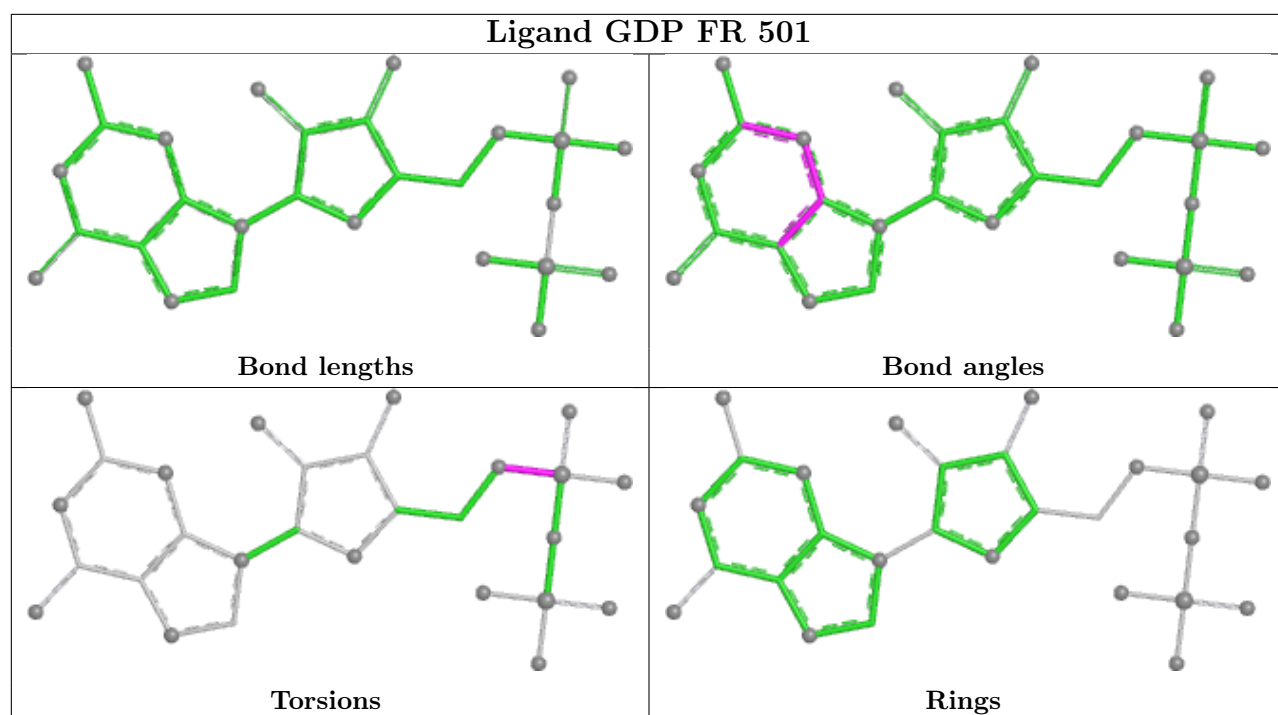
## Ligand GTP HC 602

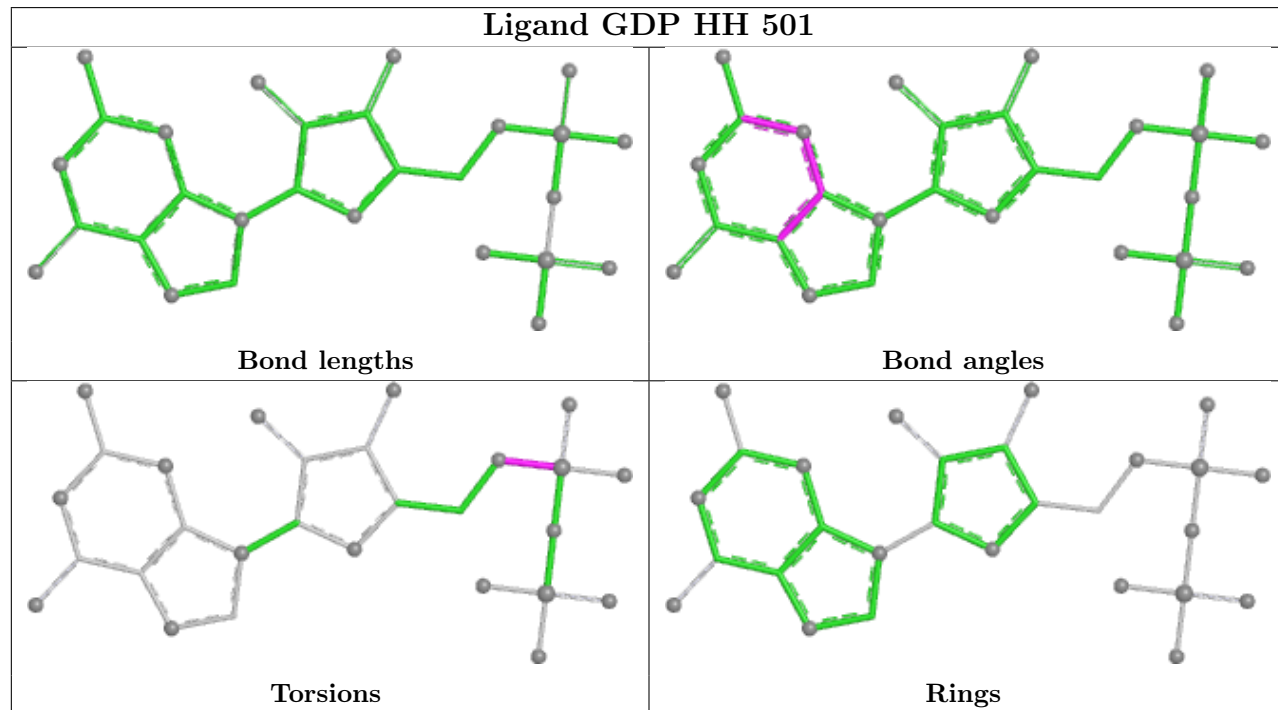
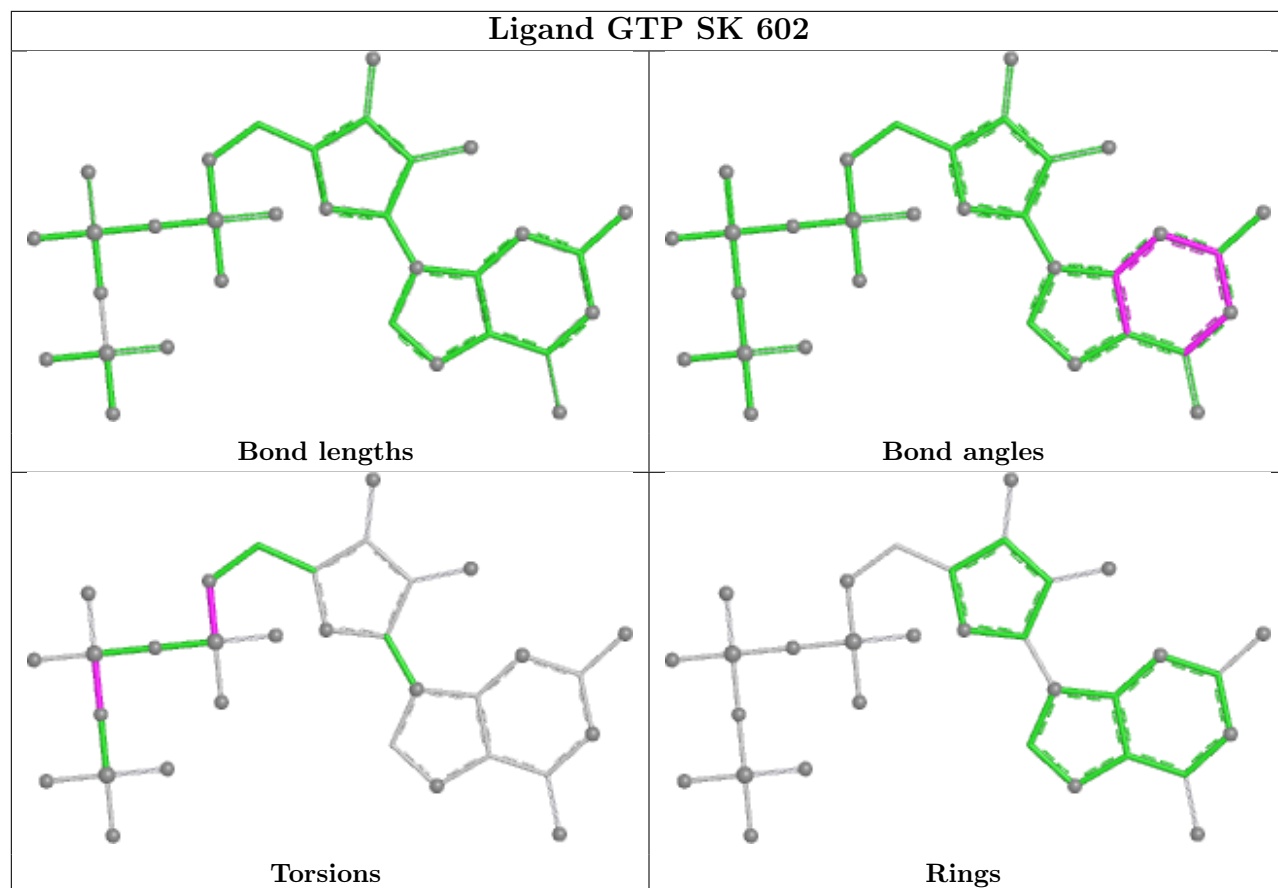


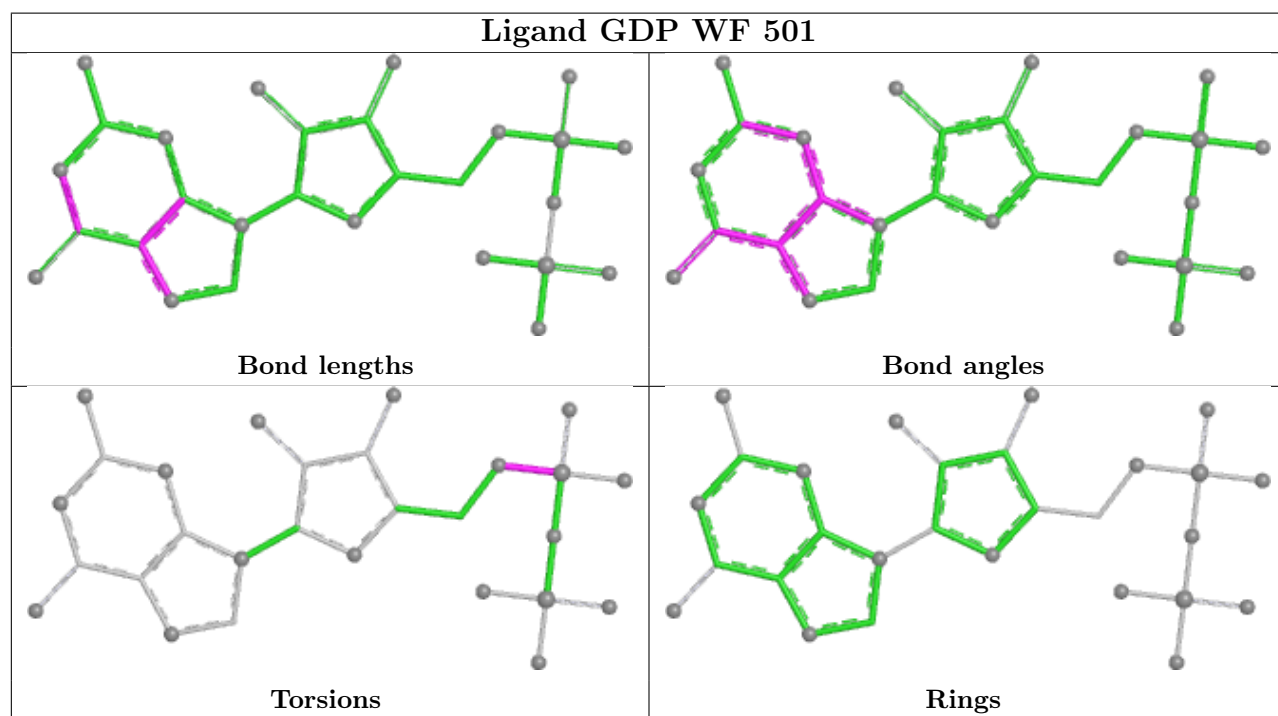
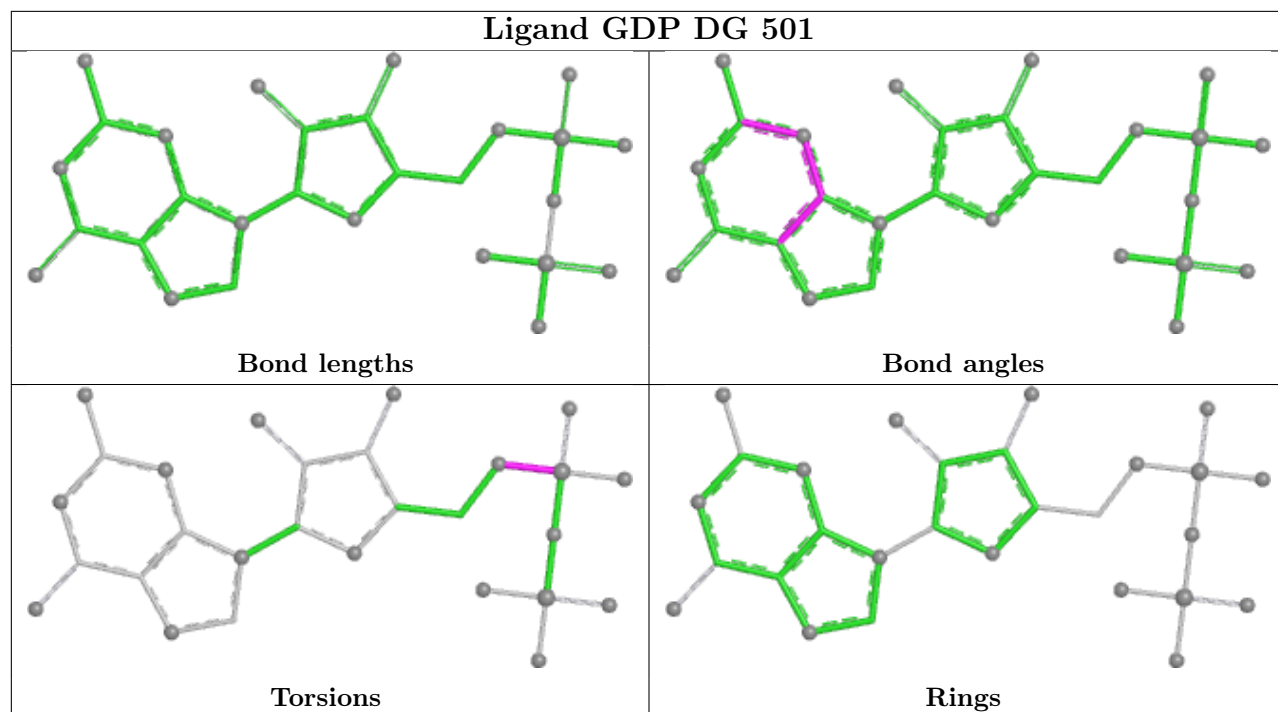




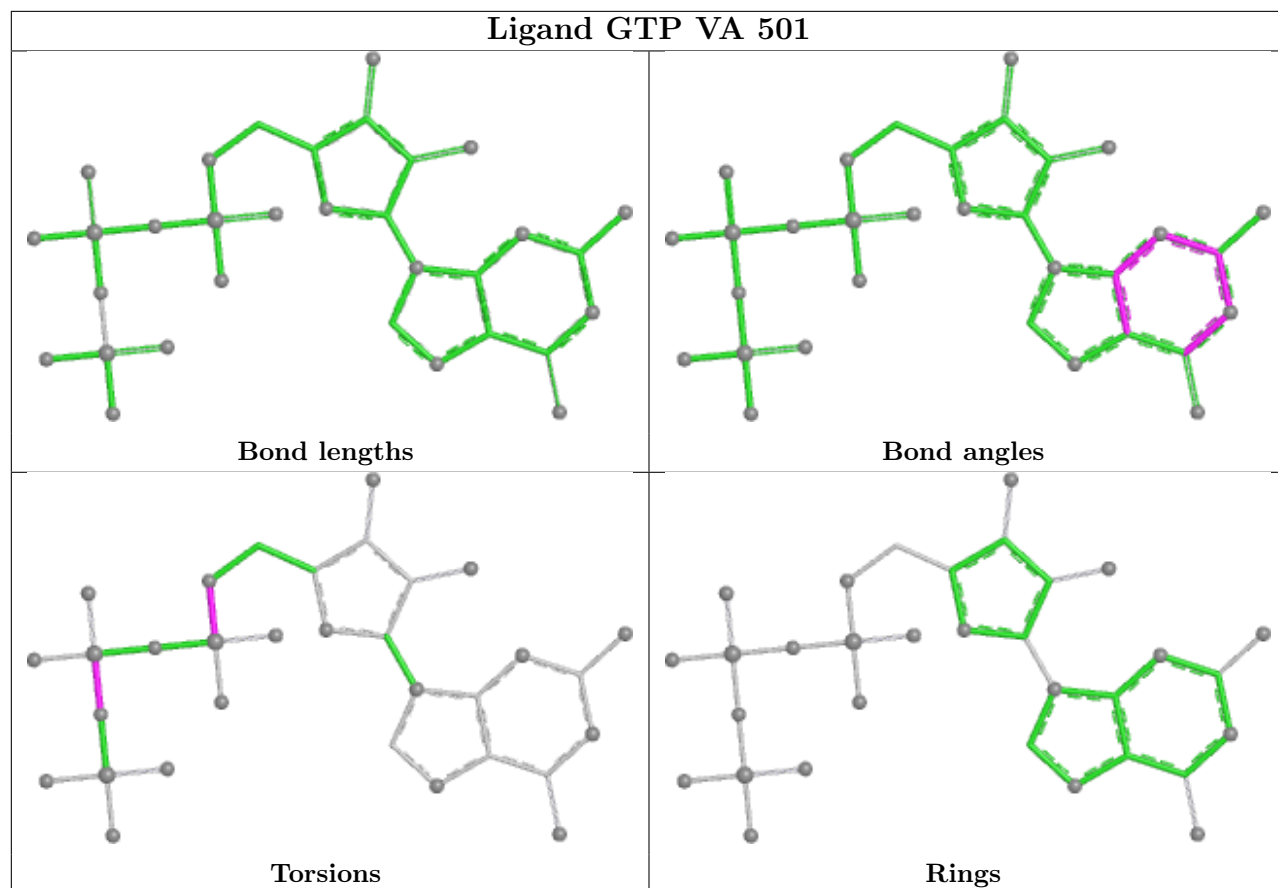




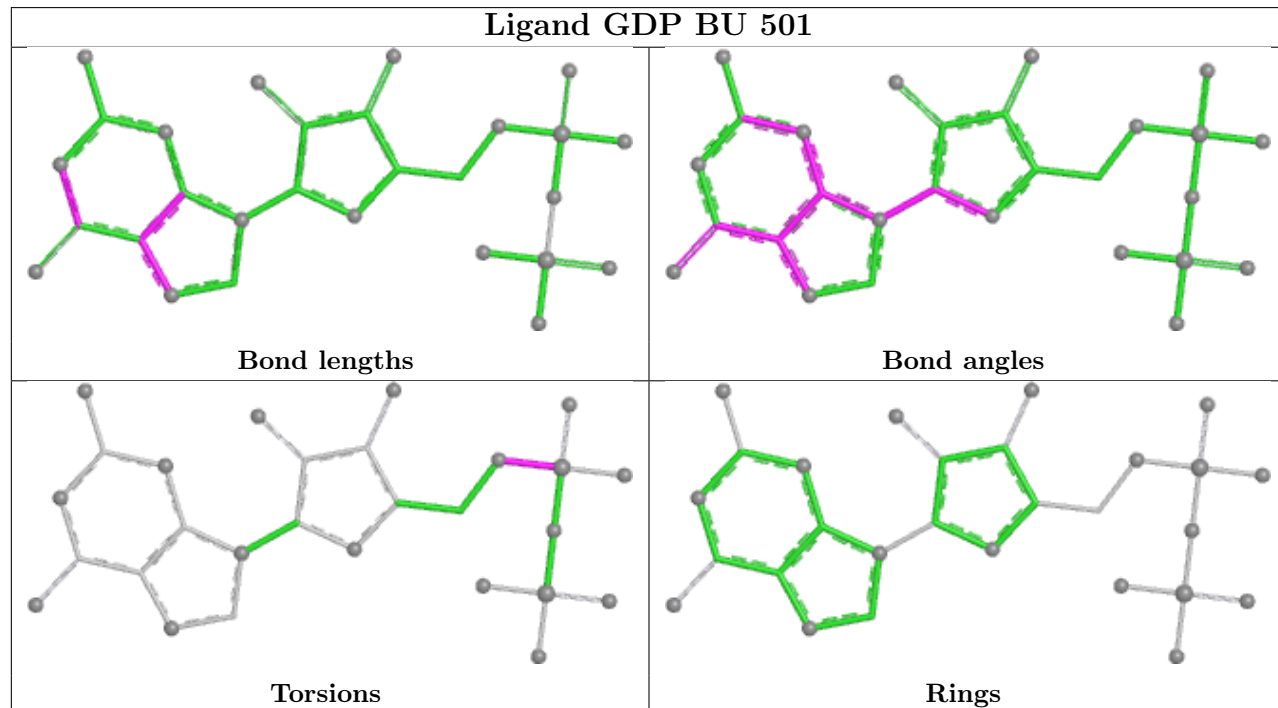


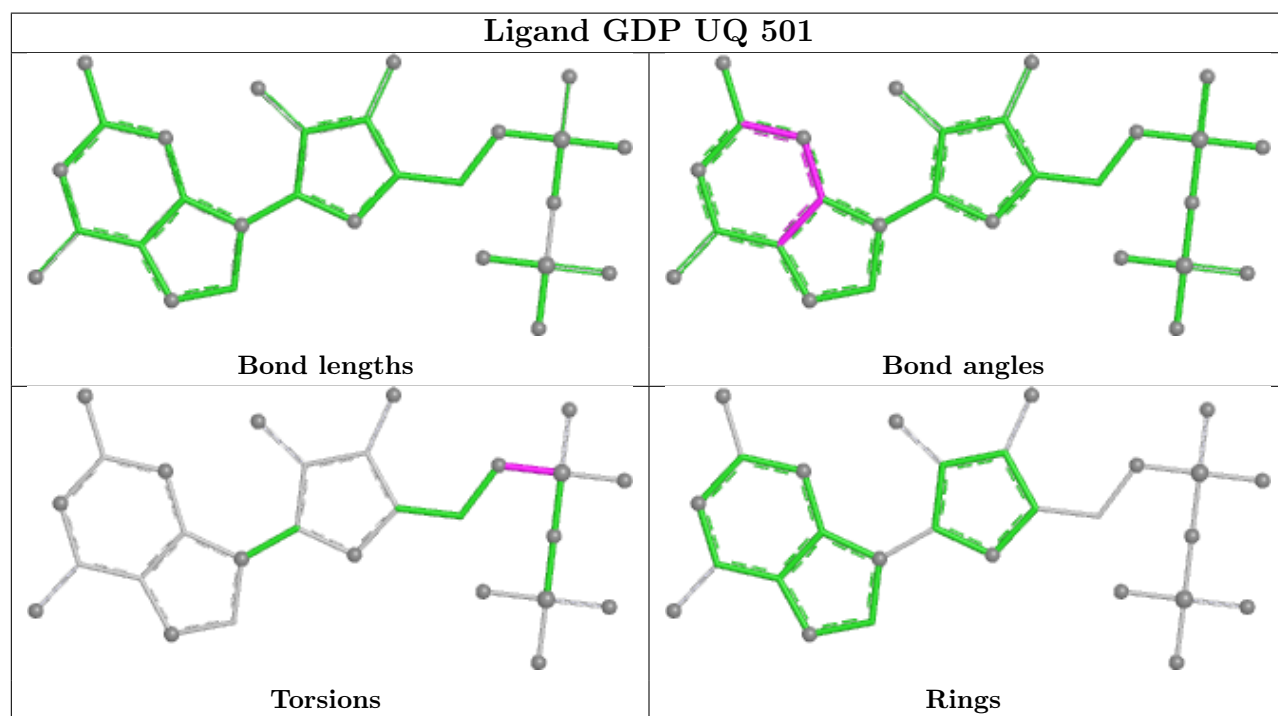
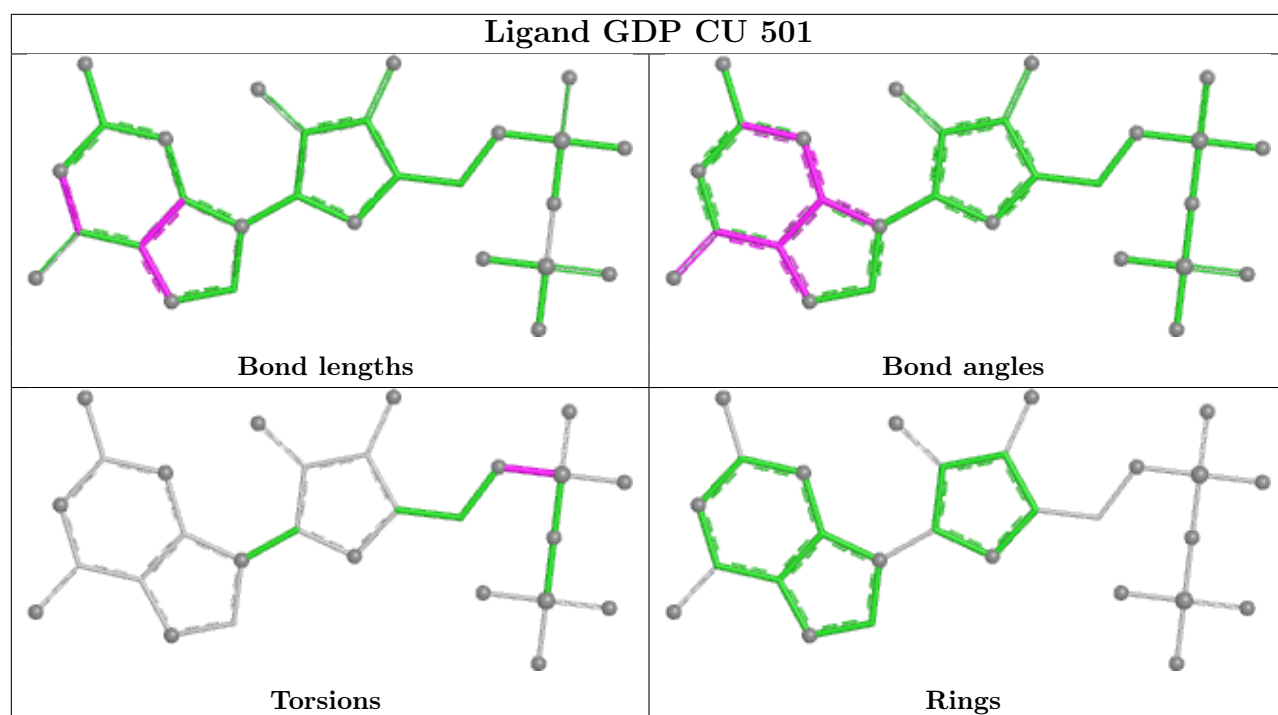


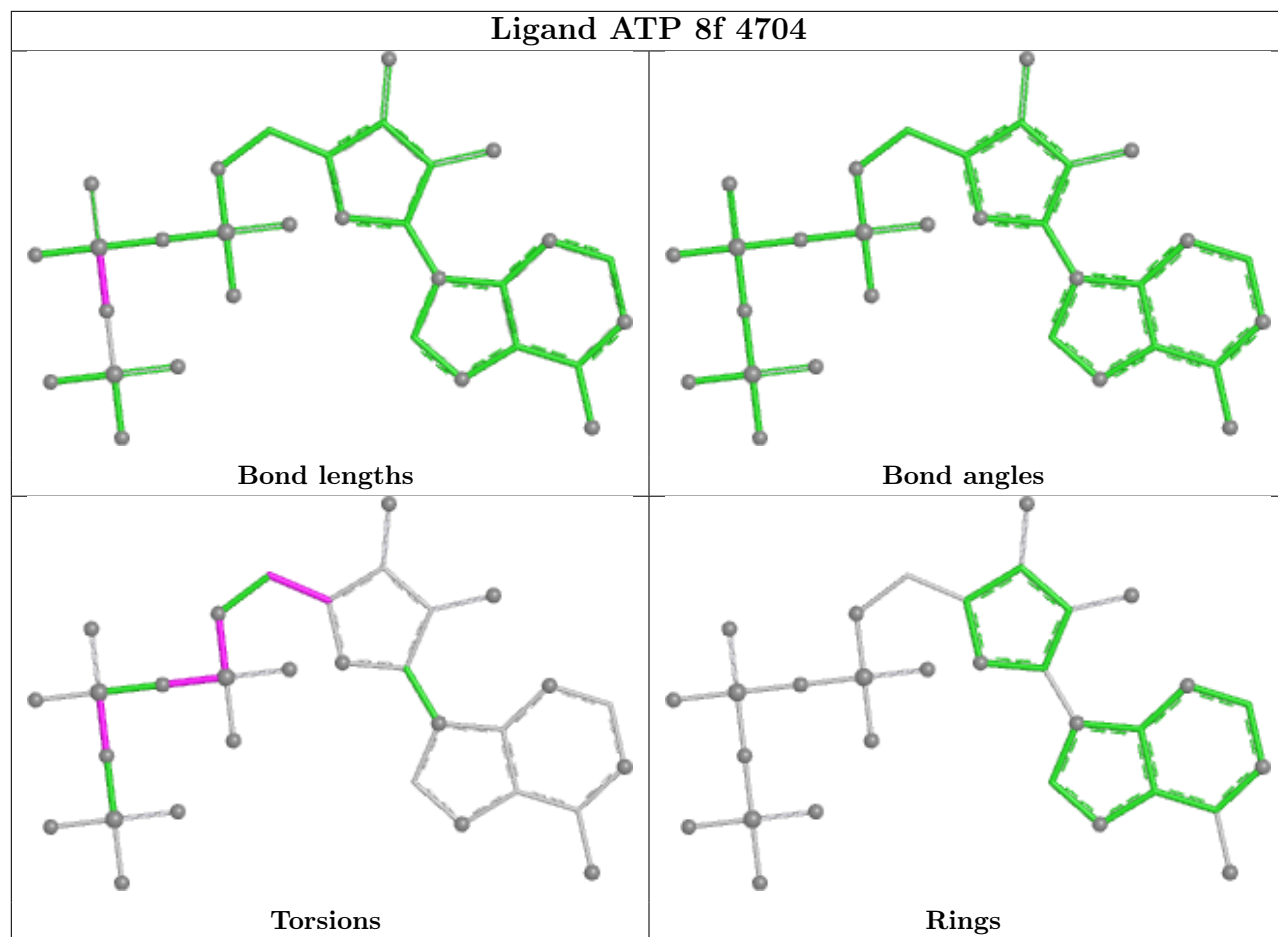
## Ligand GTP VA 501



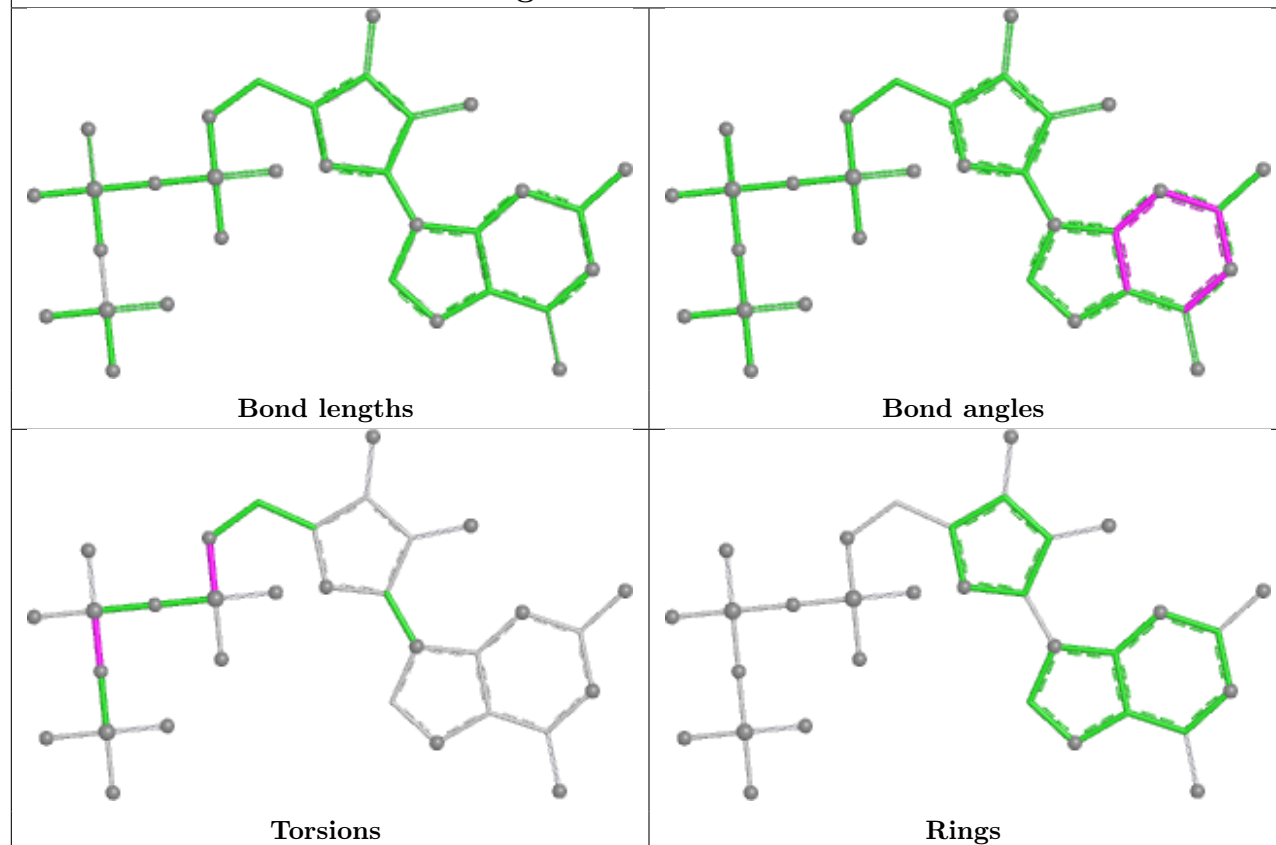
## Ligand GDP BU 501



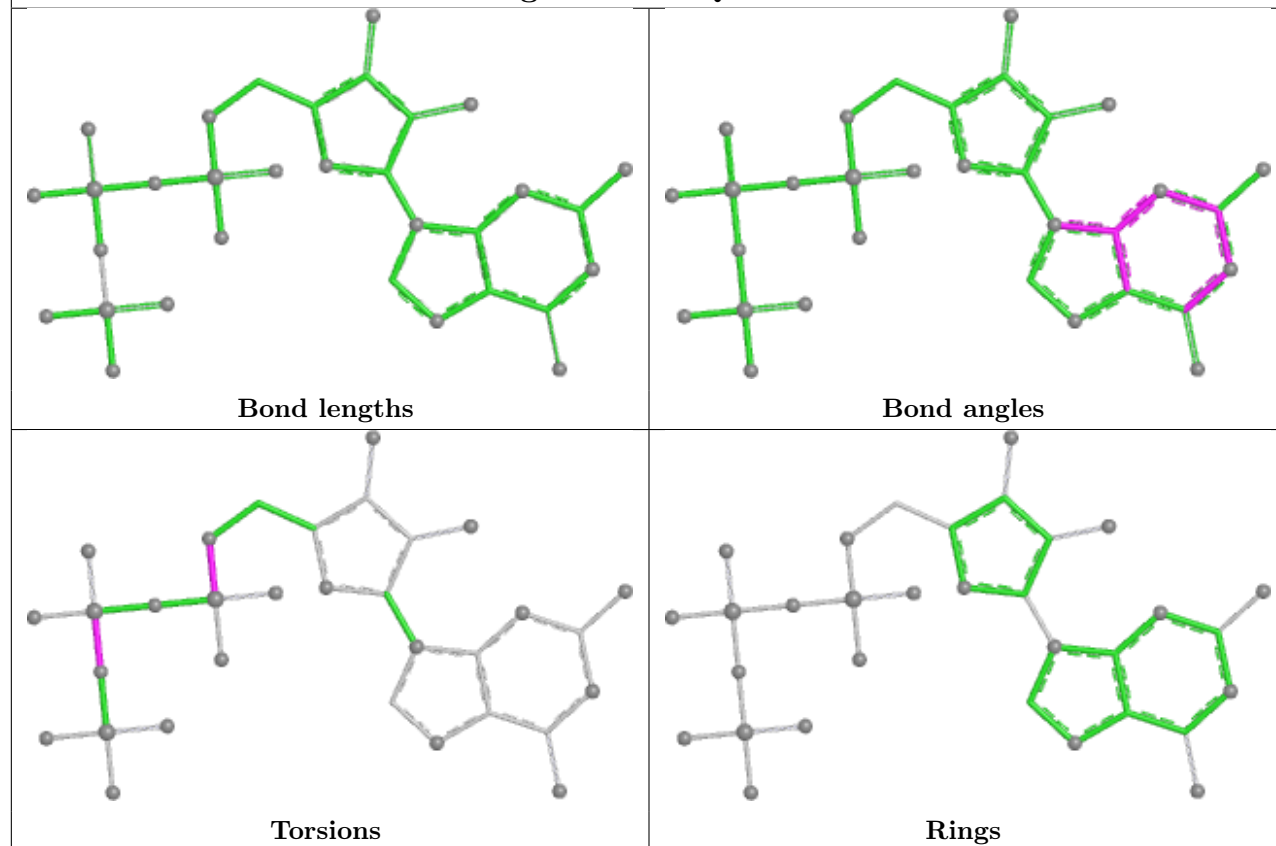




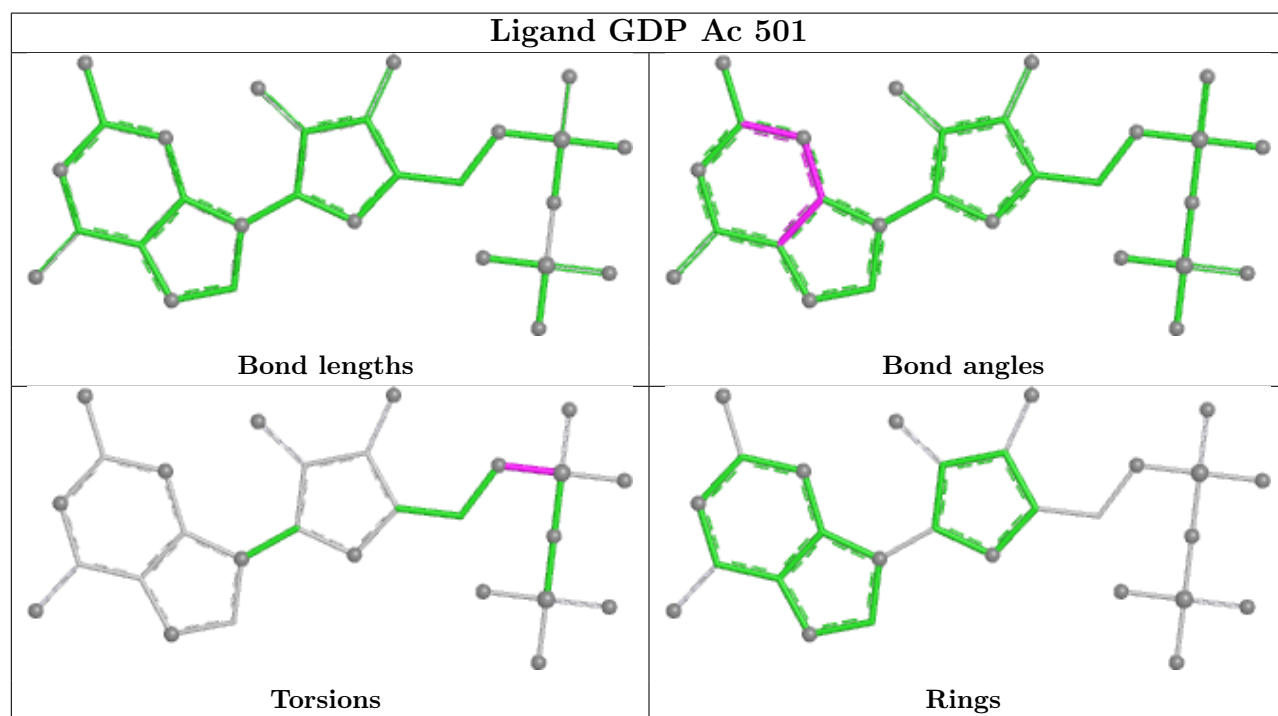
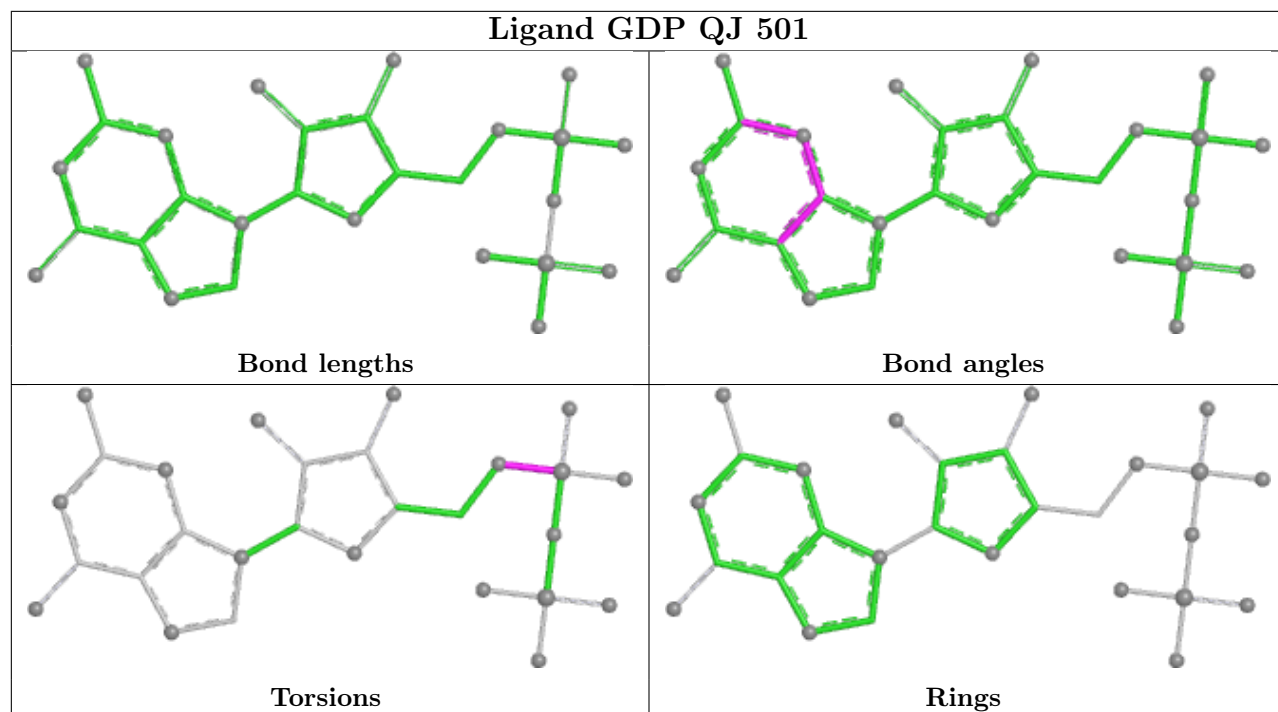
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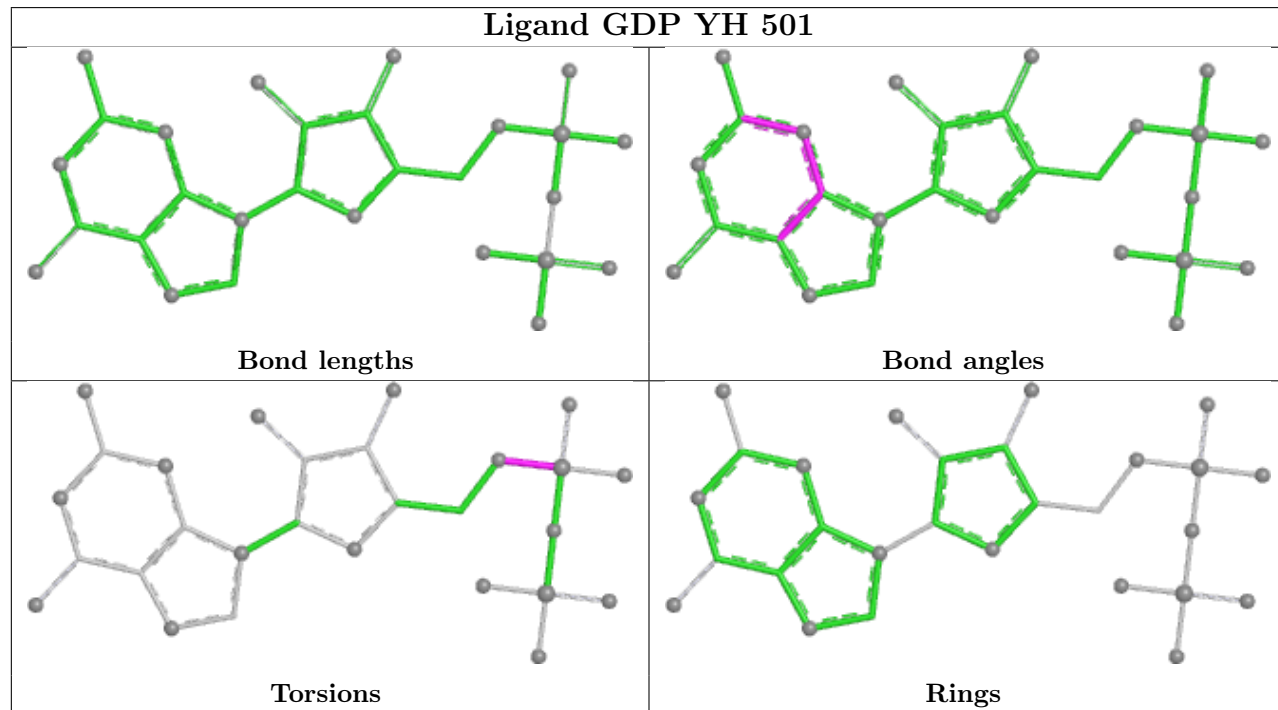
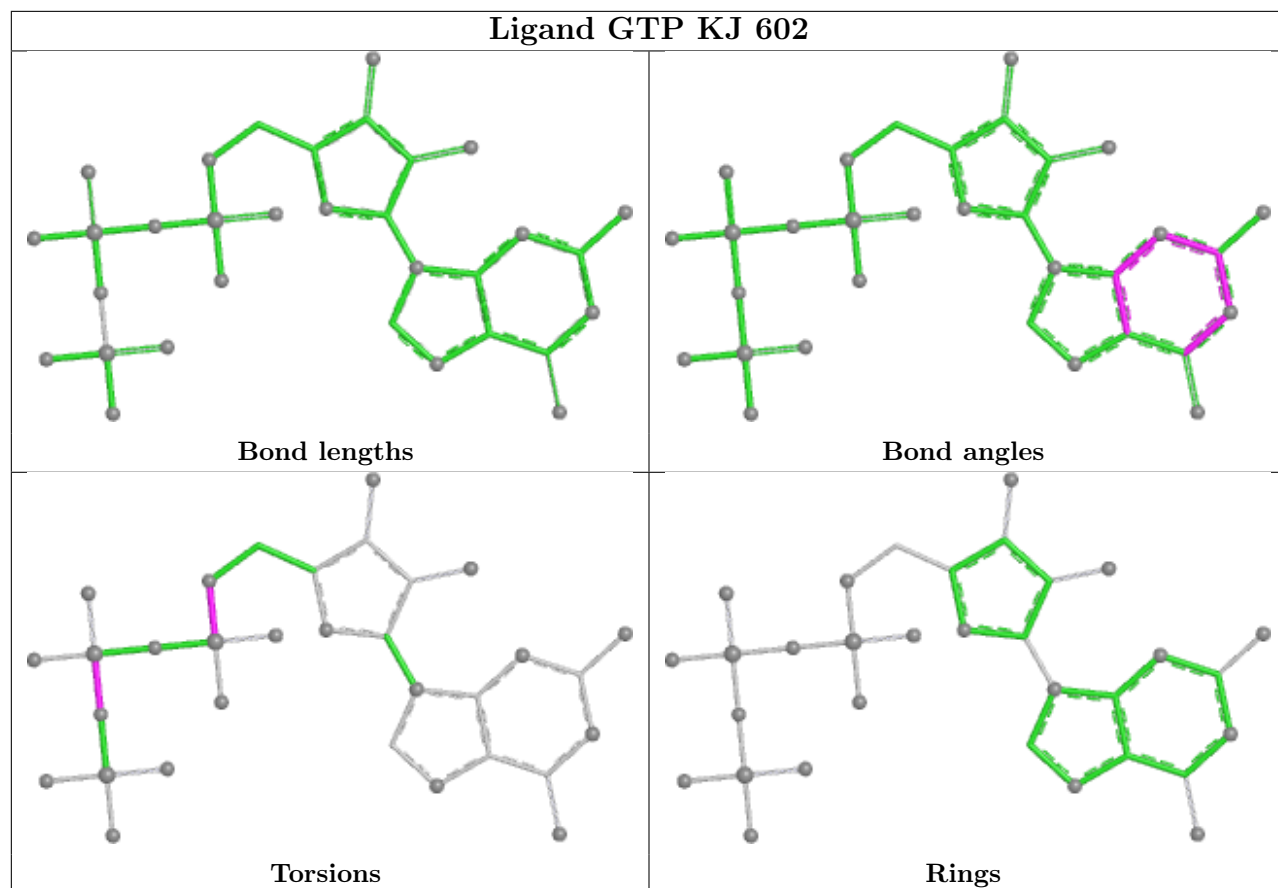


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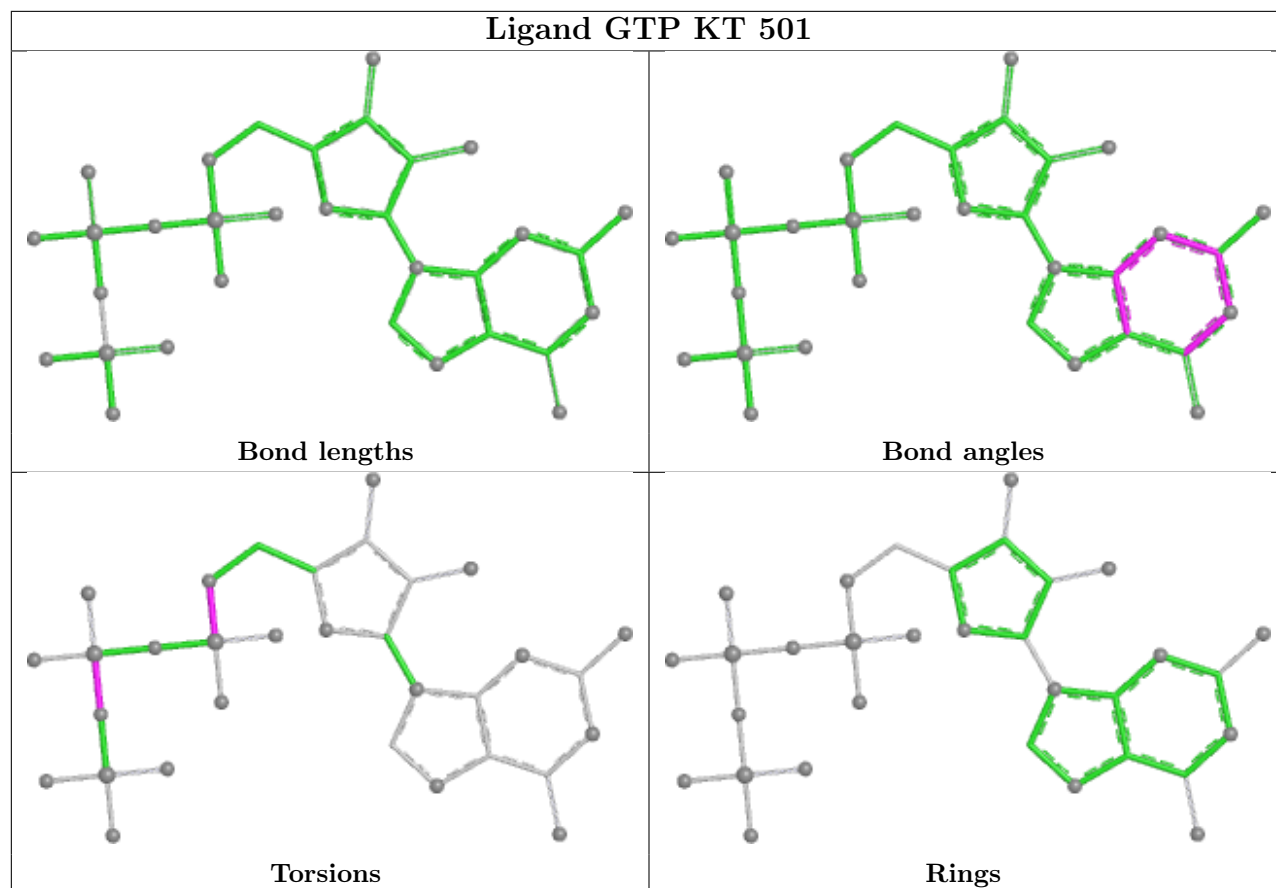




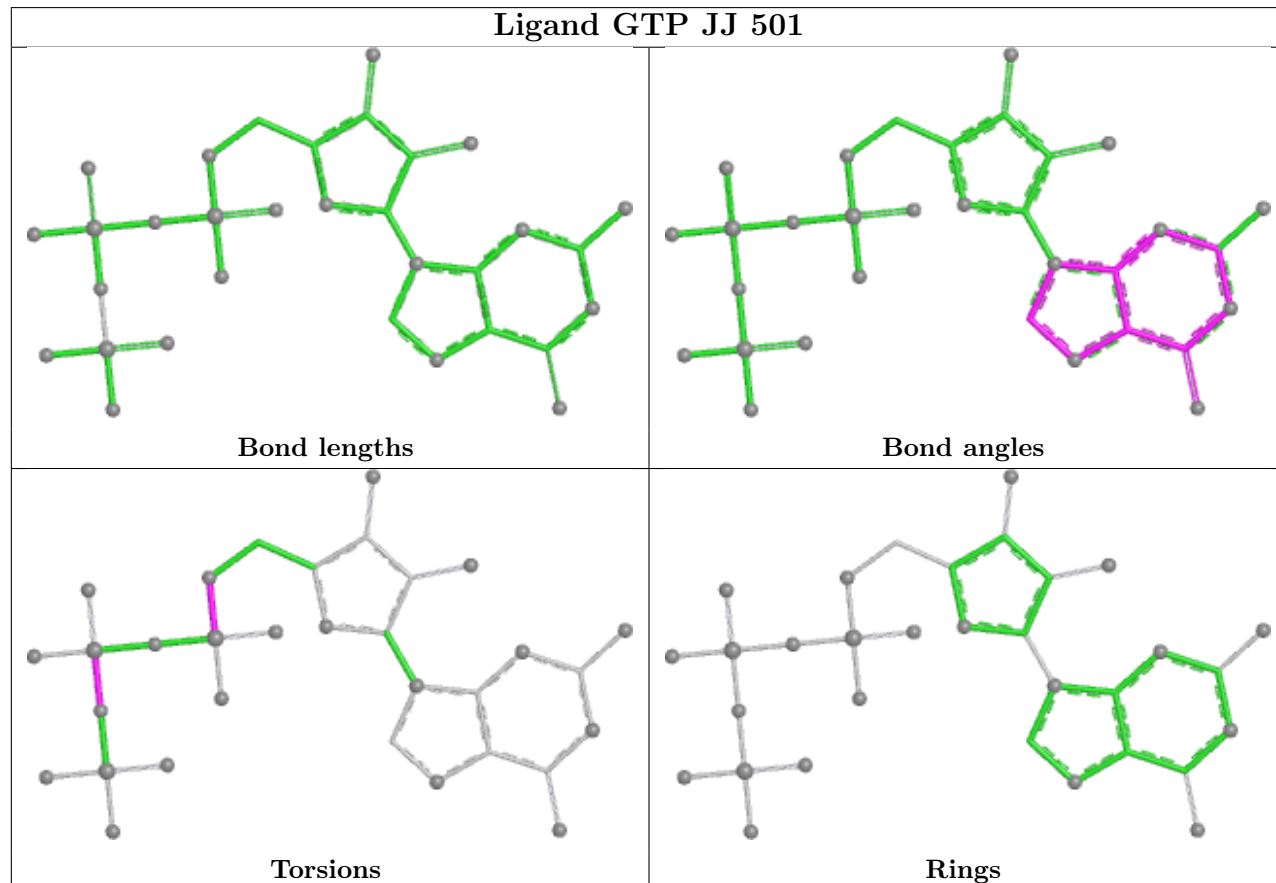




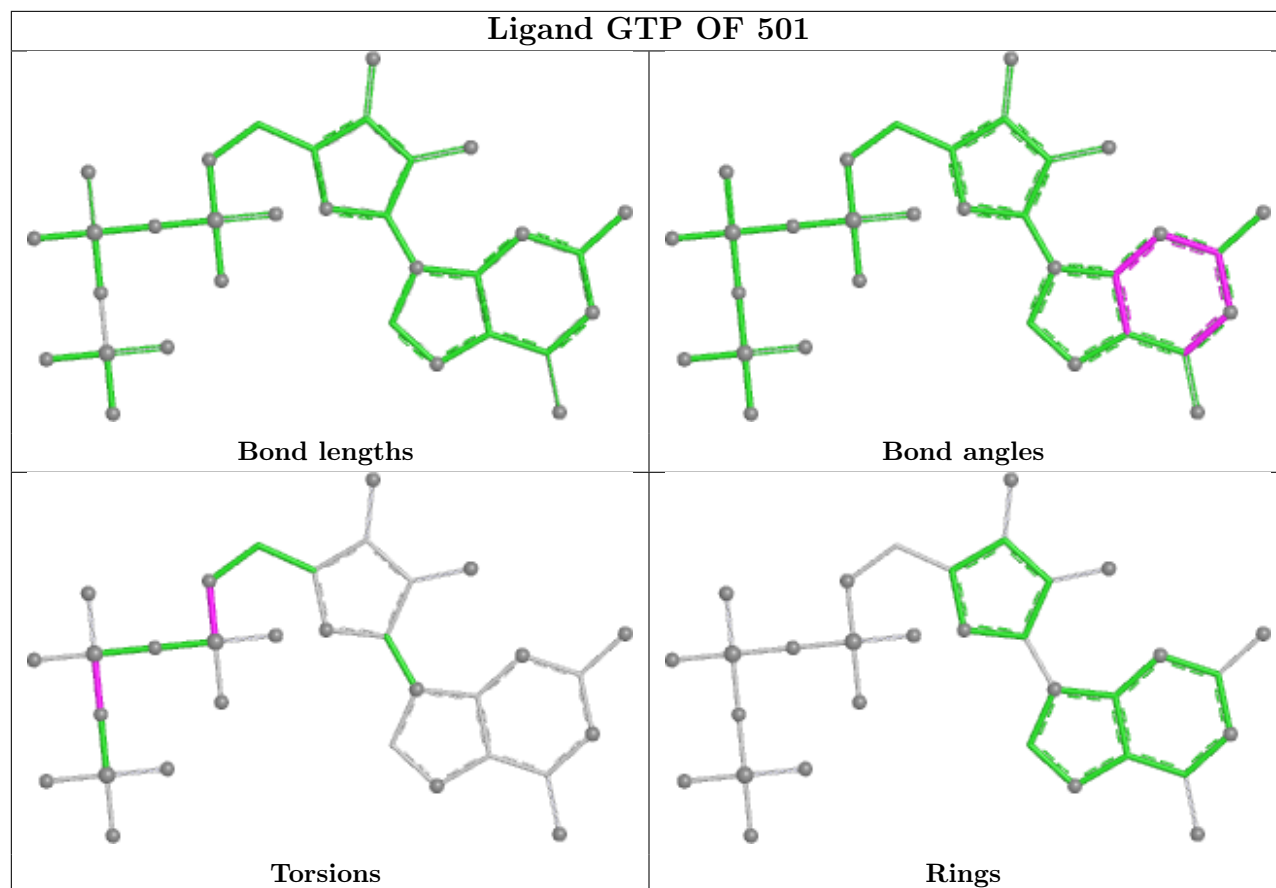
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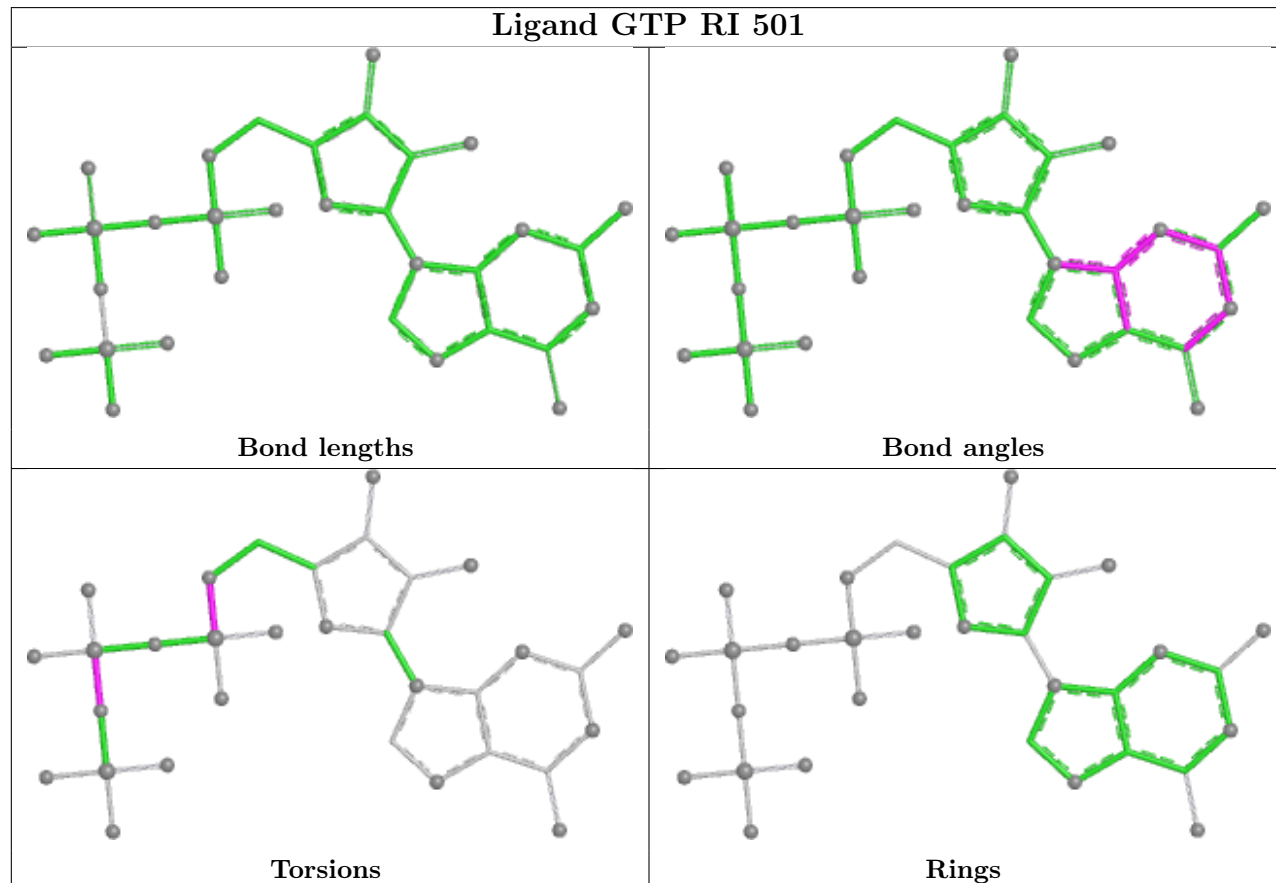
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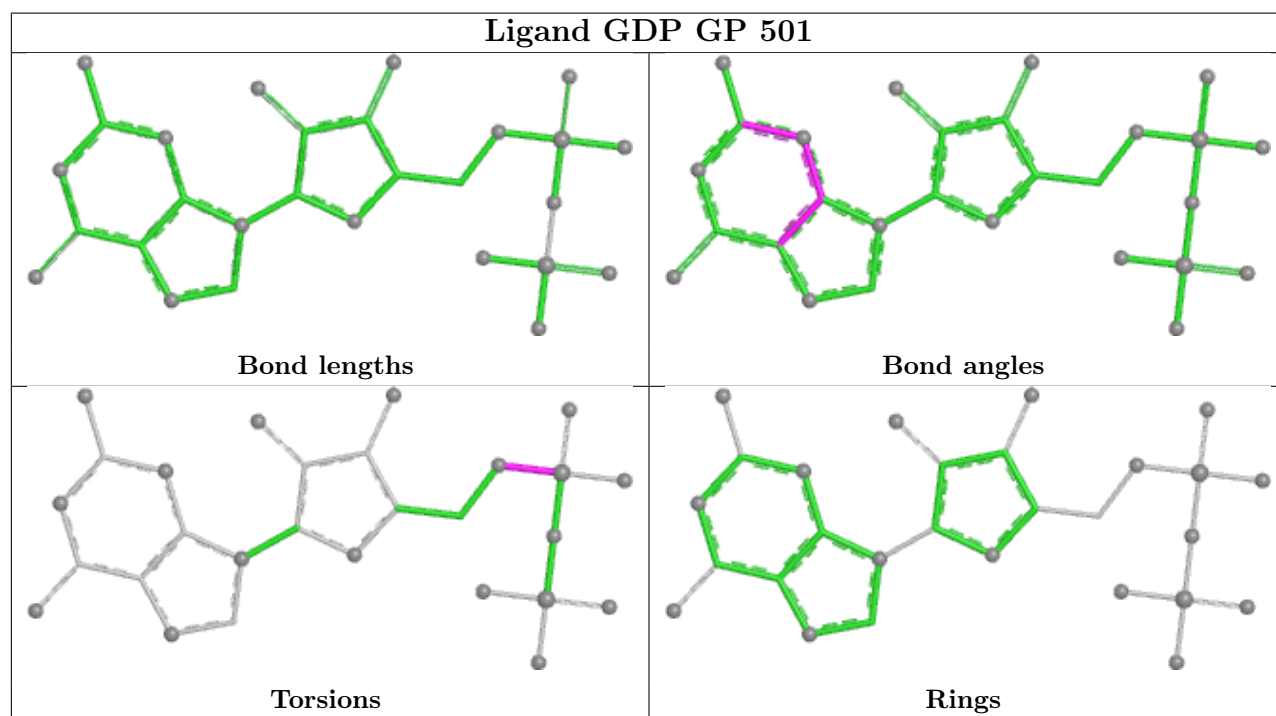
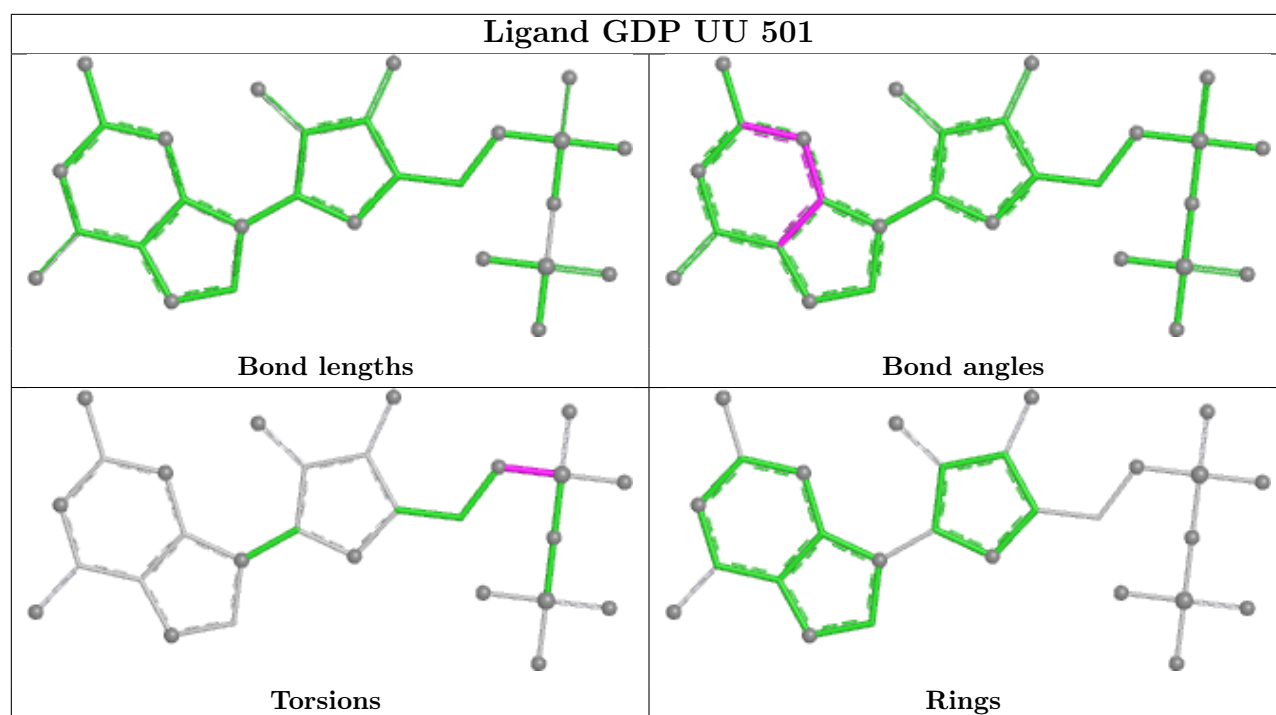


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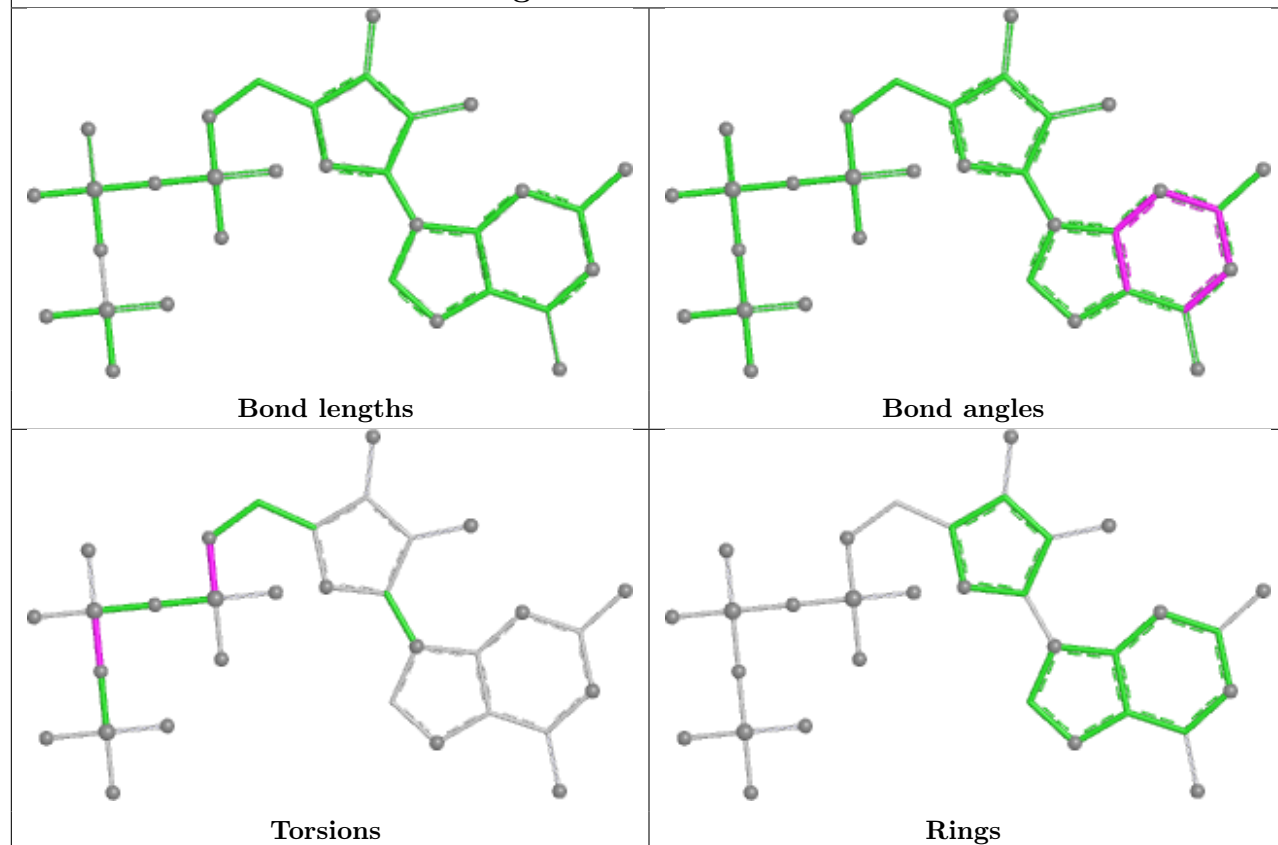


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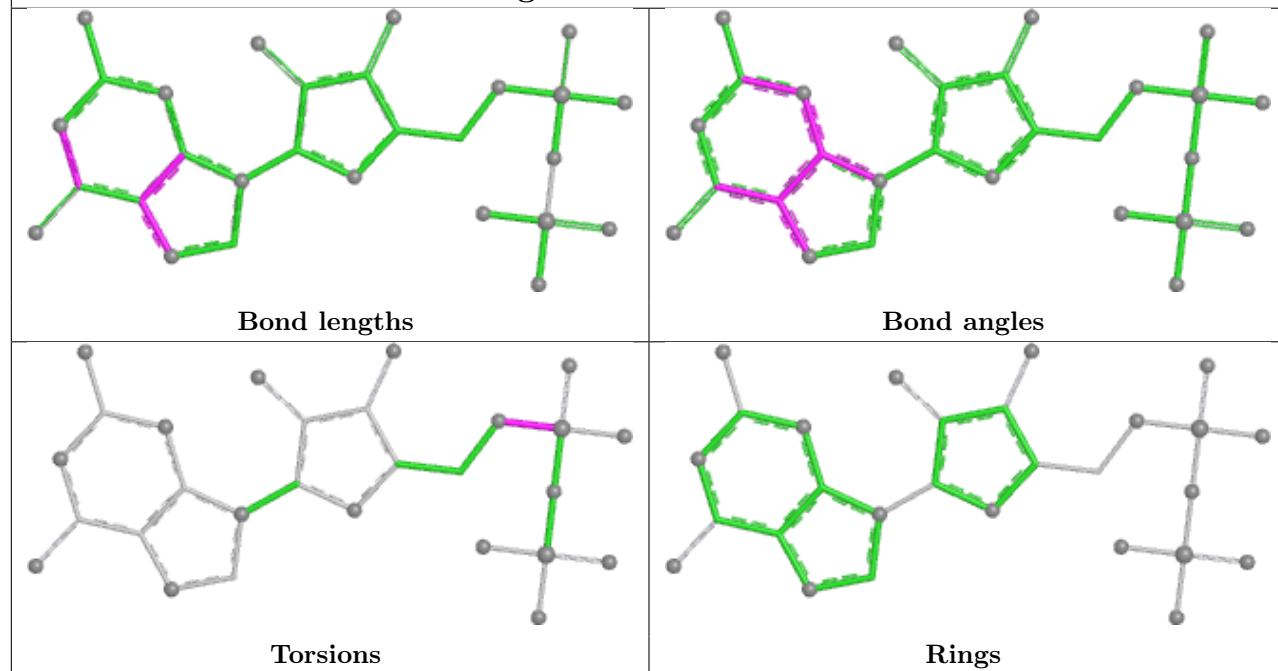


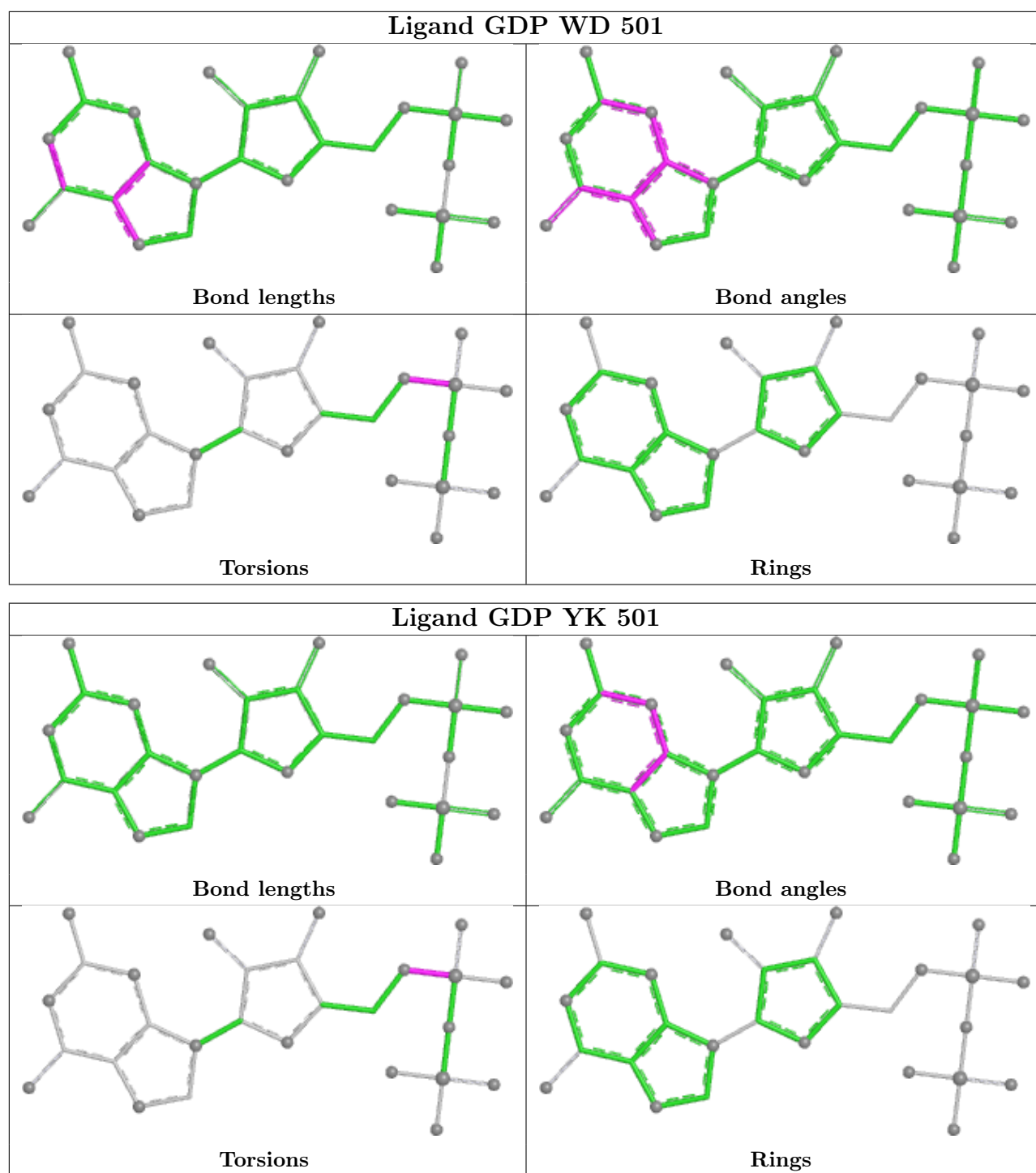


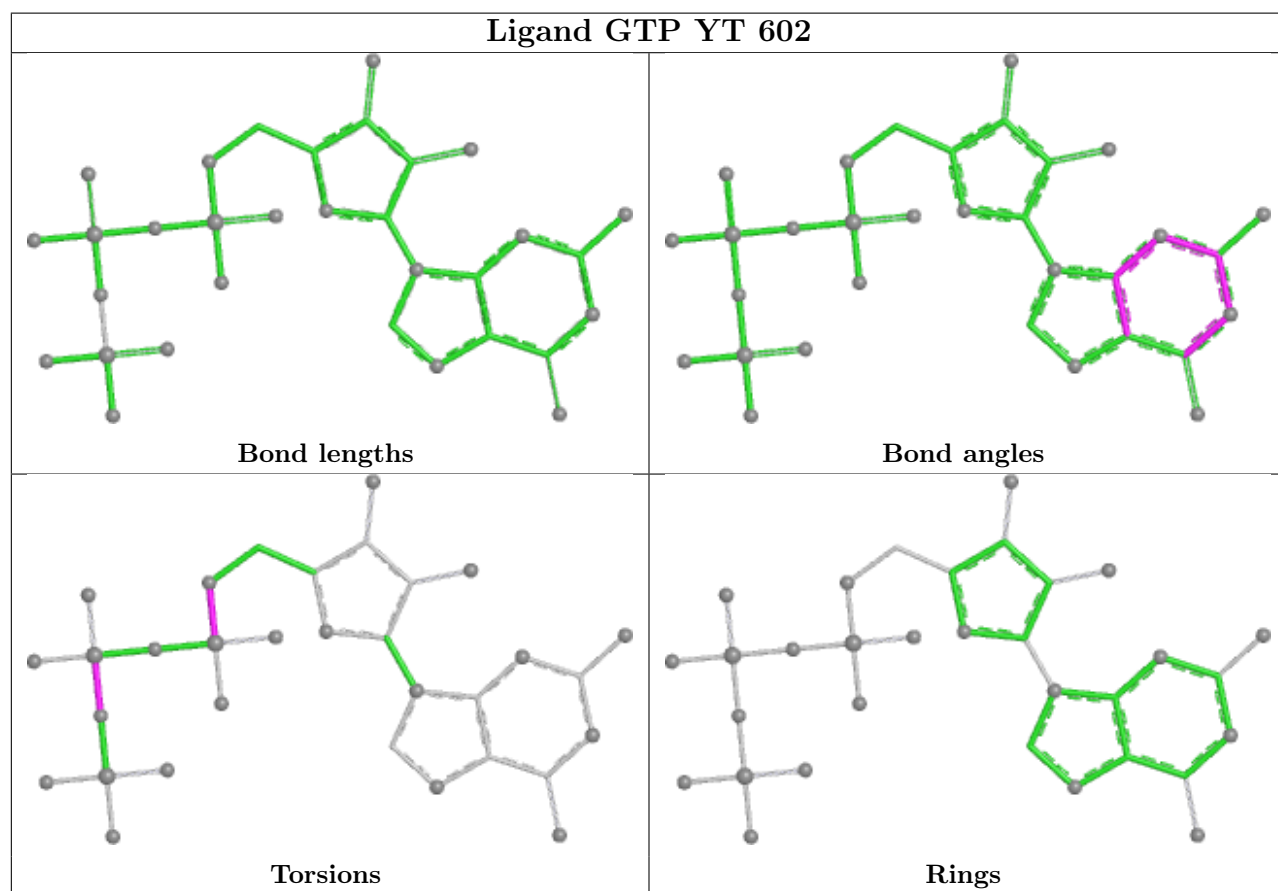
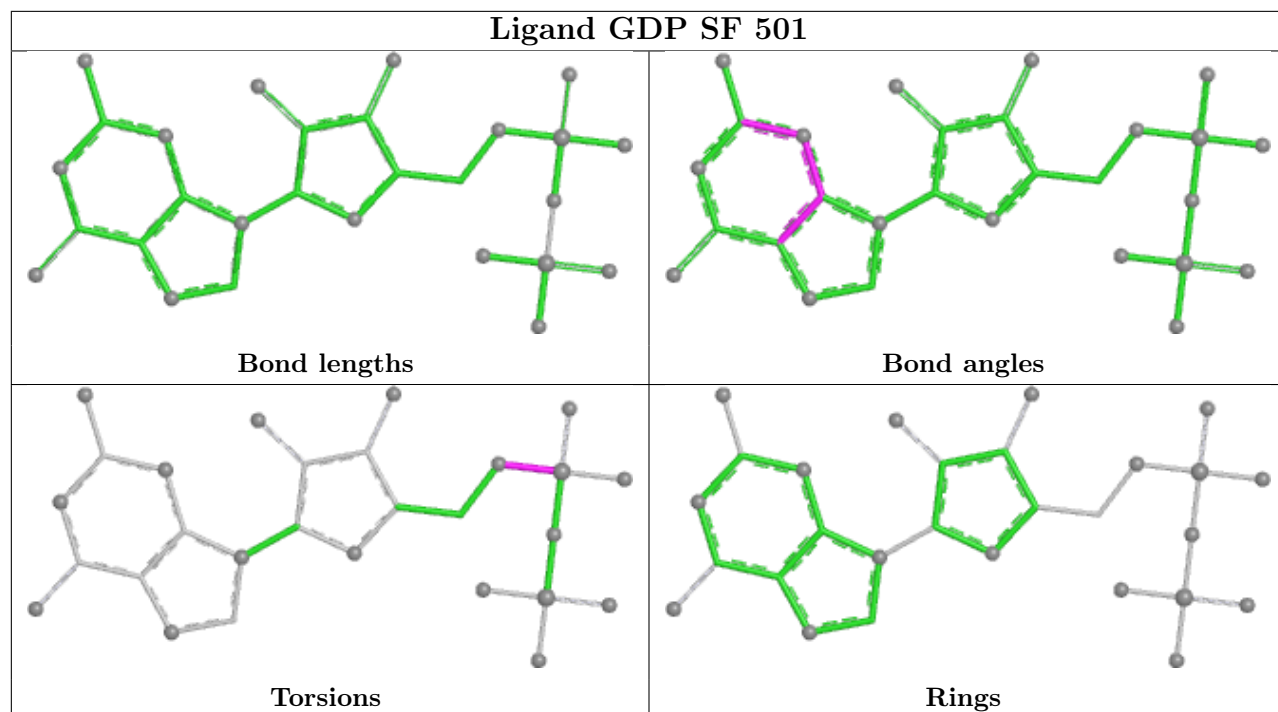
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## Ligand GDP FX 501

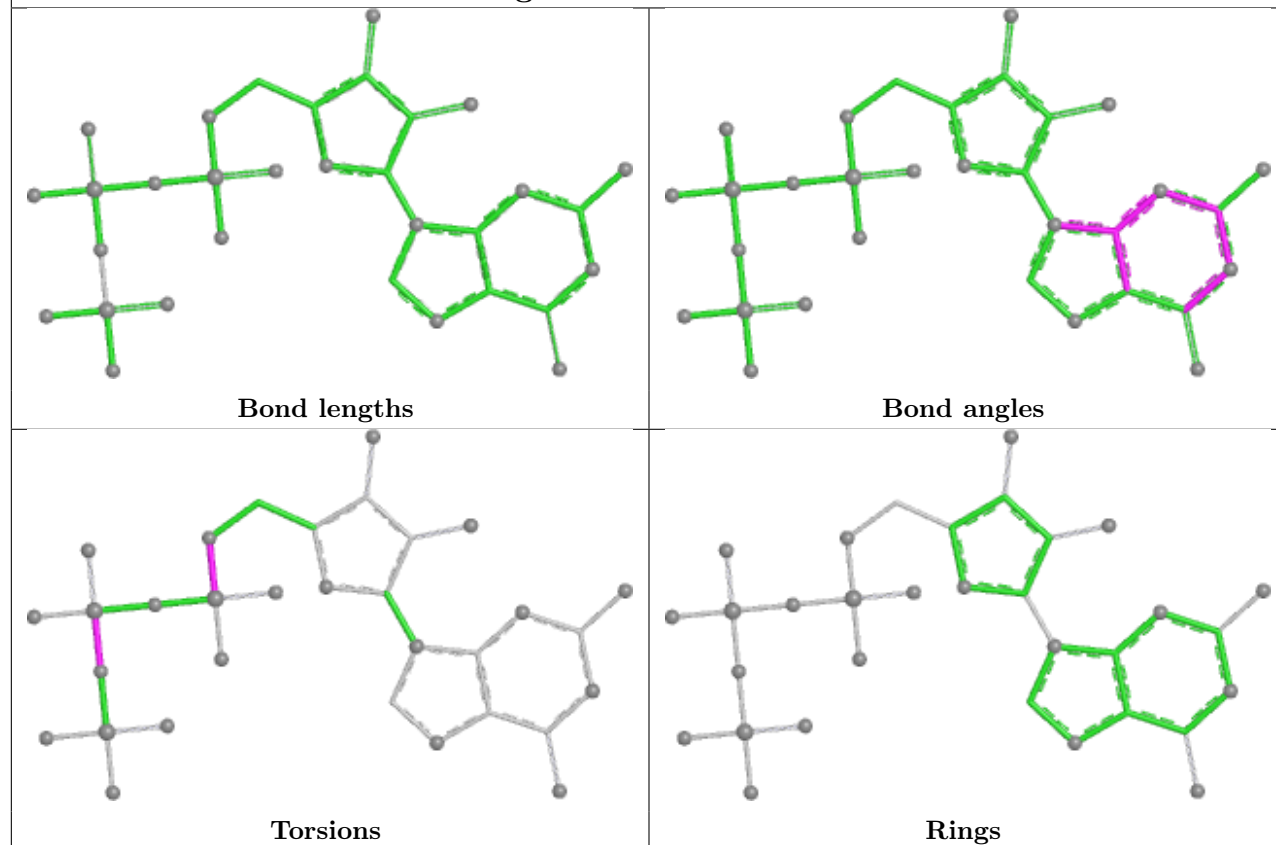




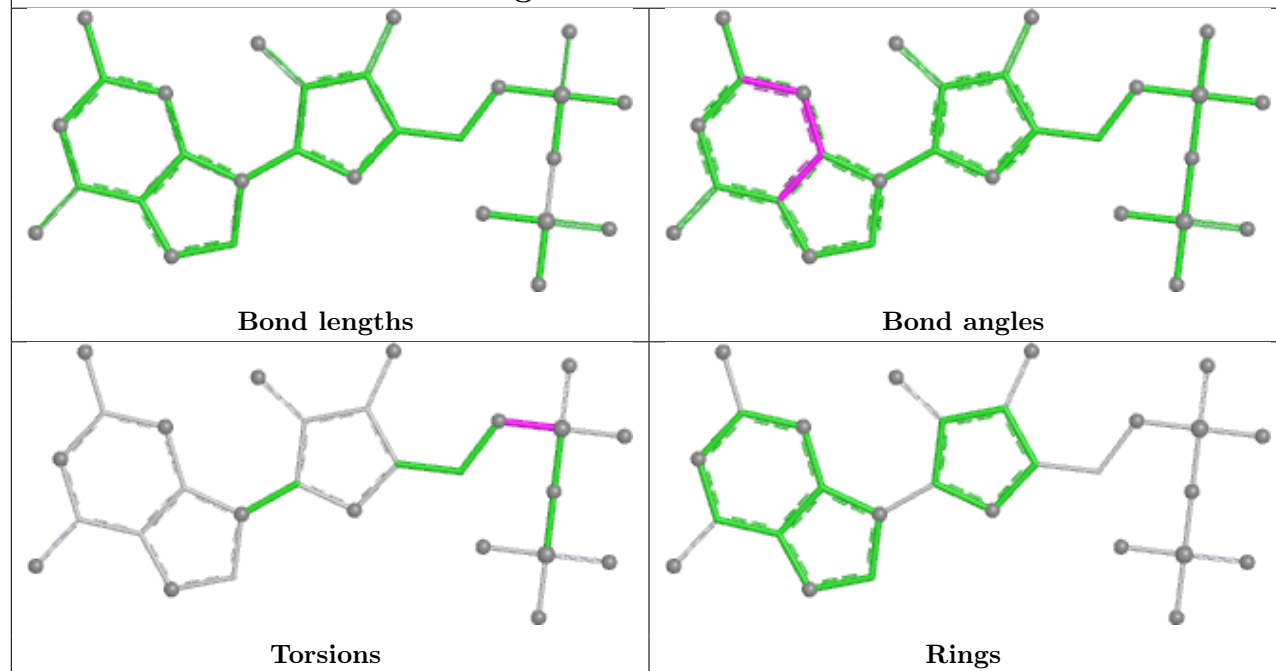


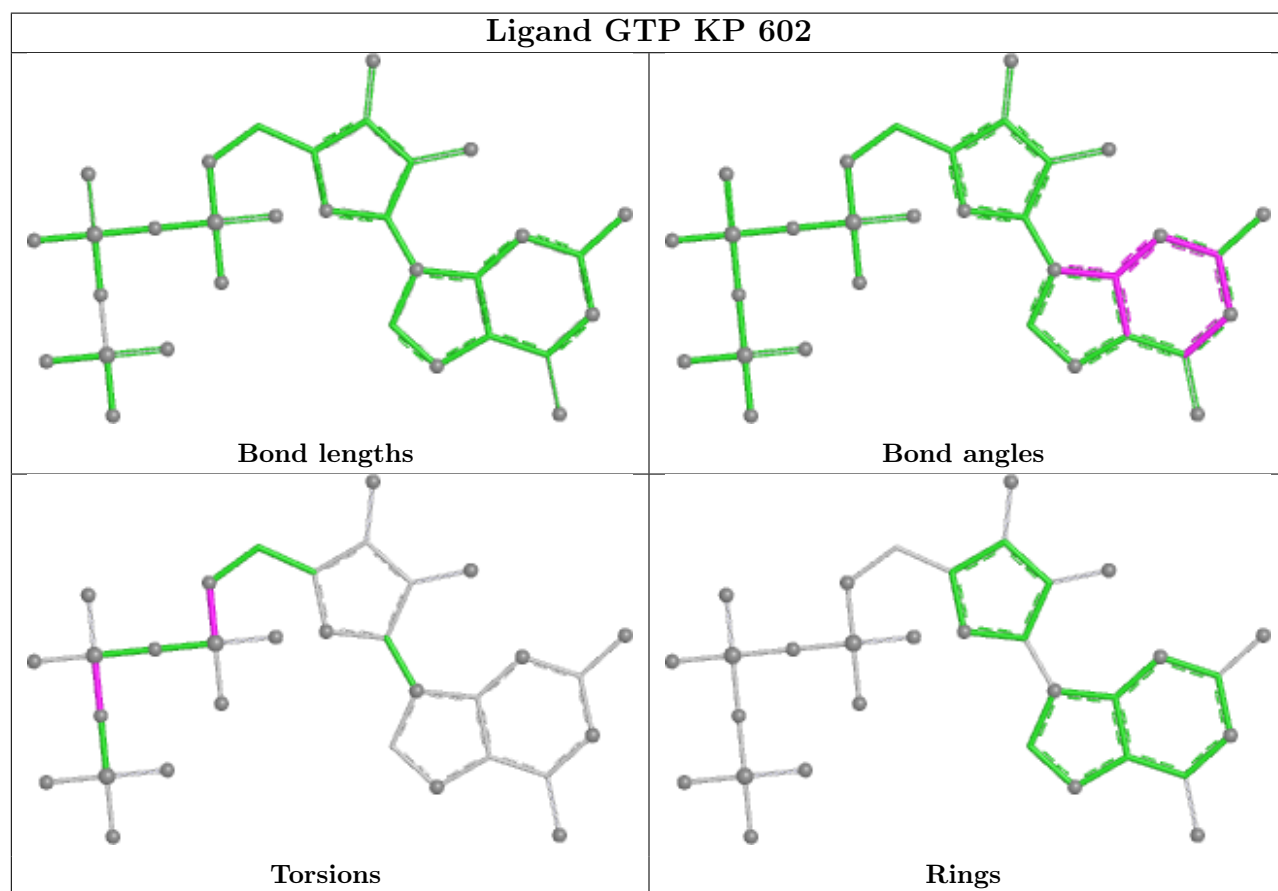
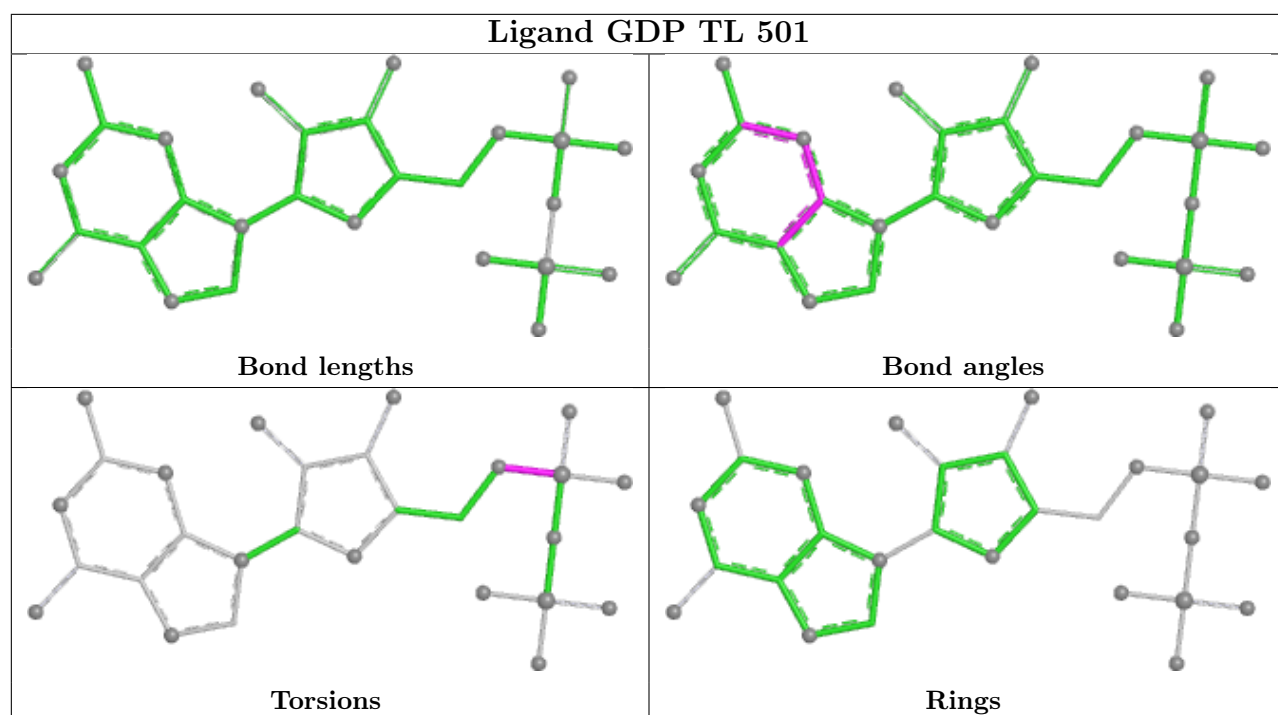


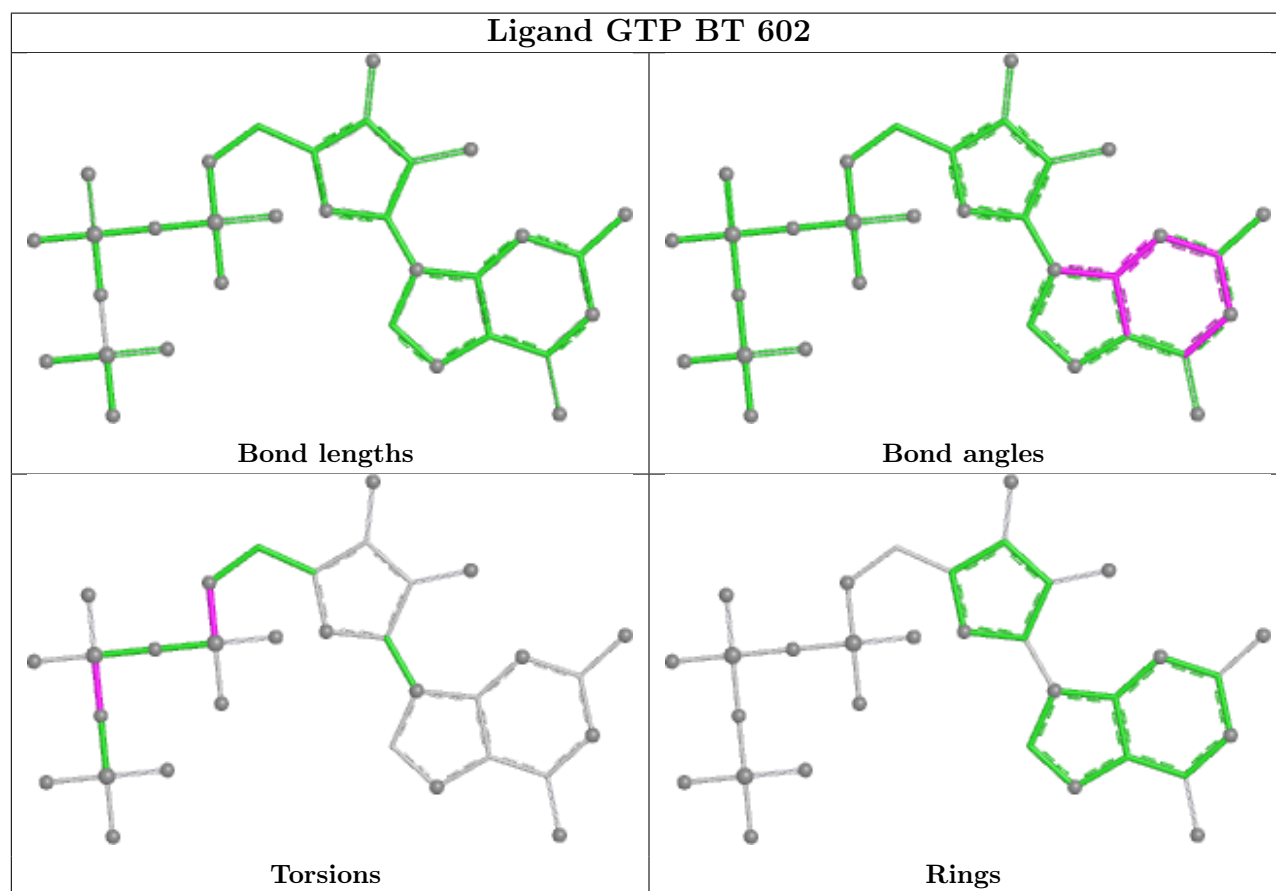
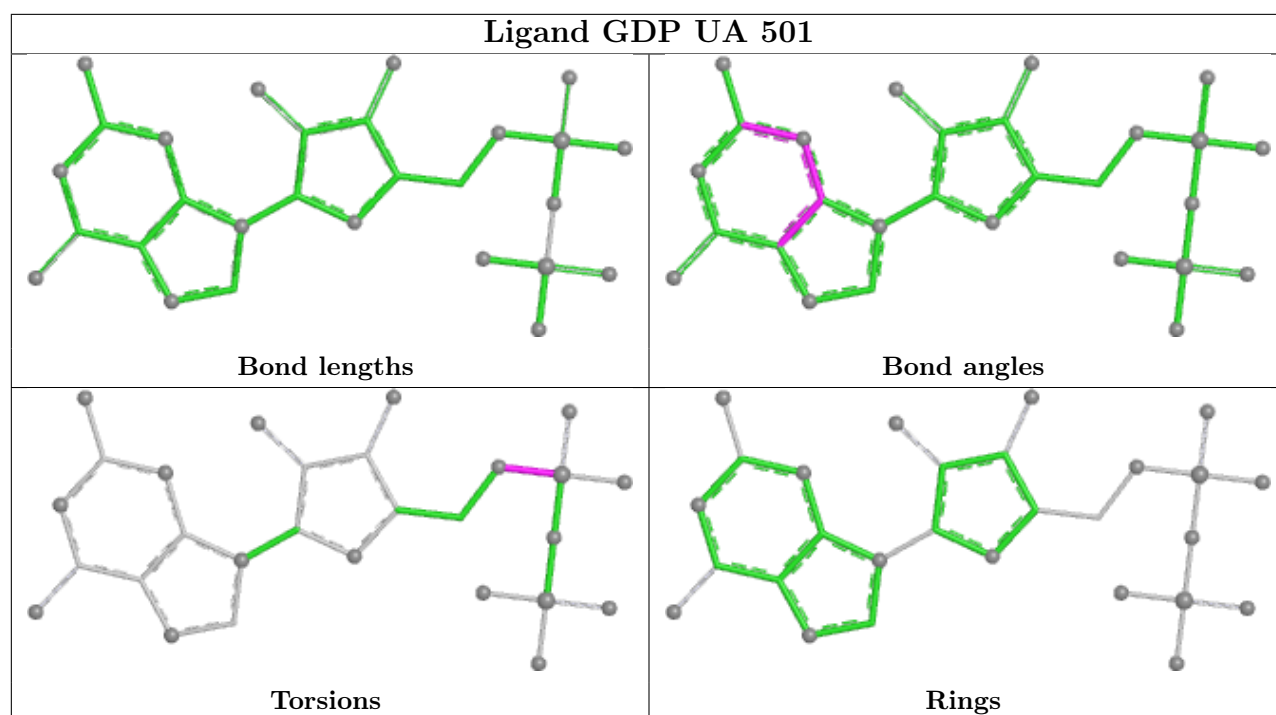
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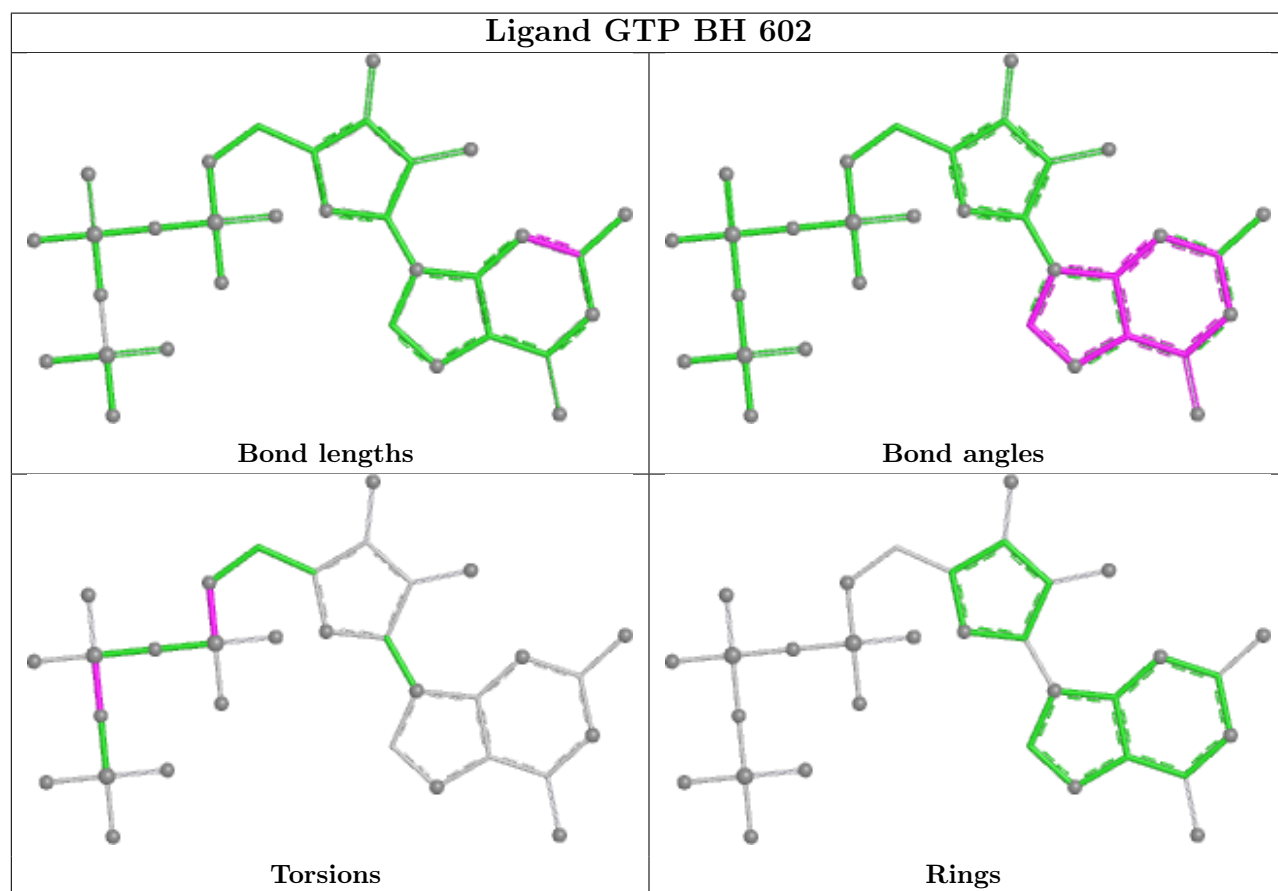
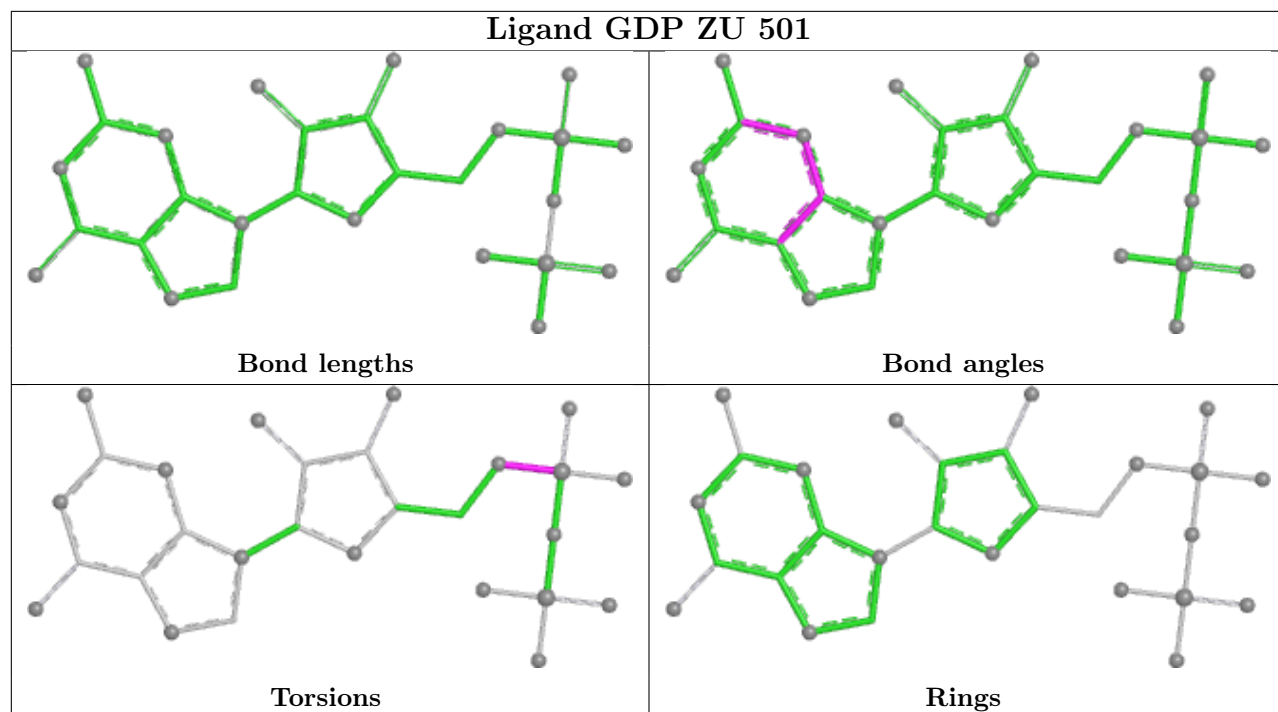


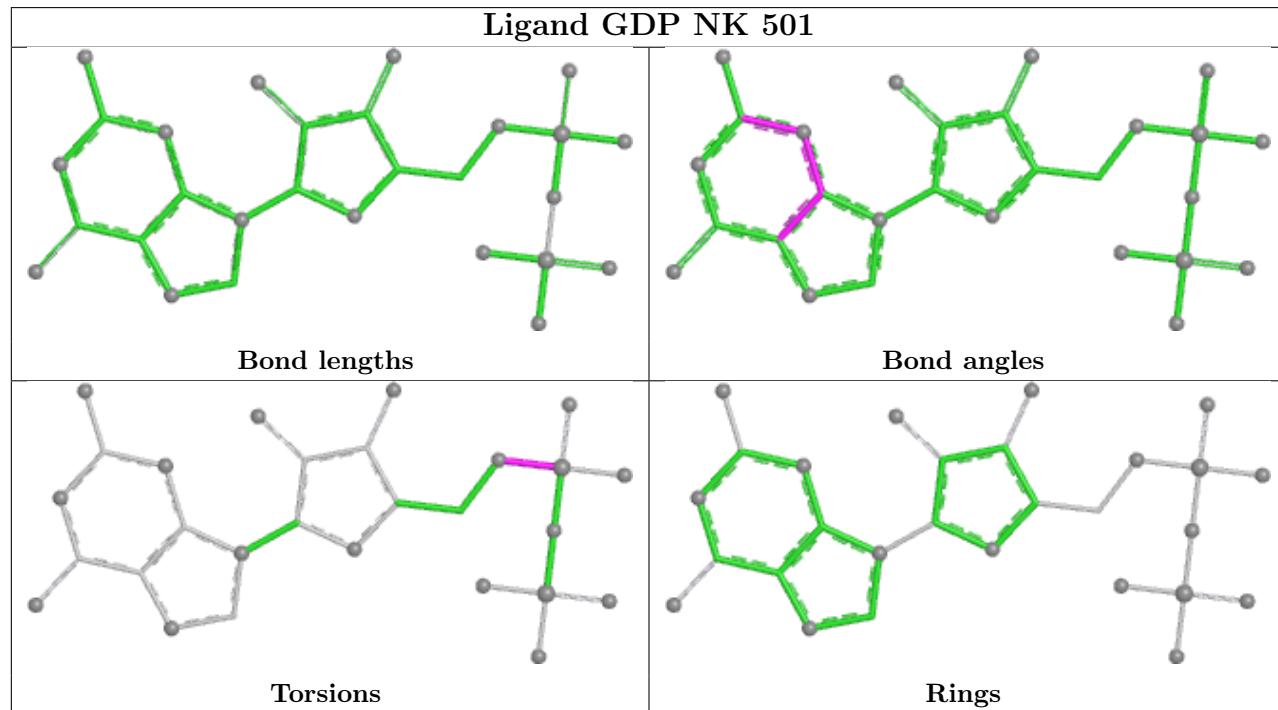
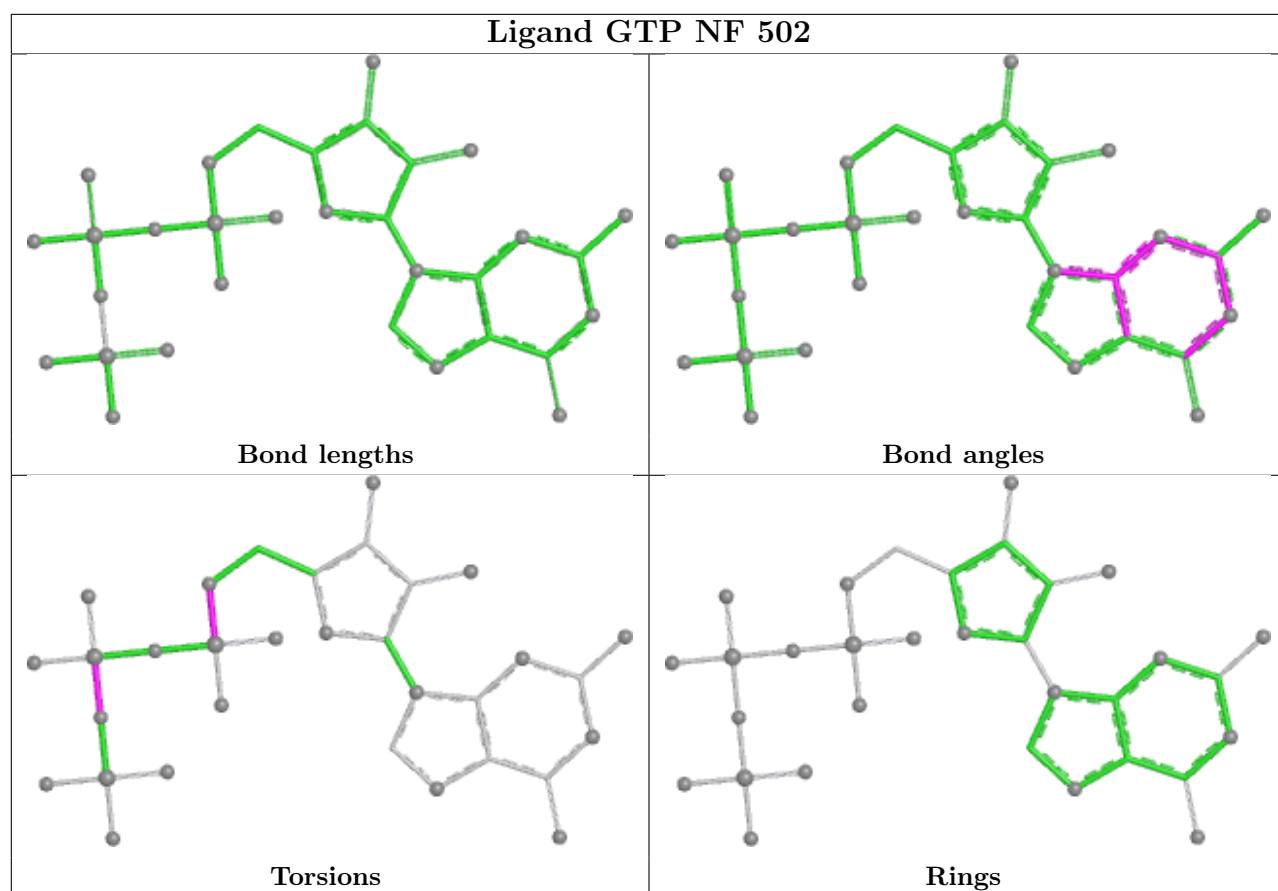
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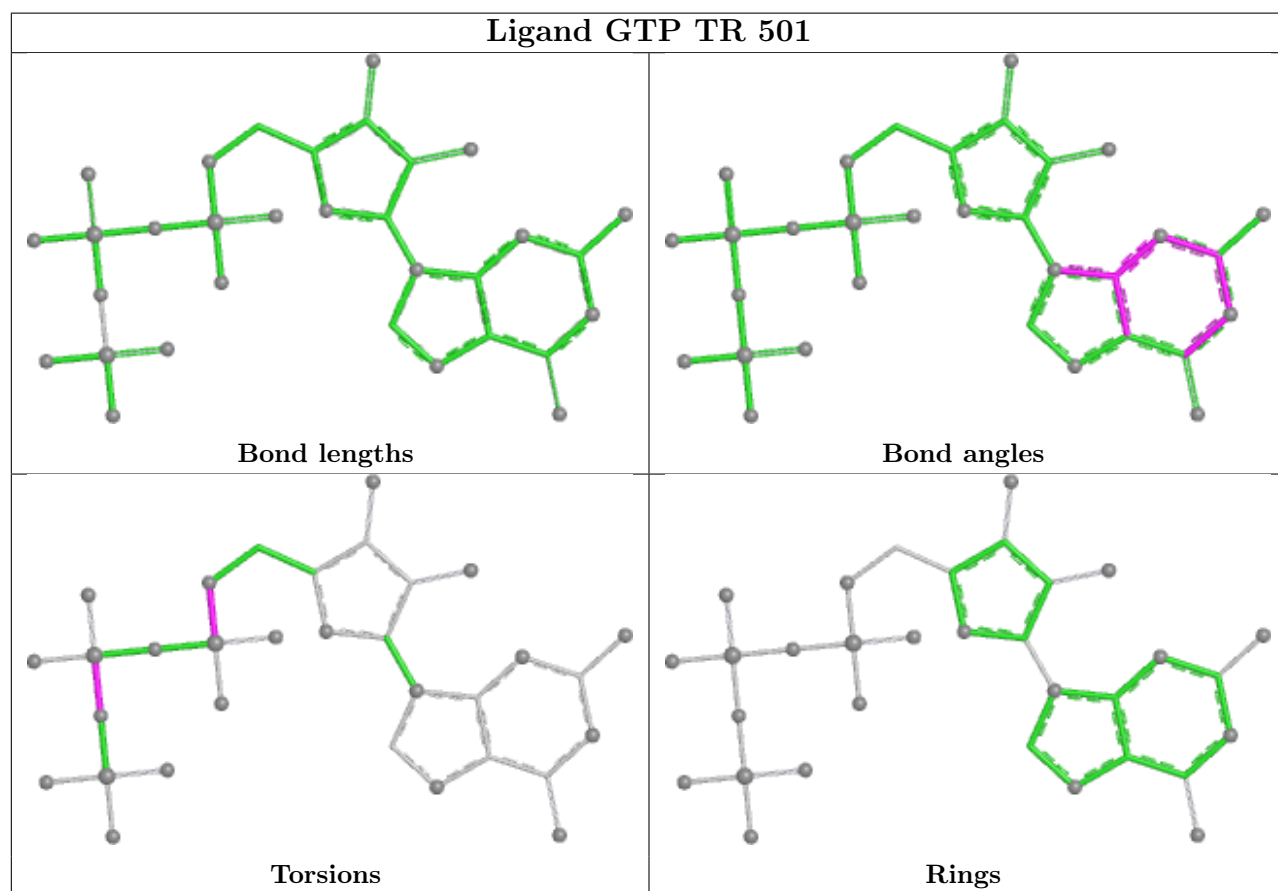
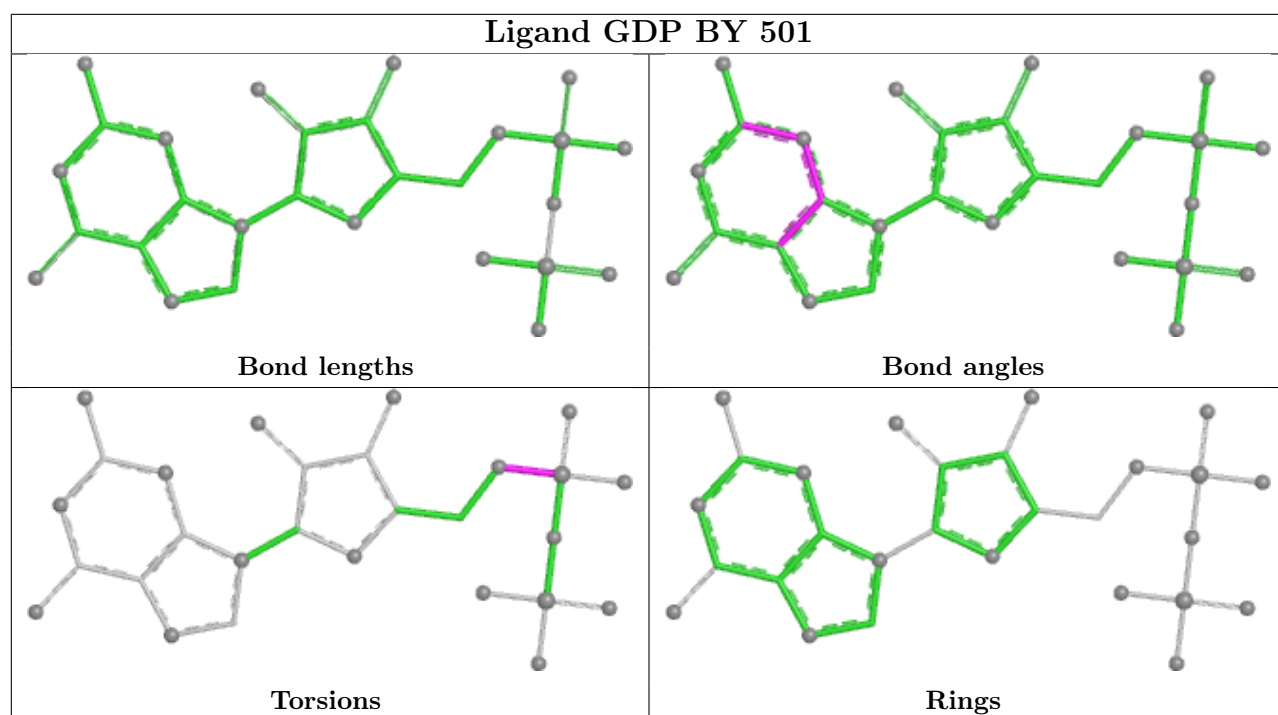


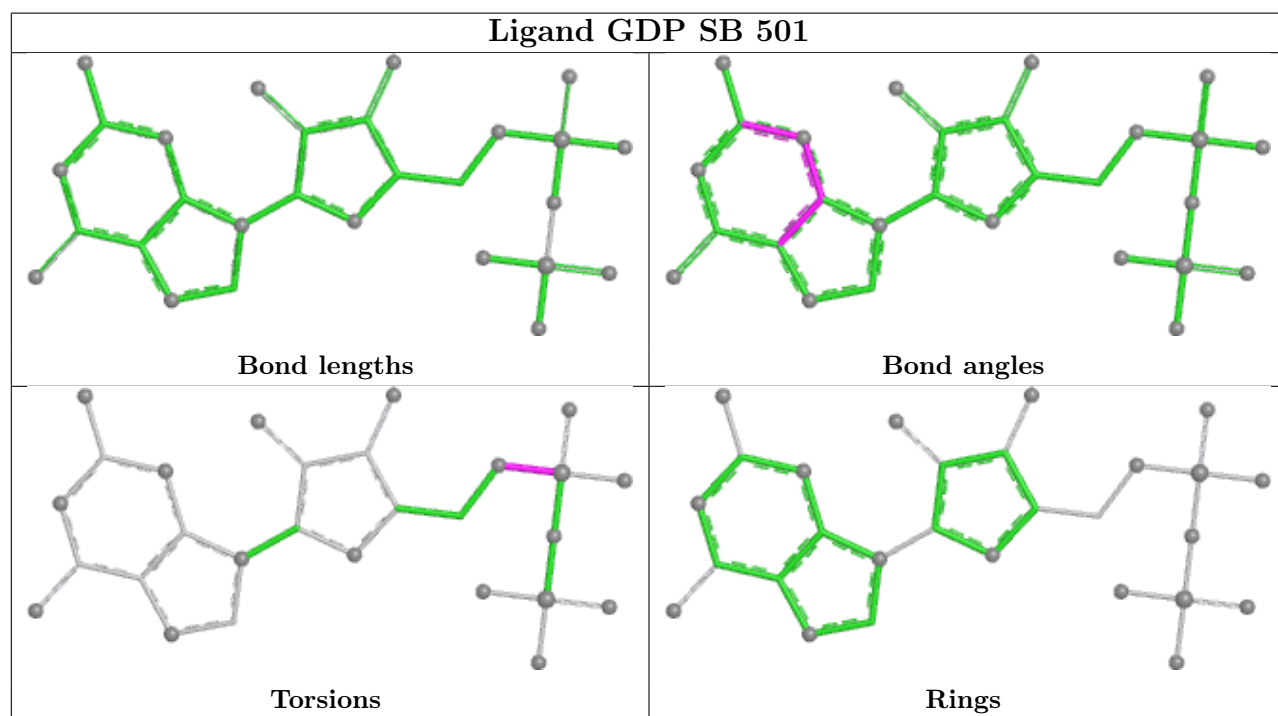
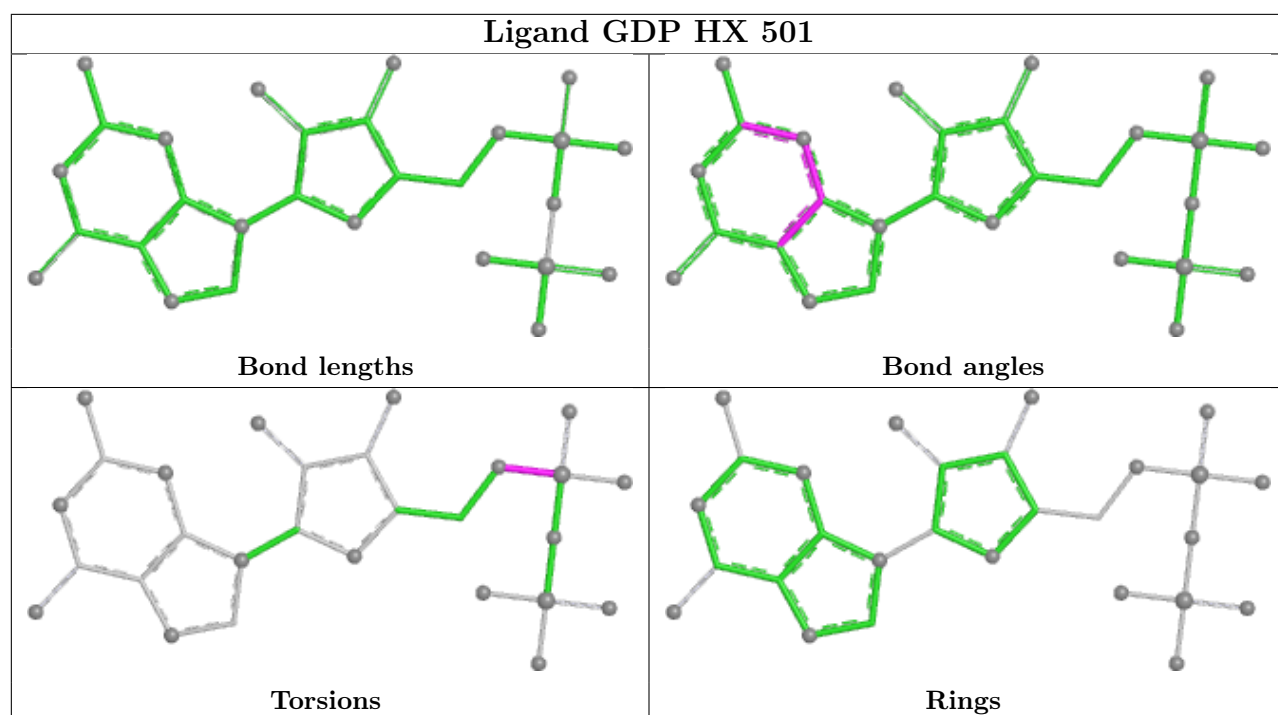


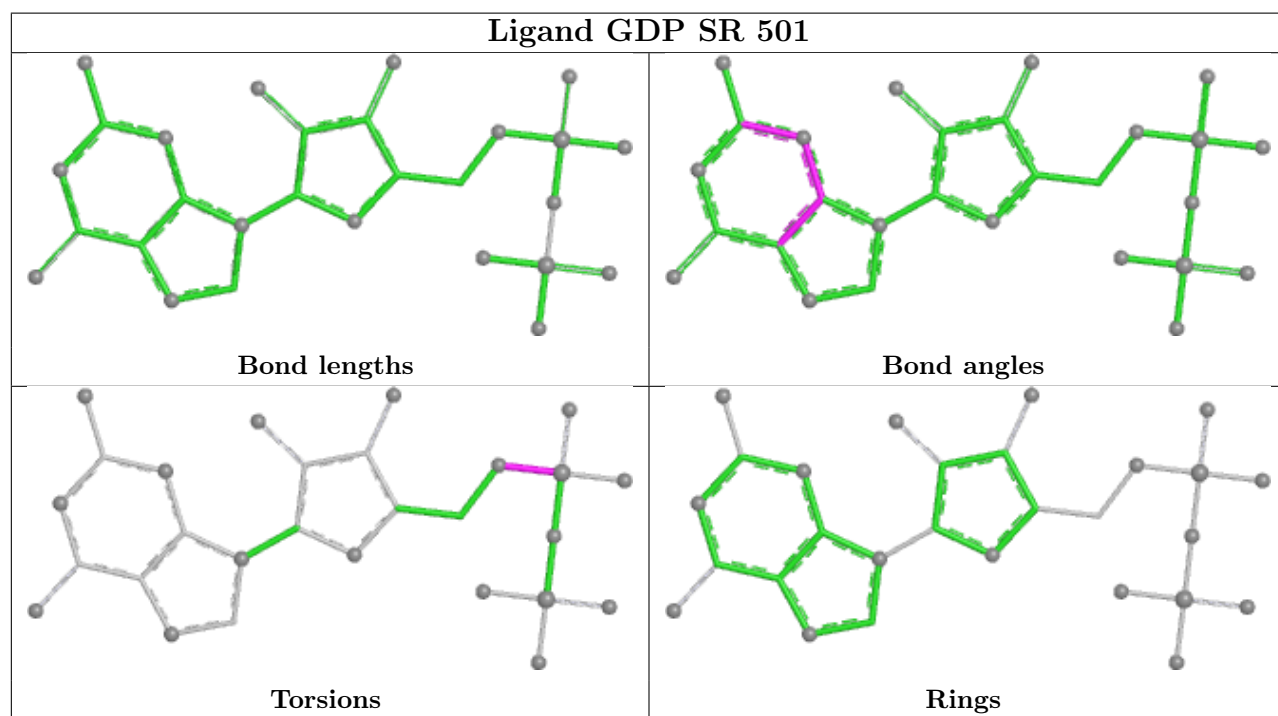
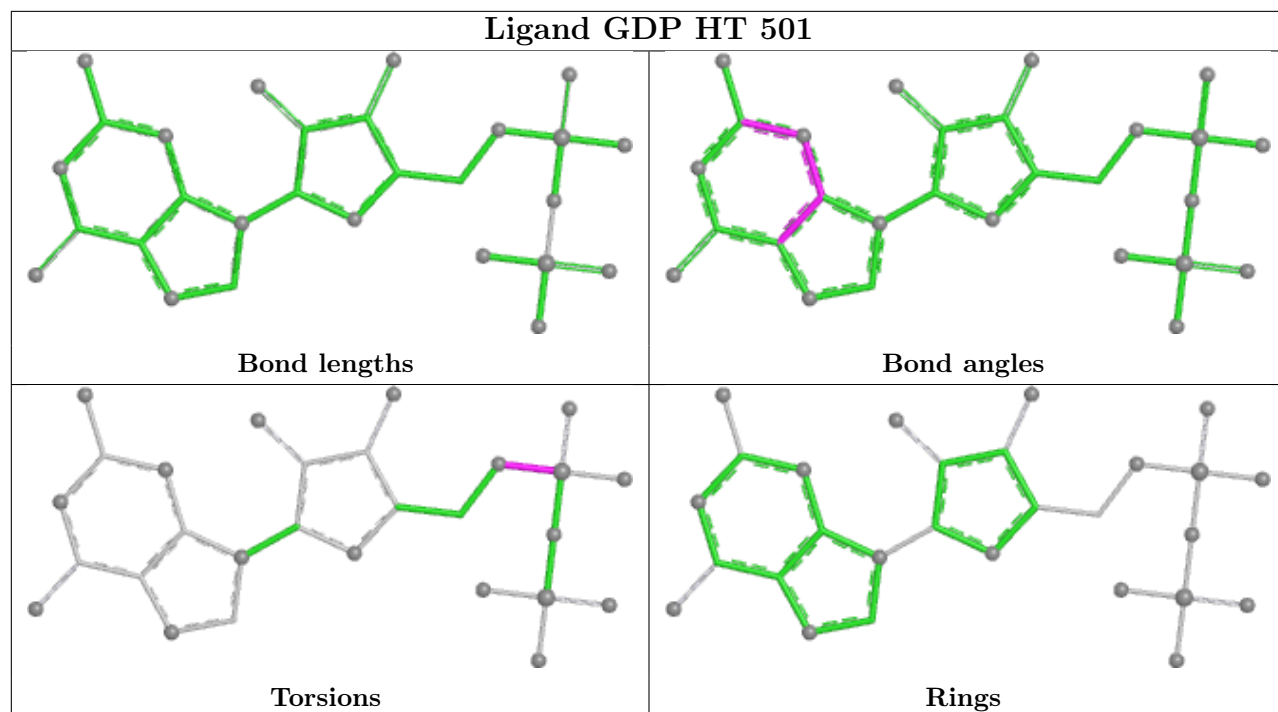






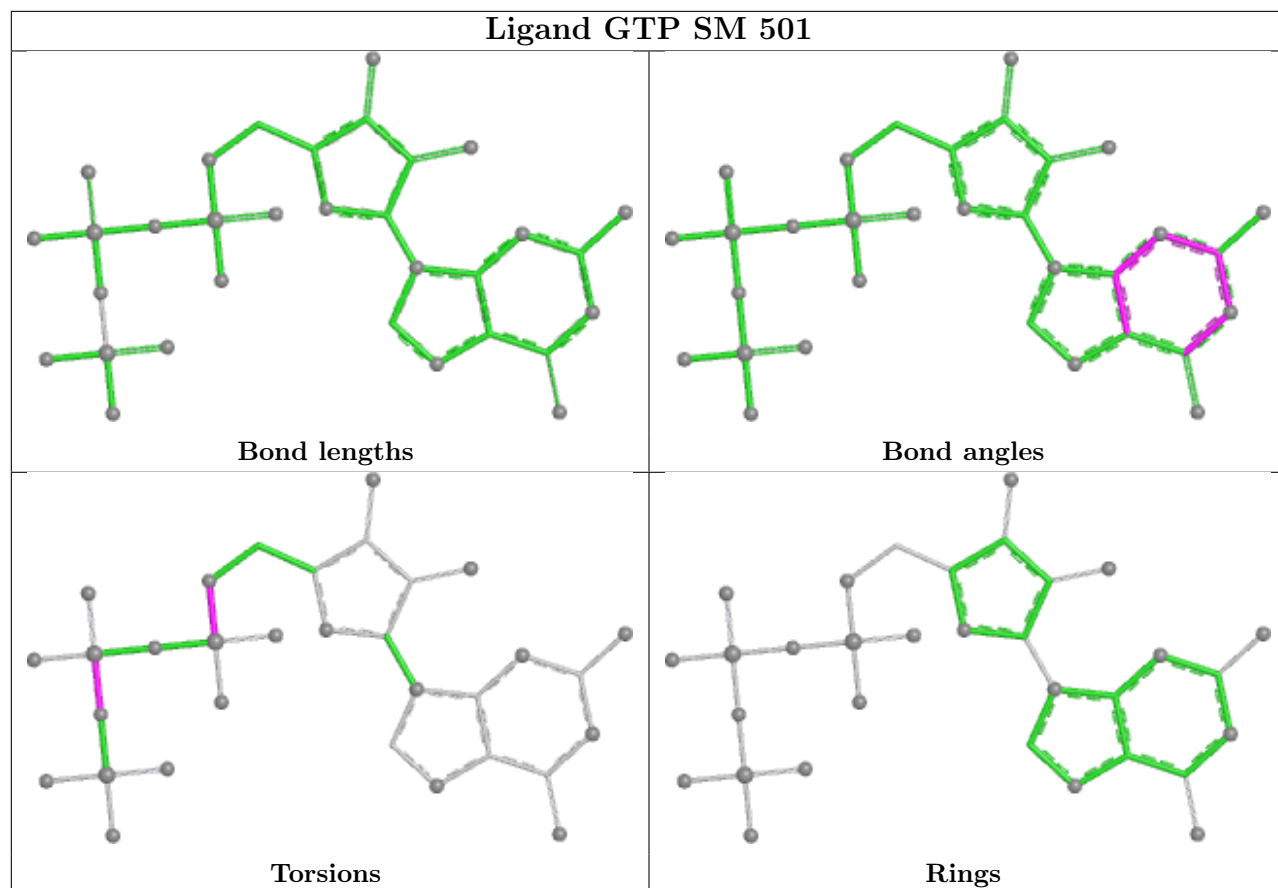




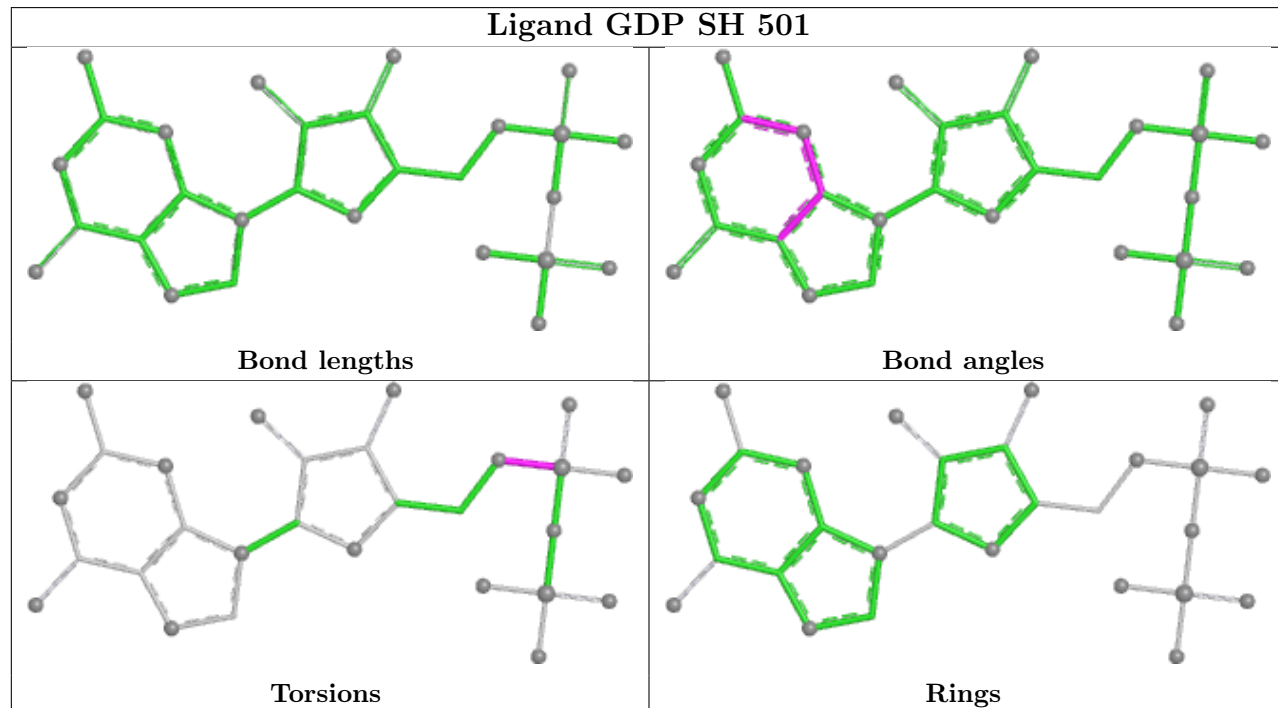


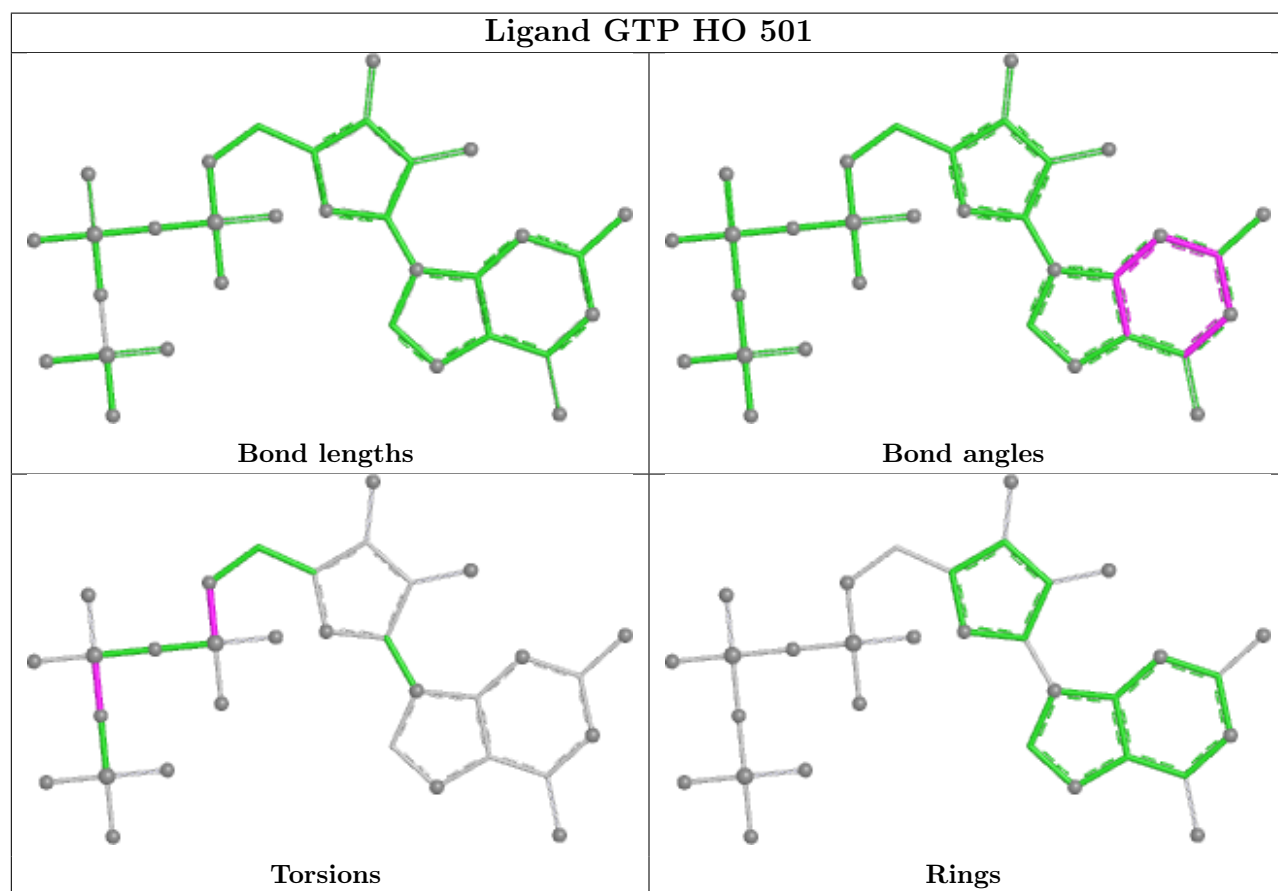
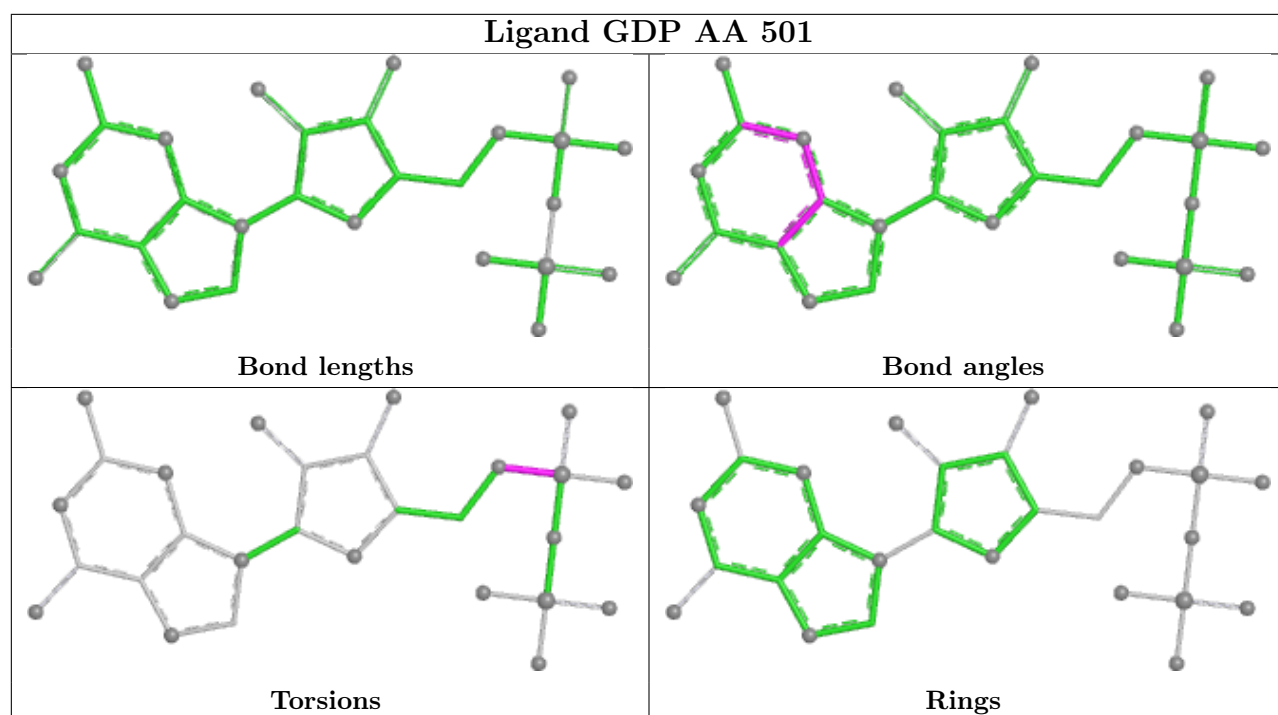


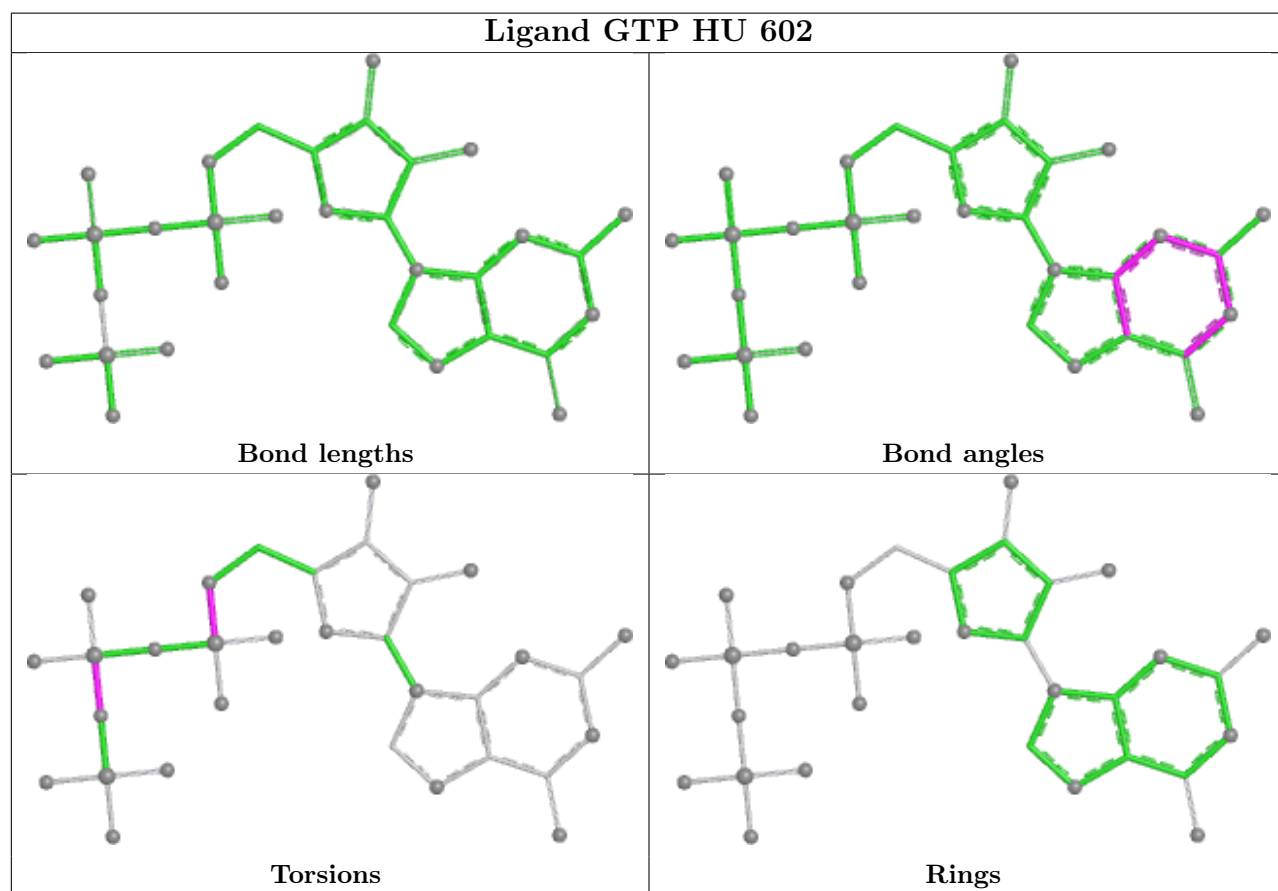
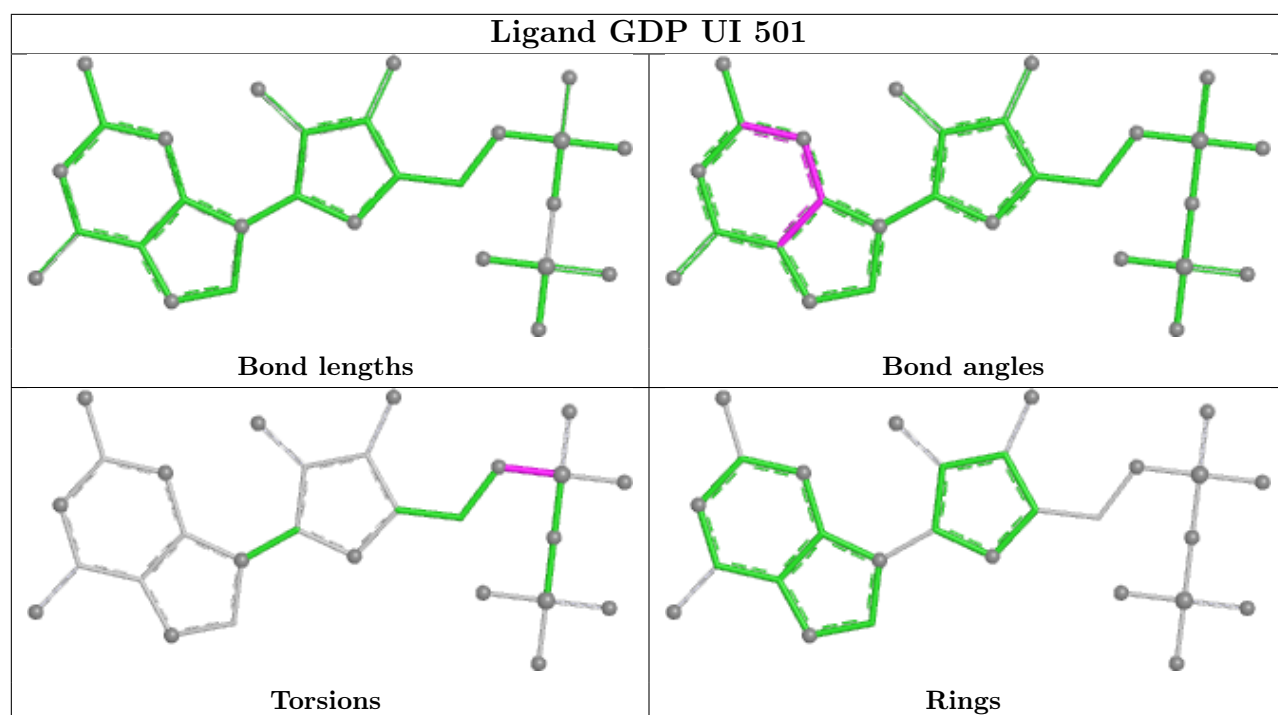
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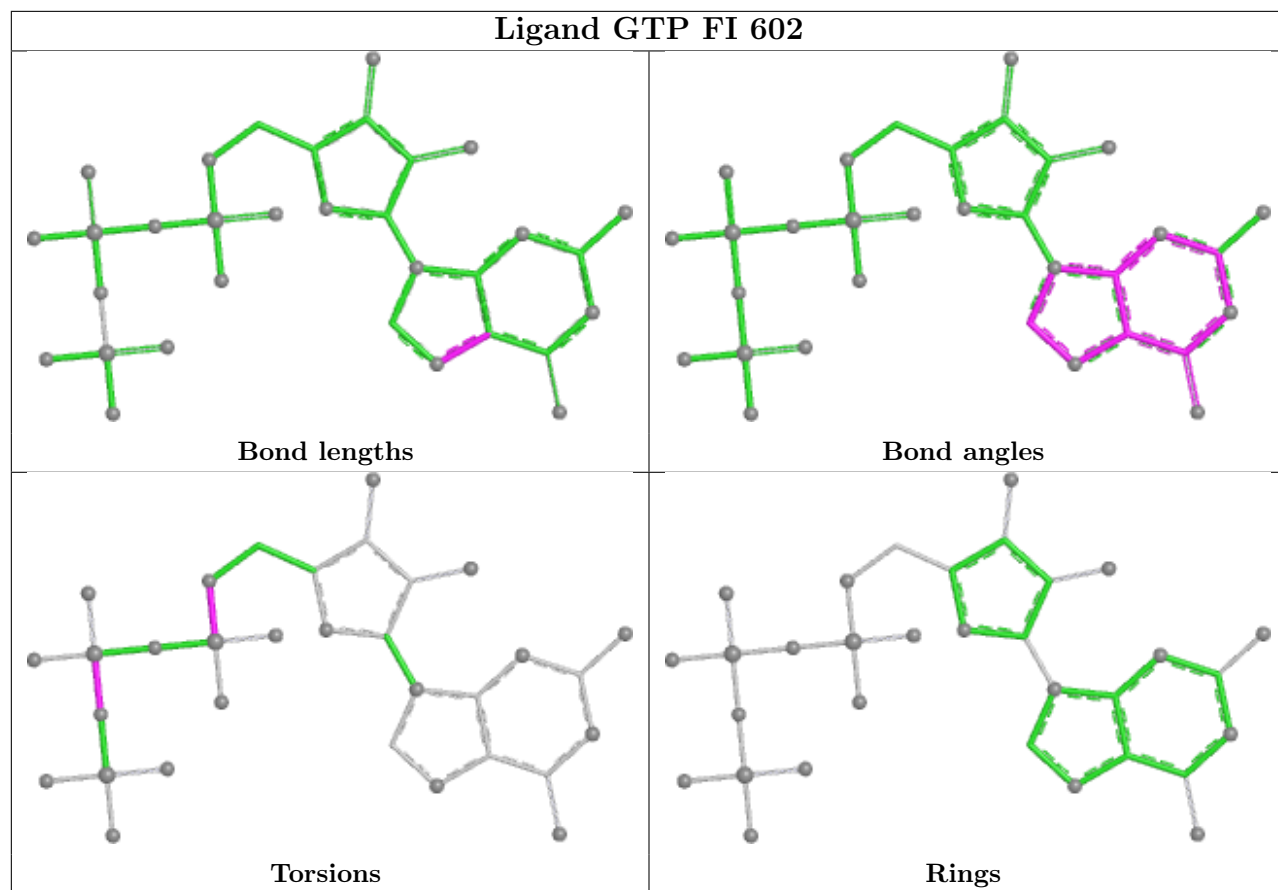


## Ligand GDP SH 501

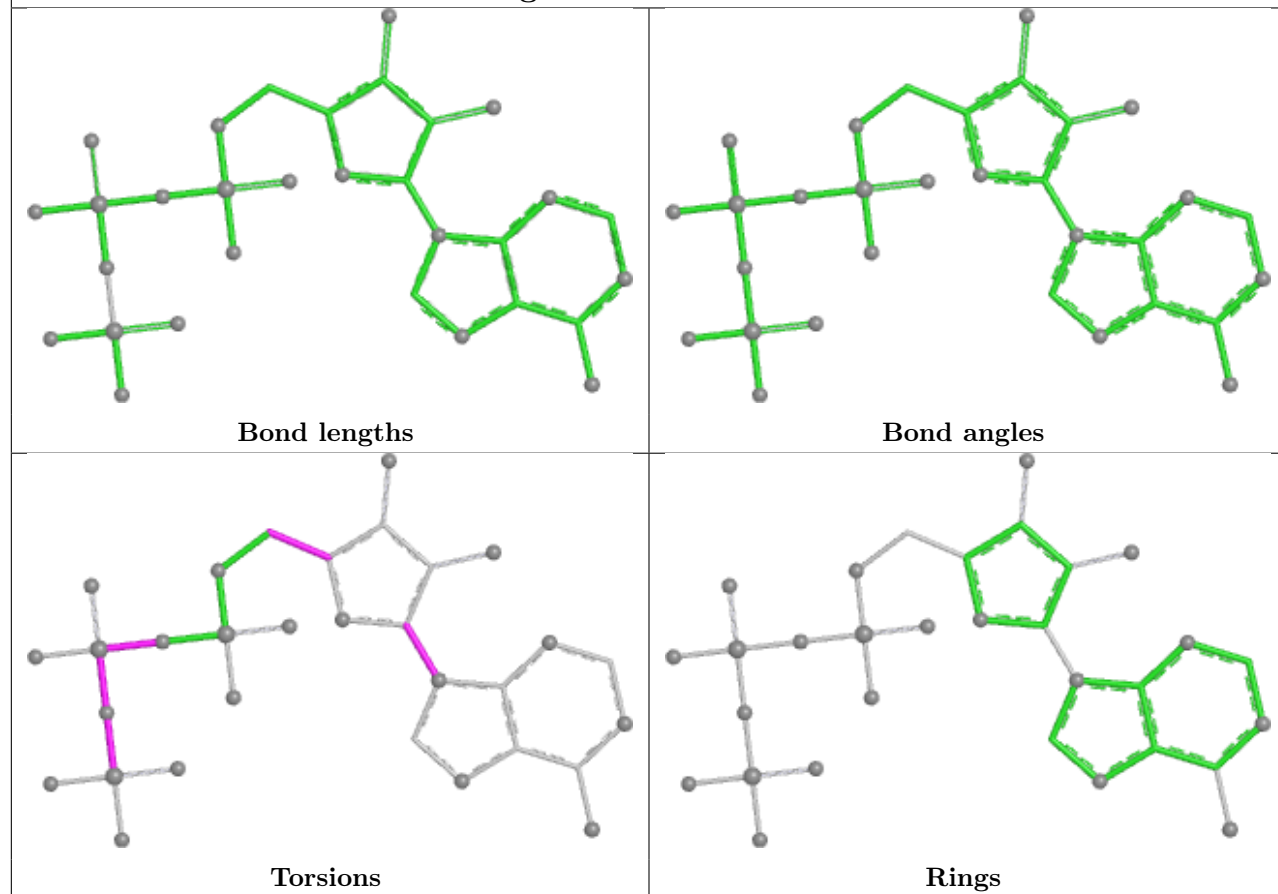




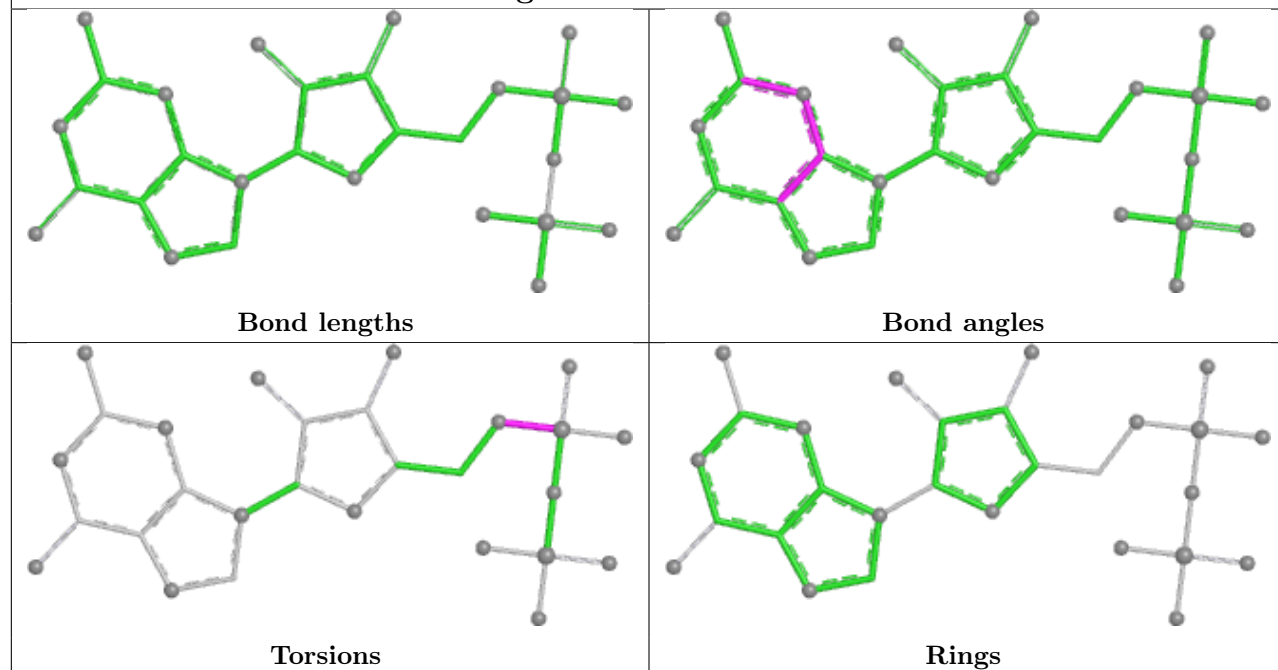




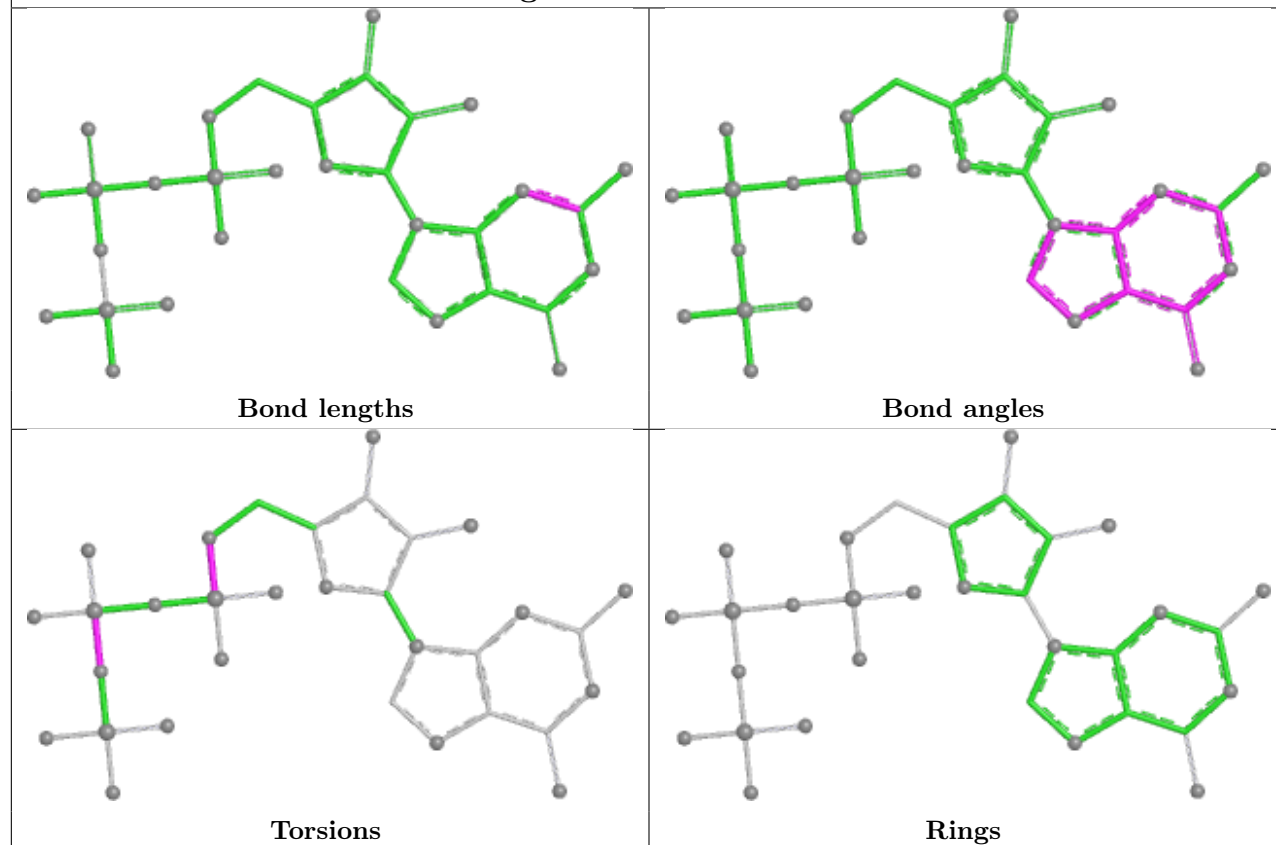
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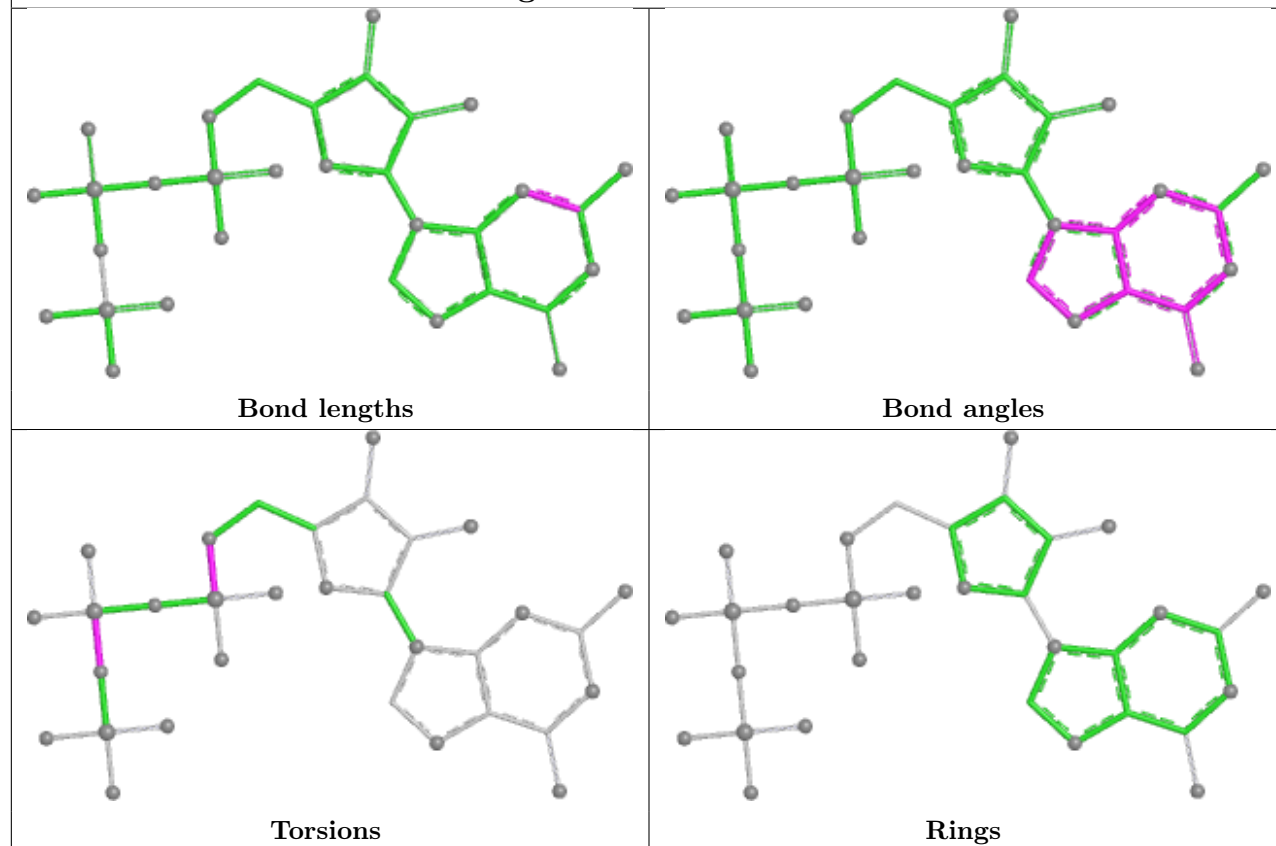
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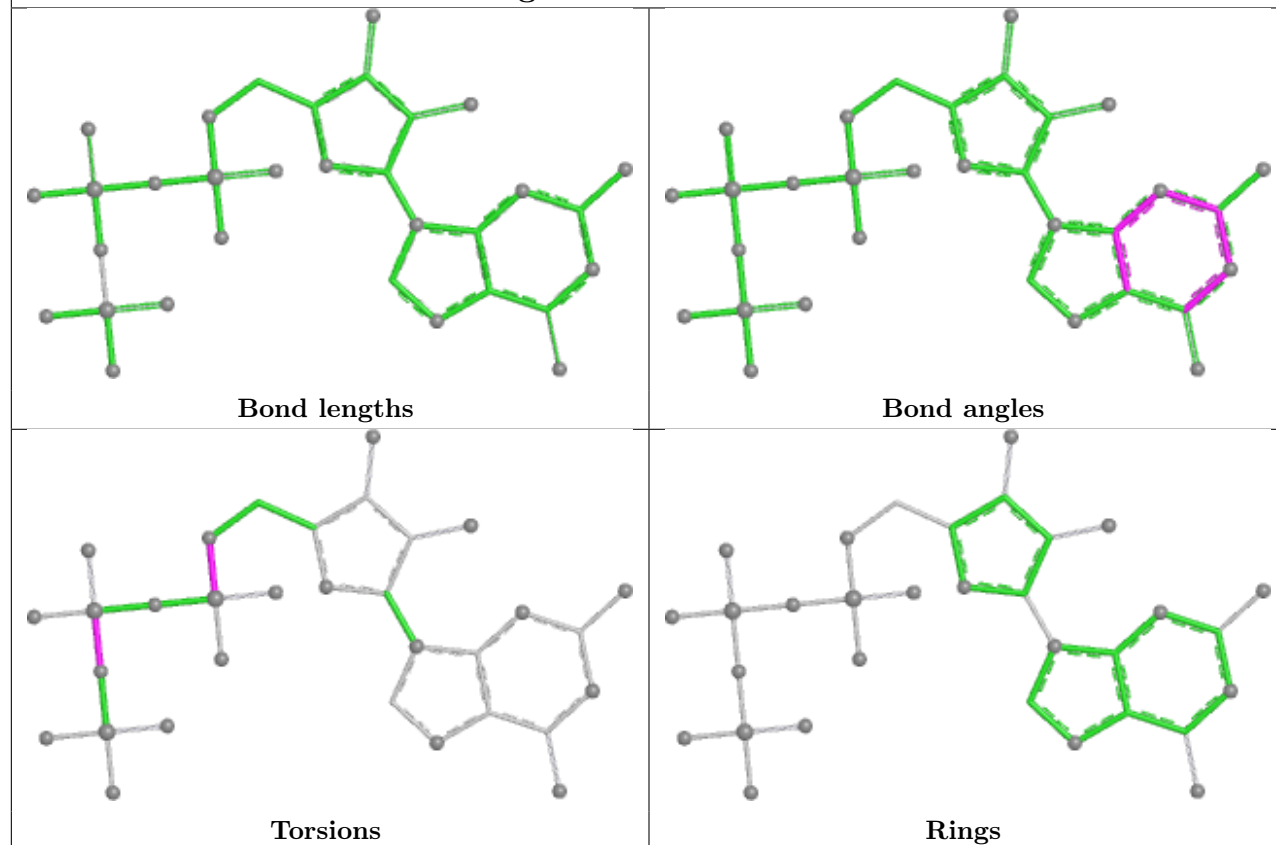
## Ligand GTP XS 501



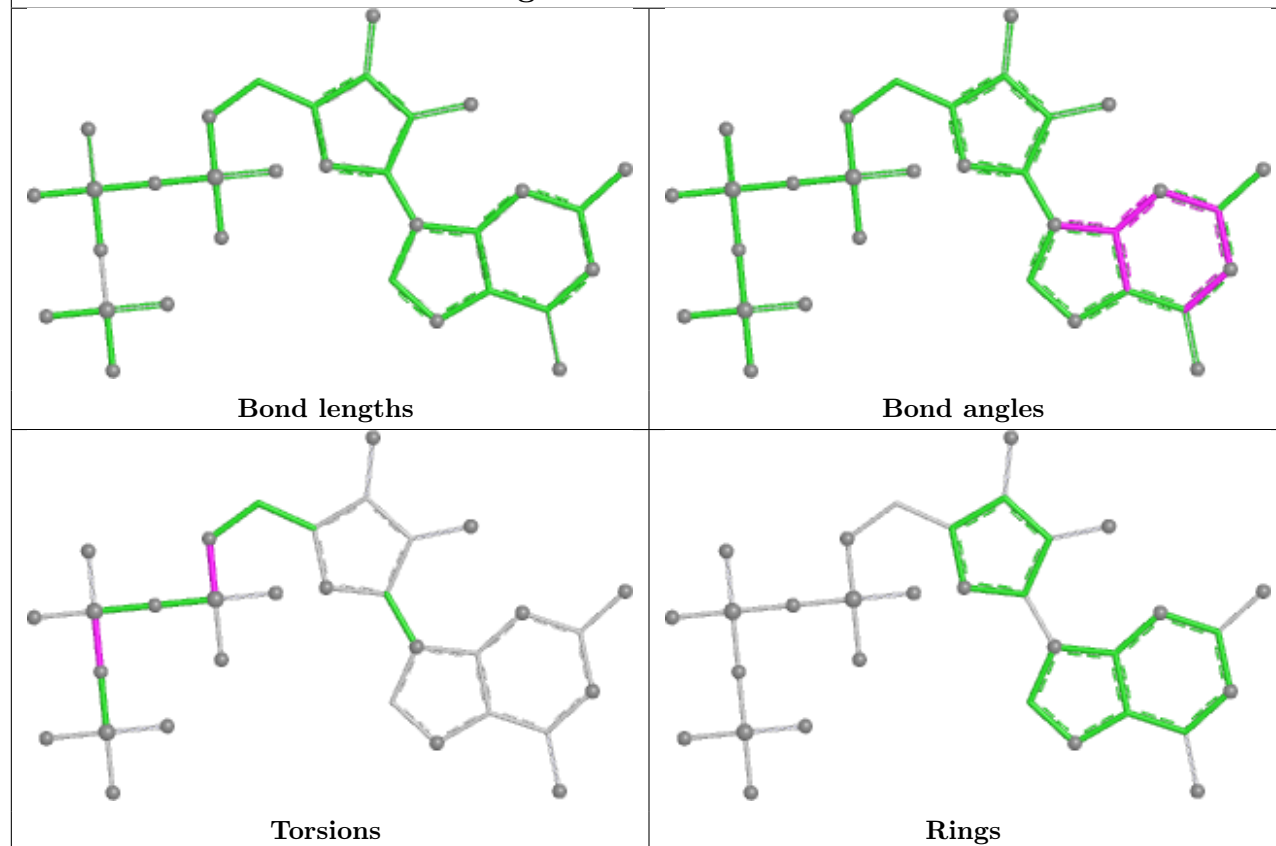
## Ligand GTP HE 602

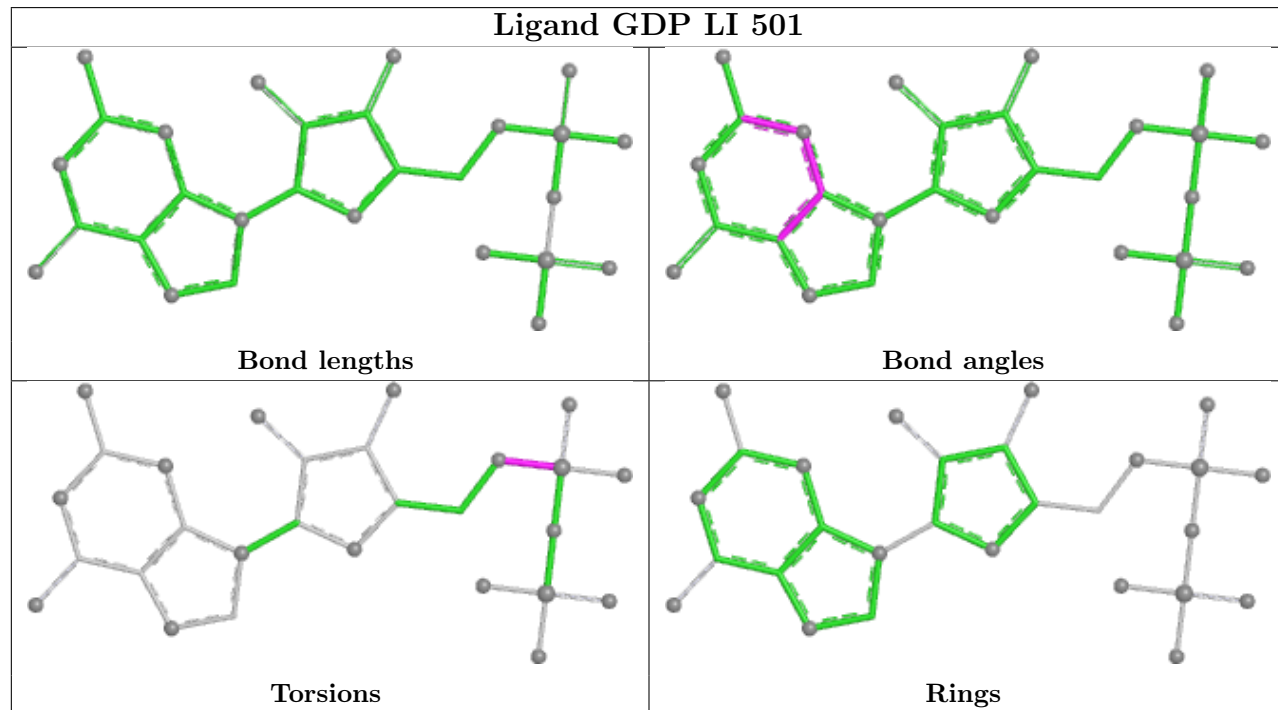
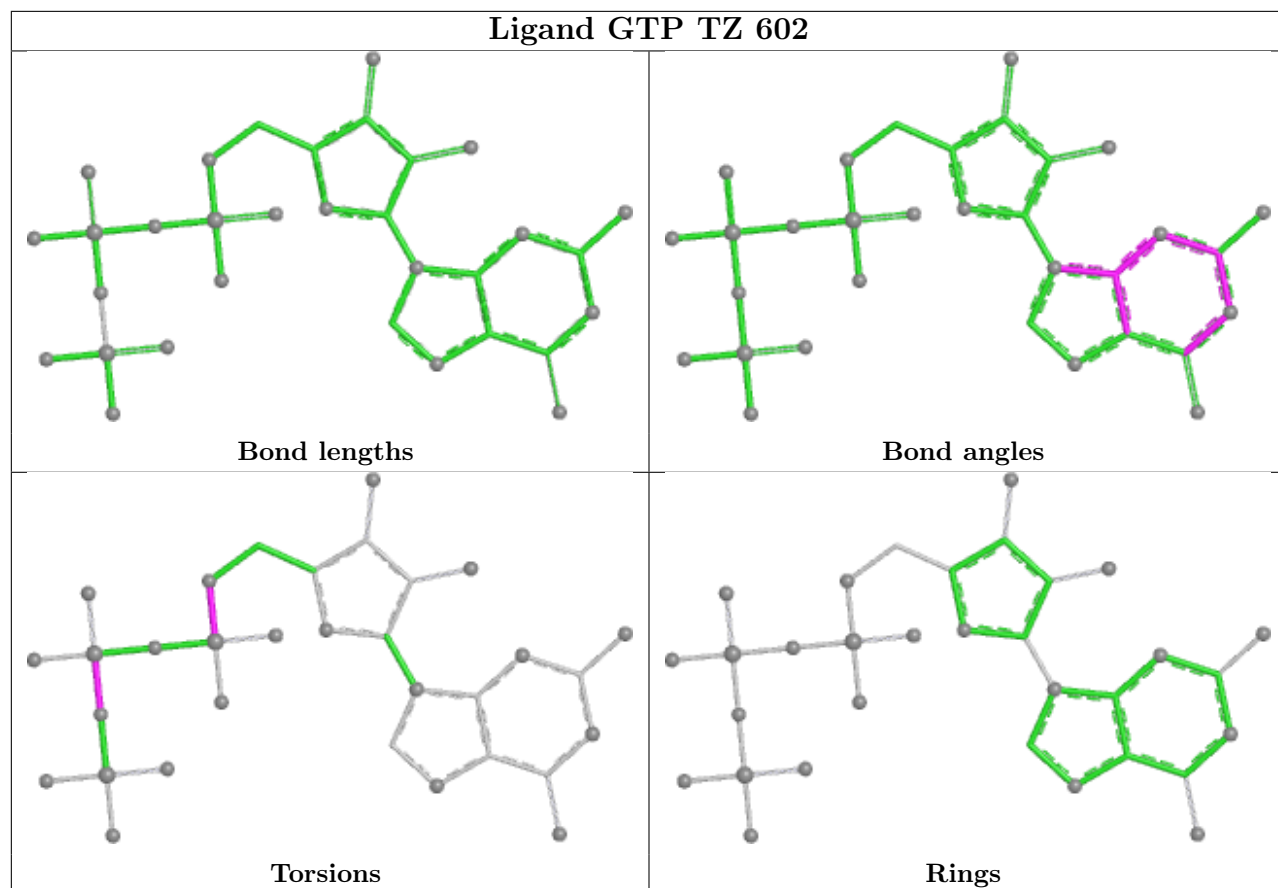


## Ligand GTP VE 501

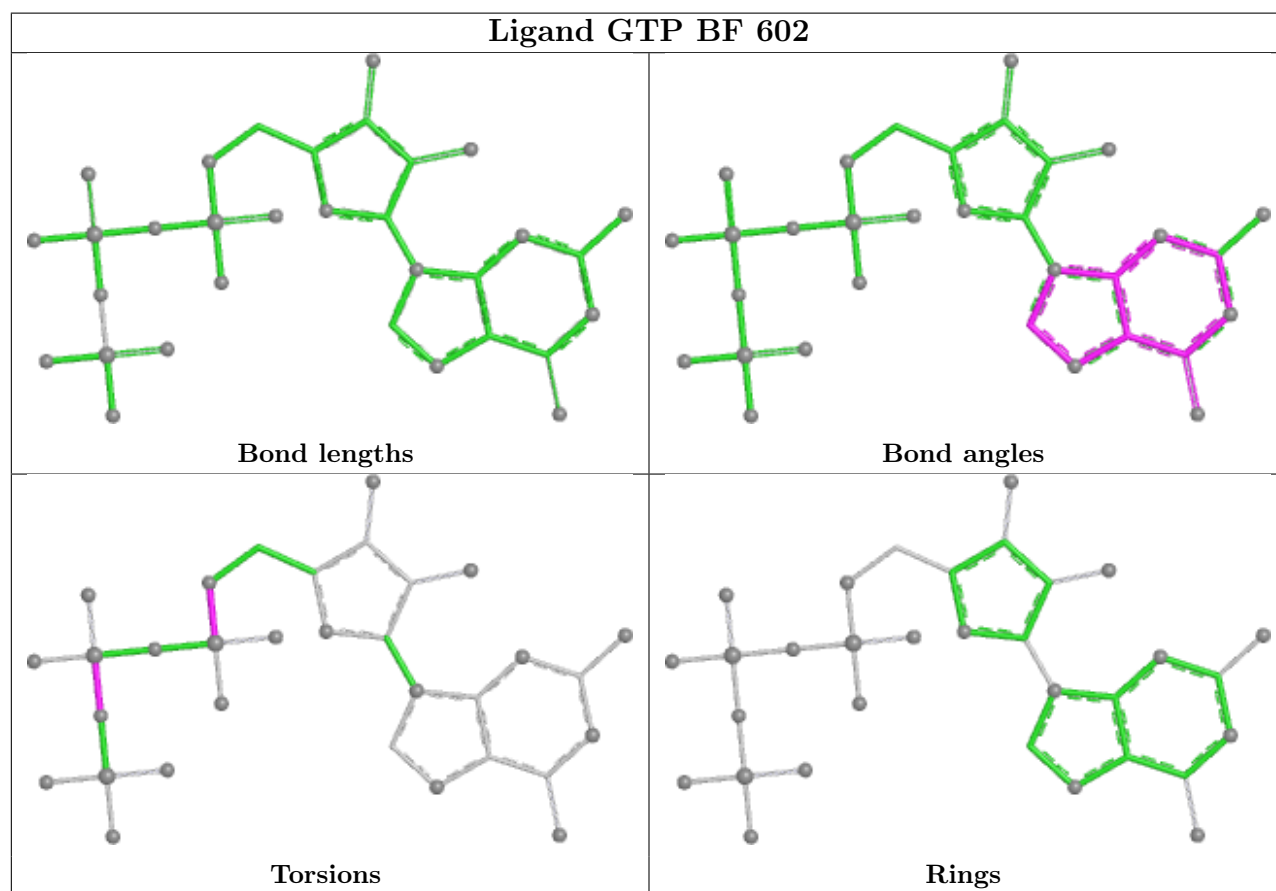
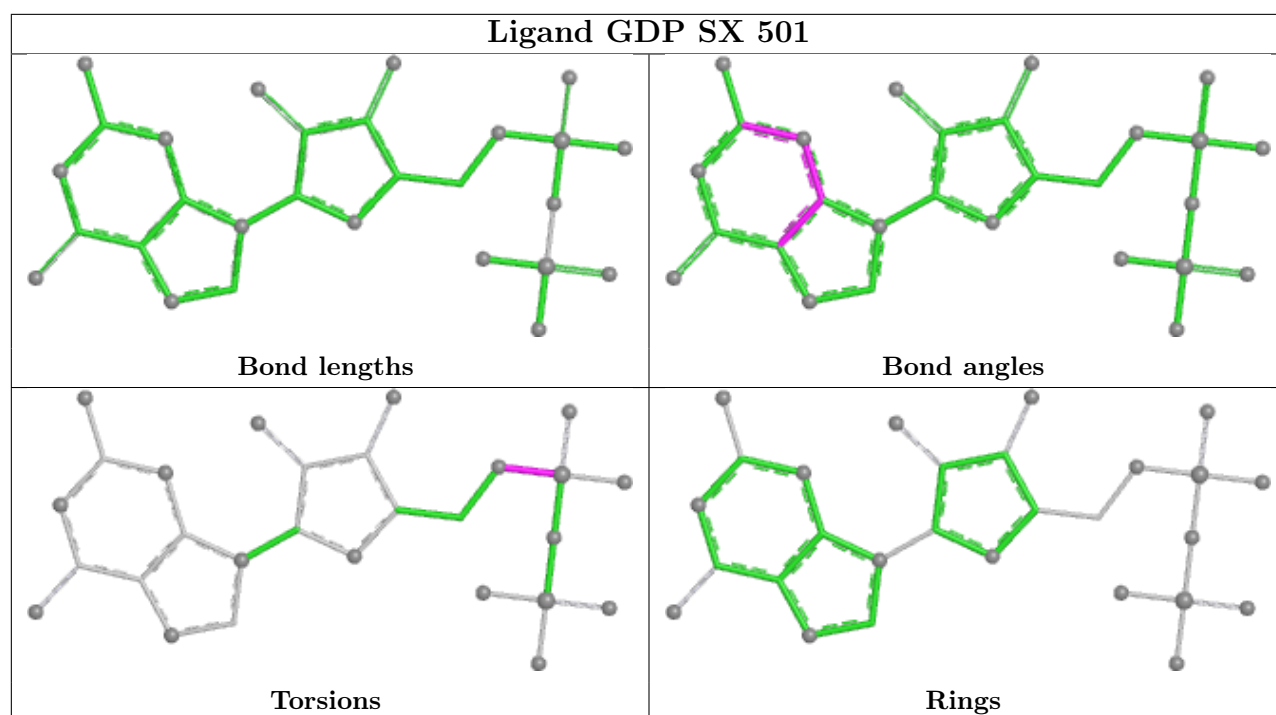


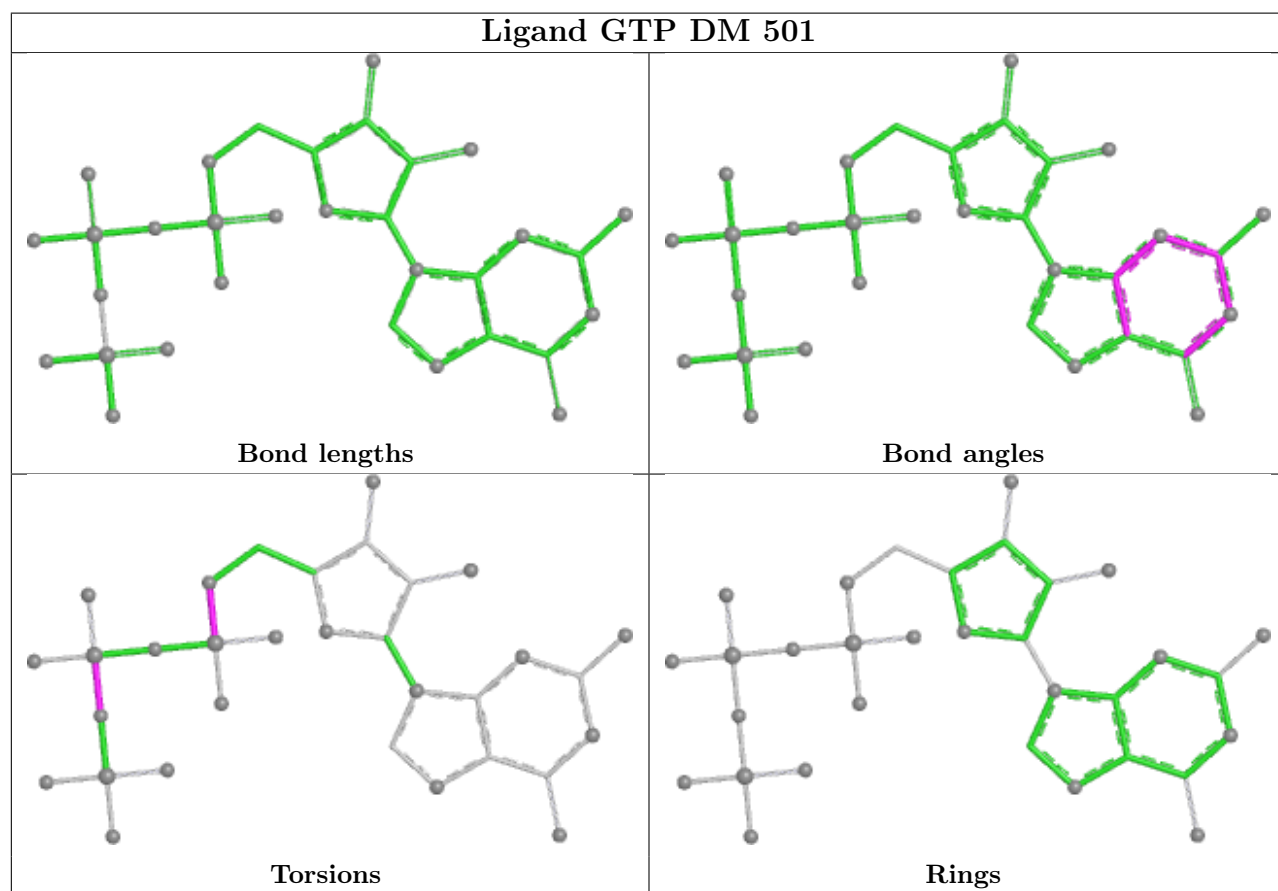
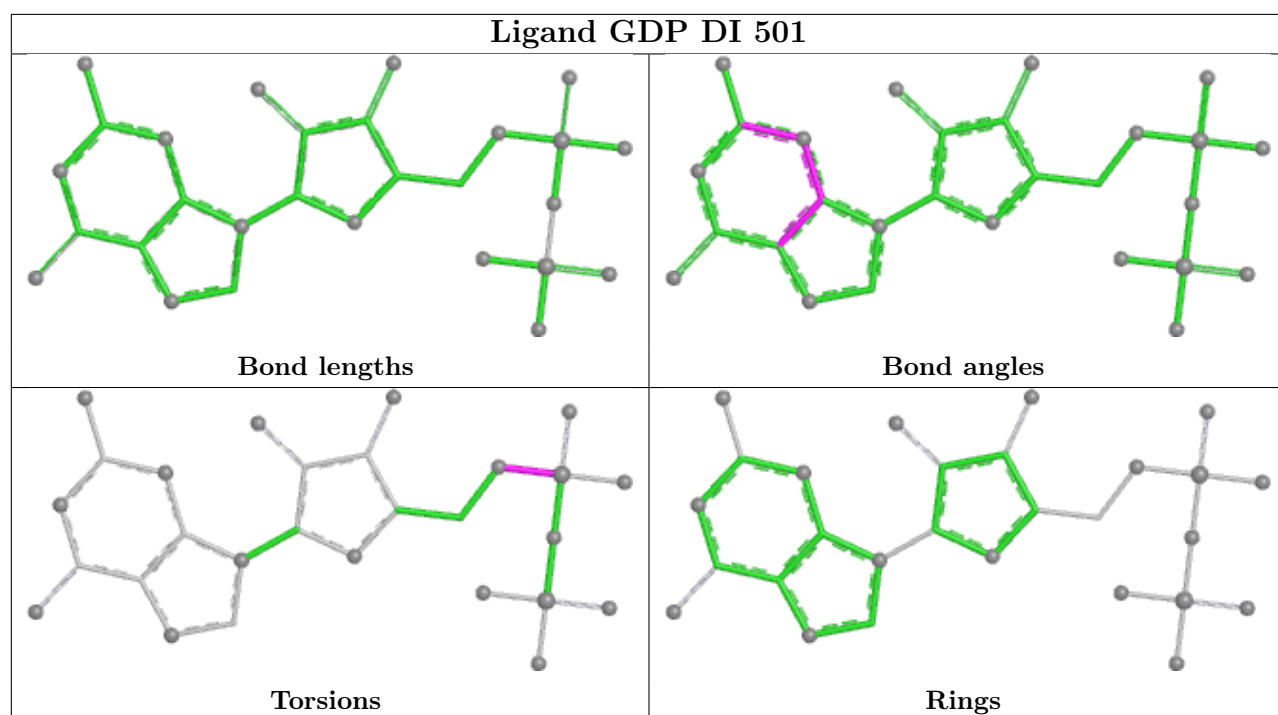
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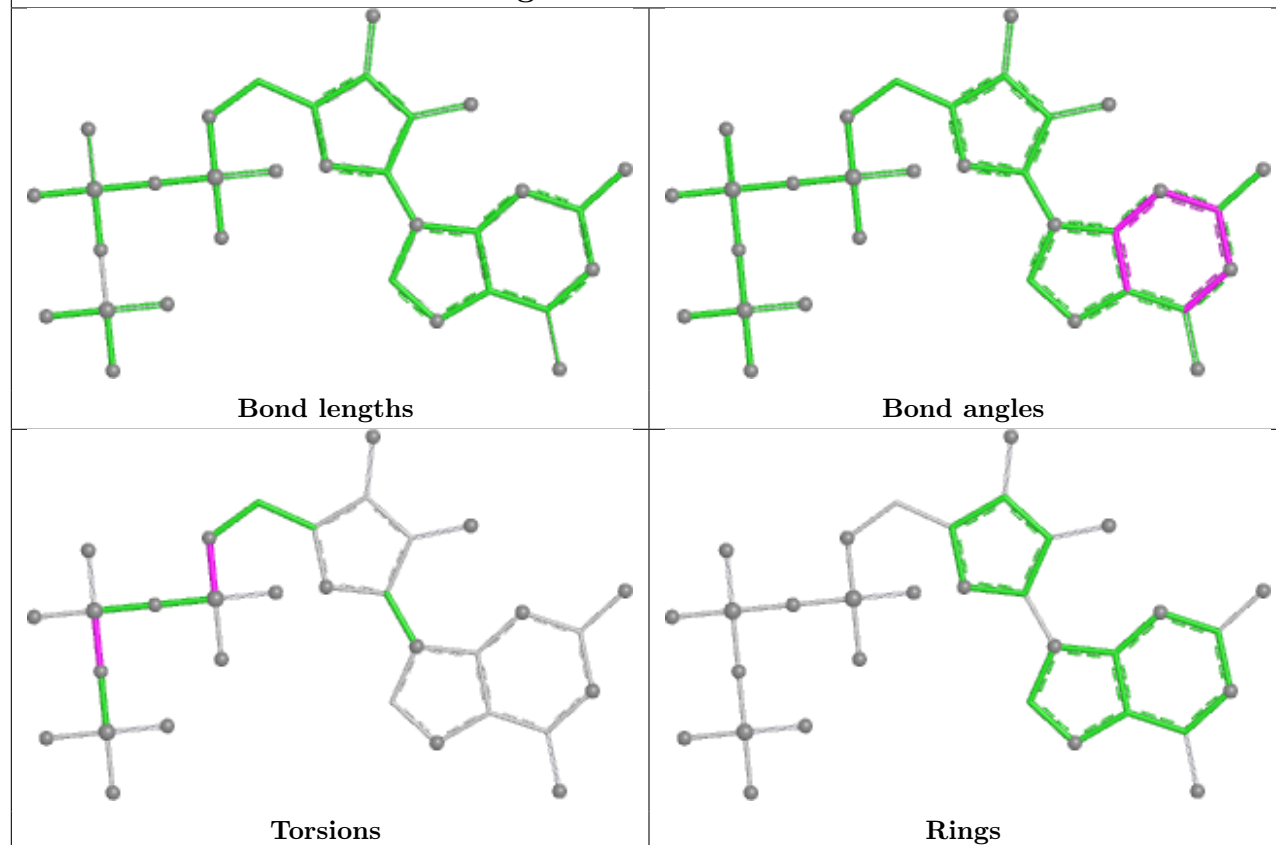




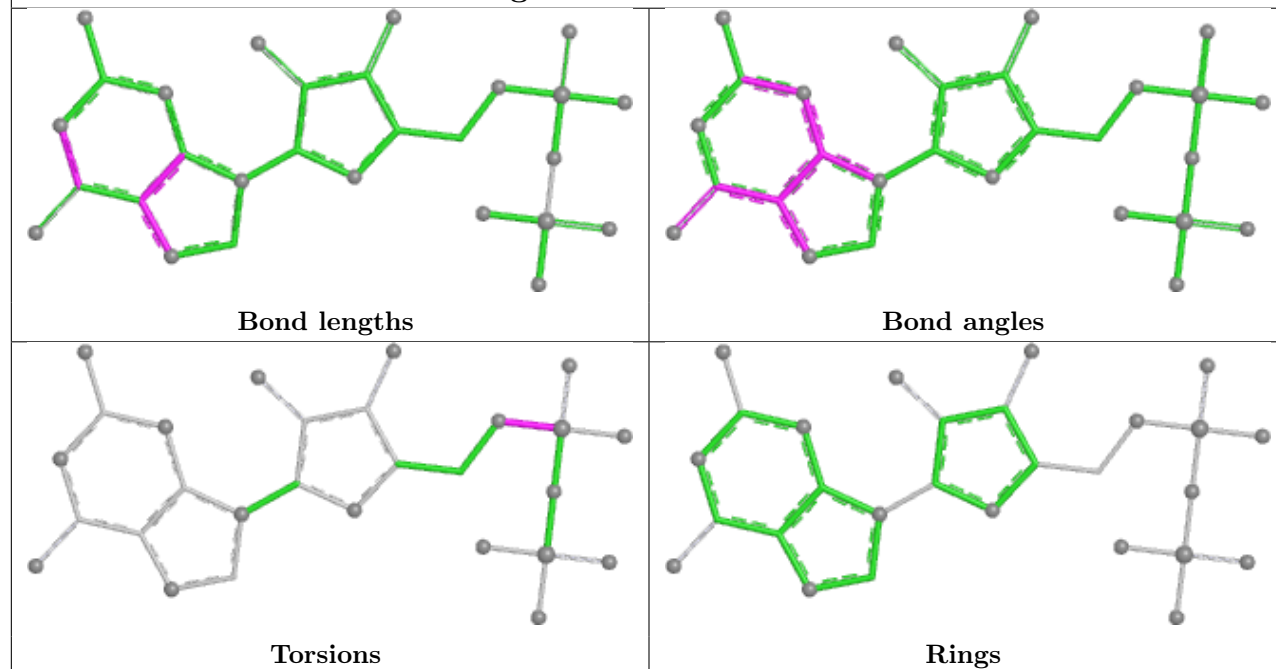




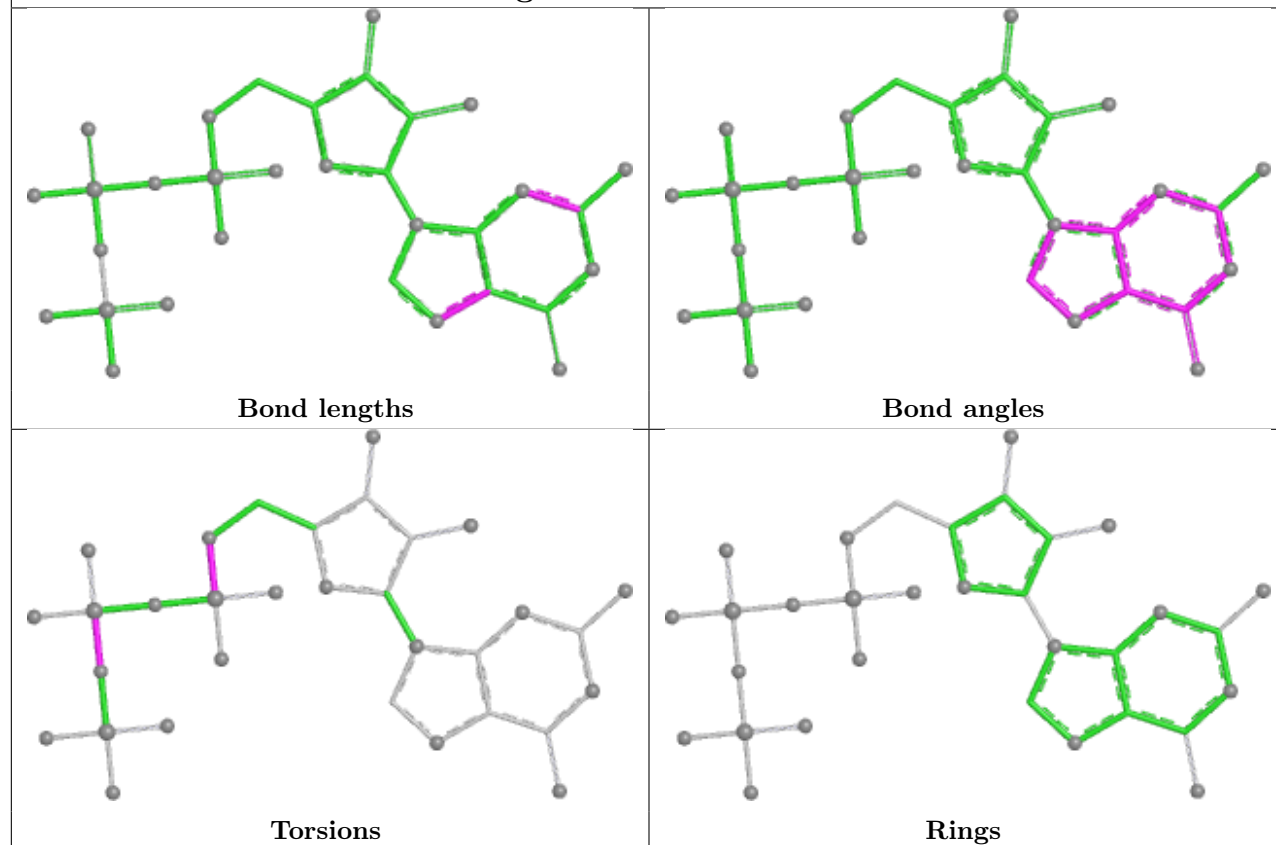
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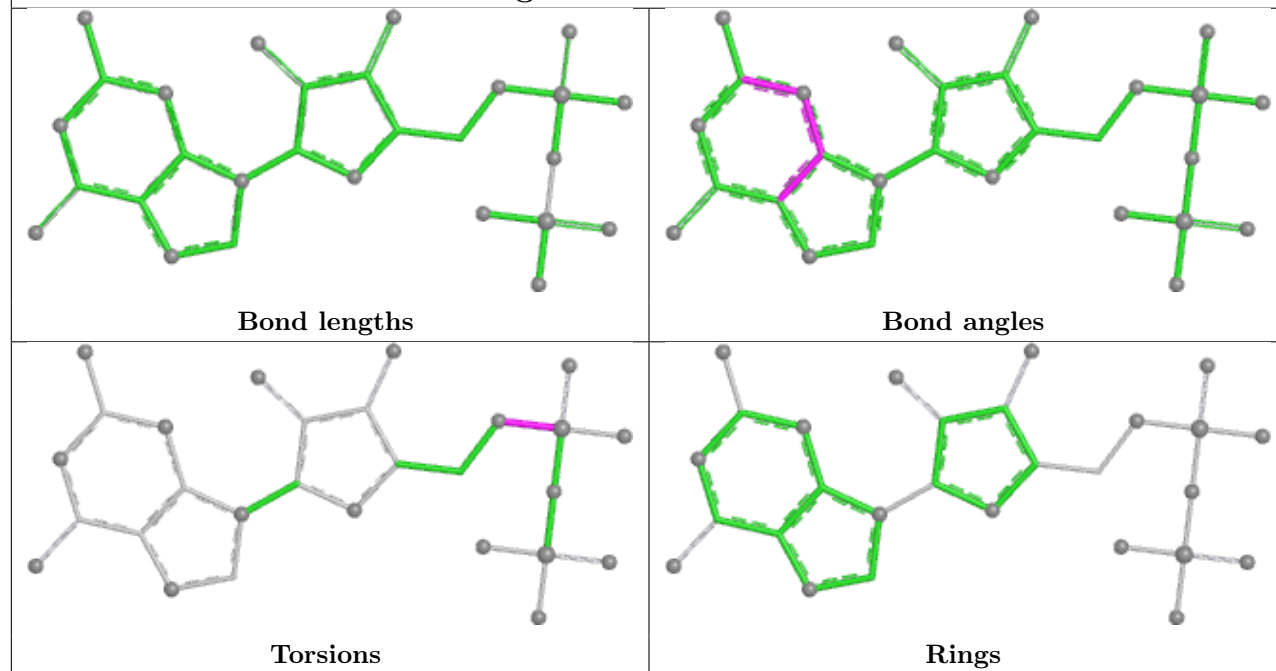
## Ligand GDP WX 501



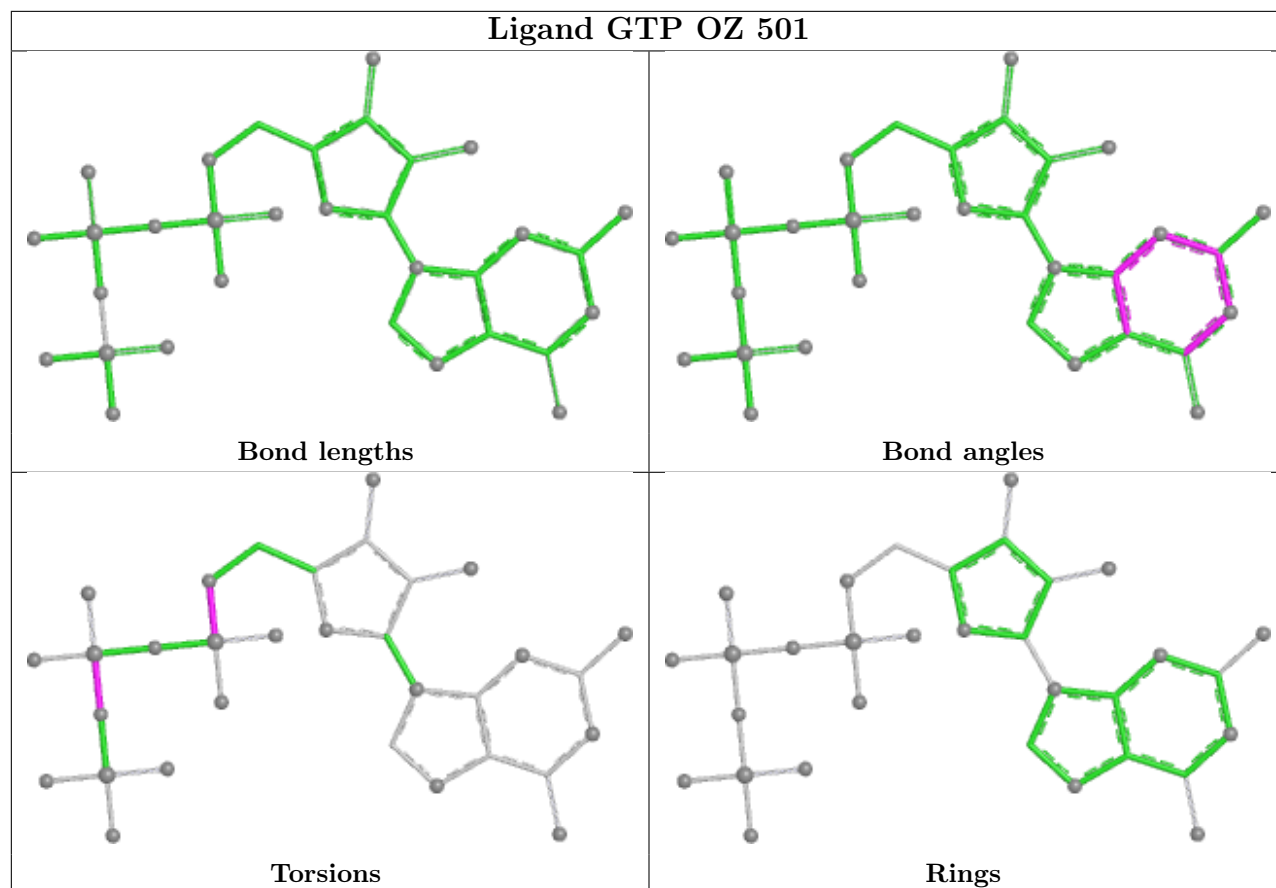
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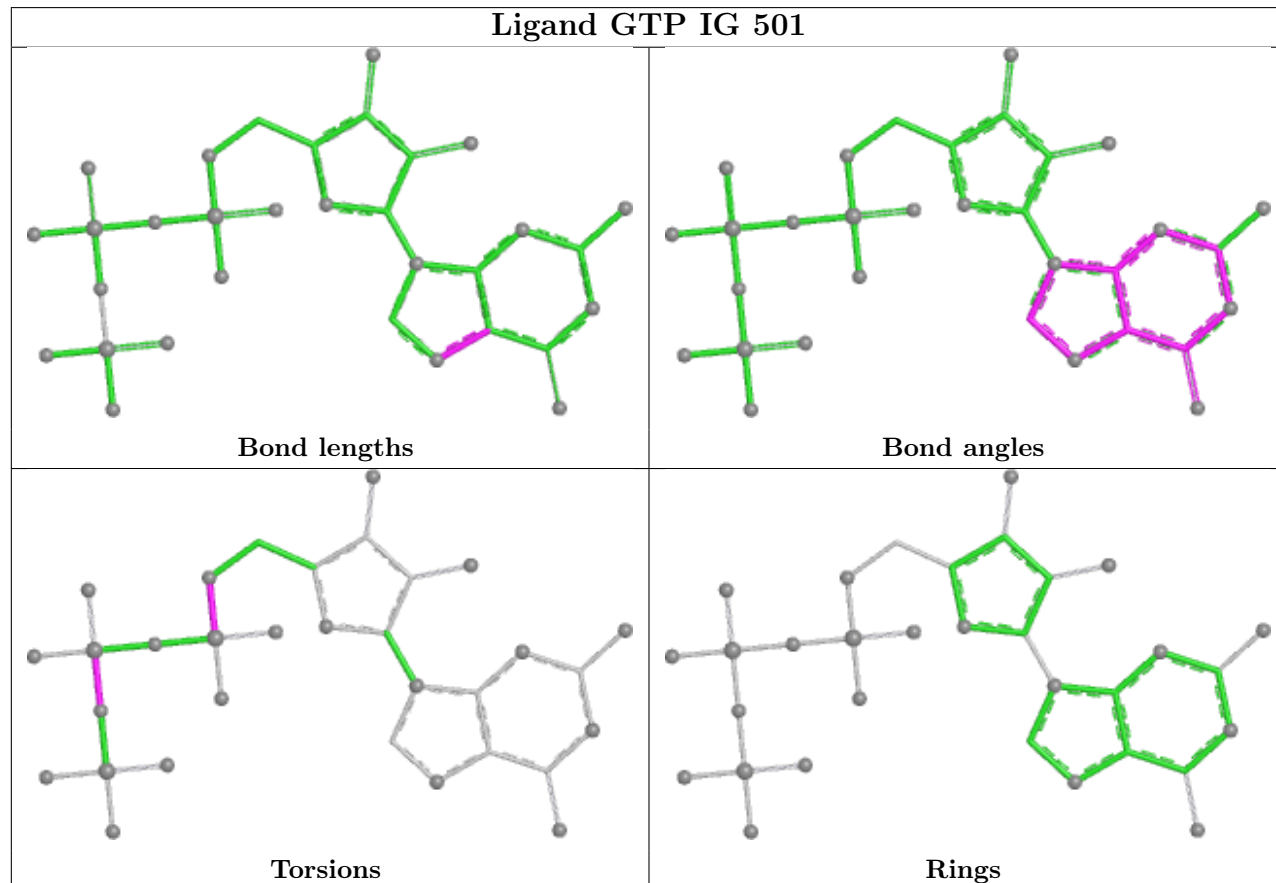
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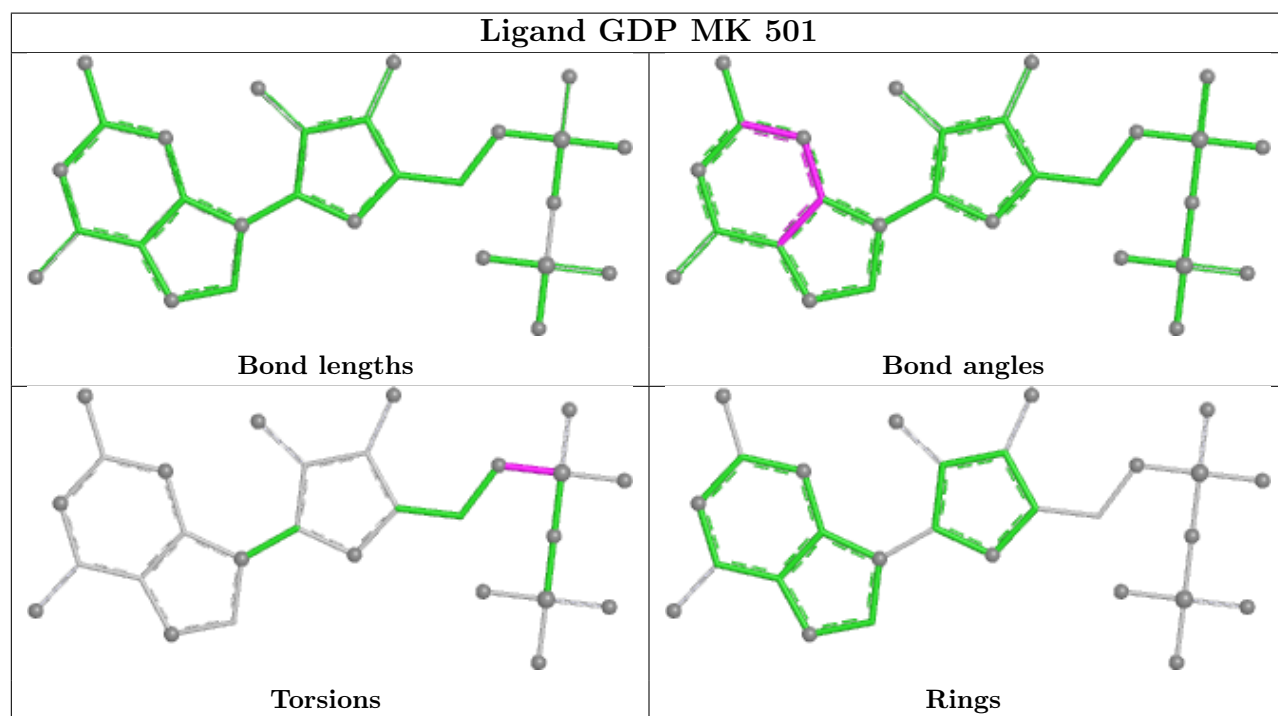
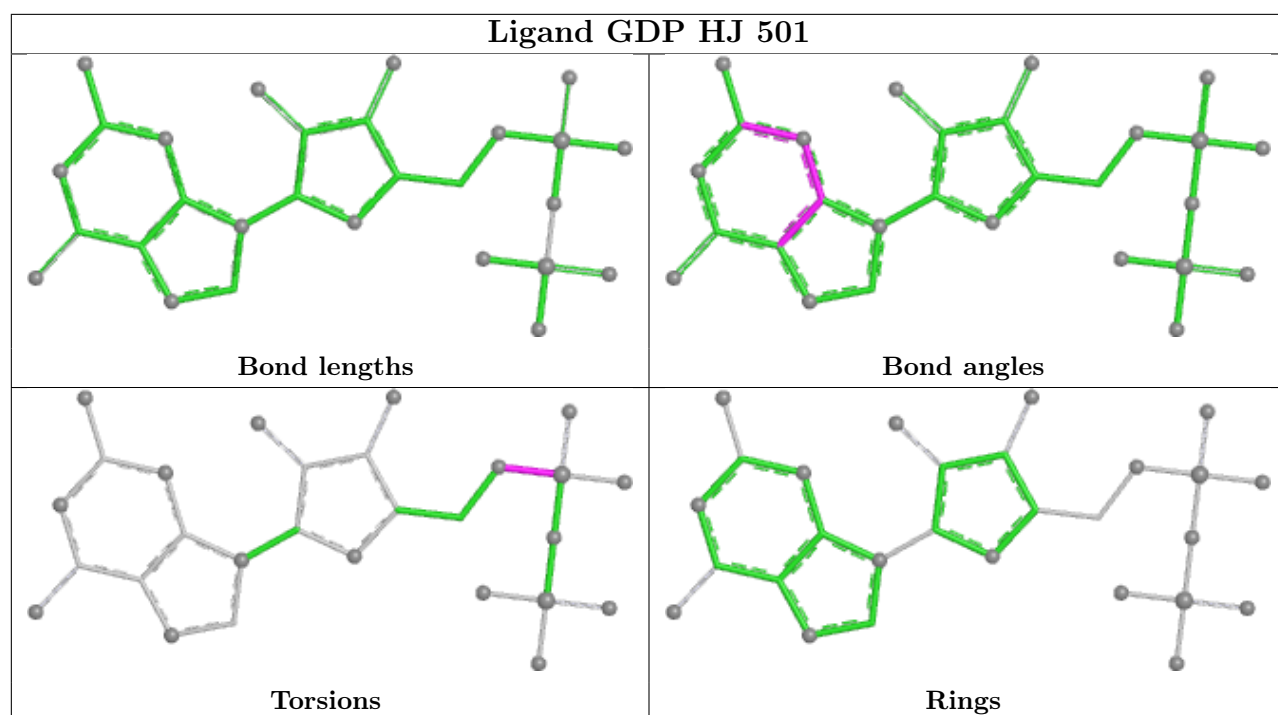


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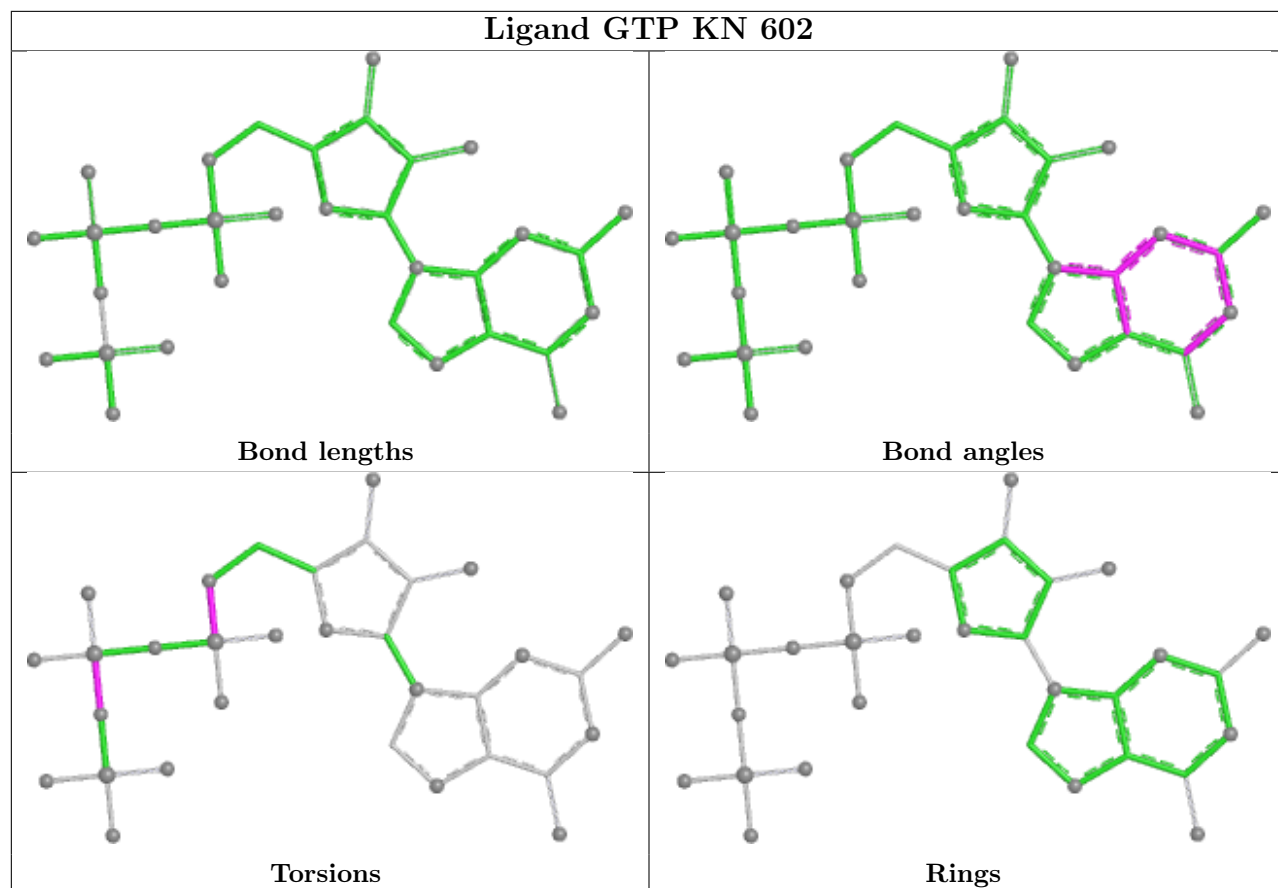


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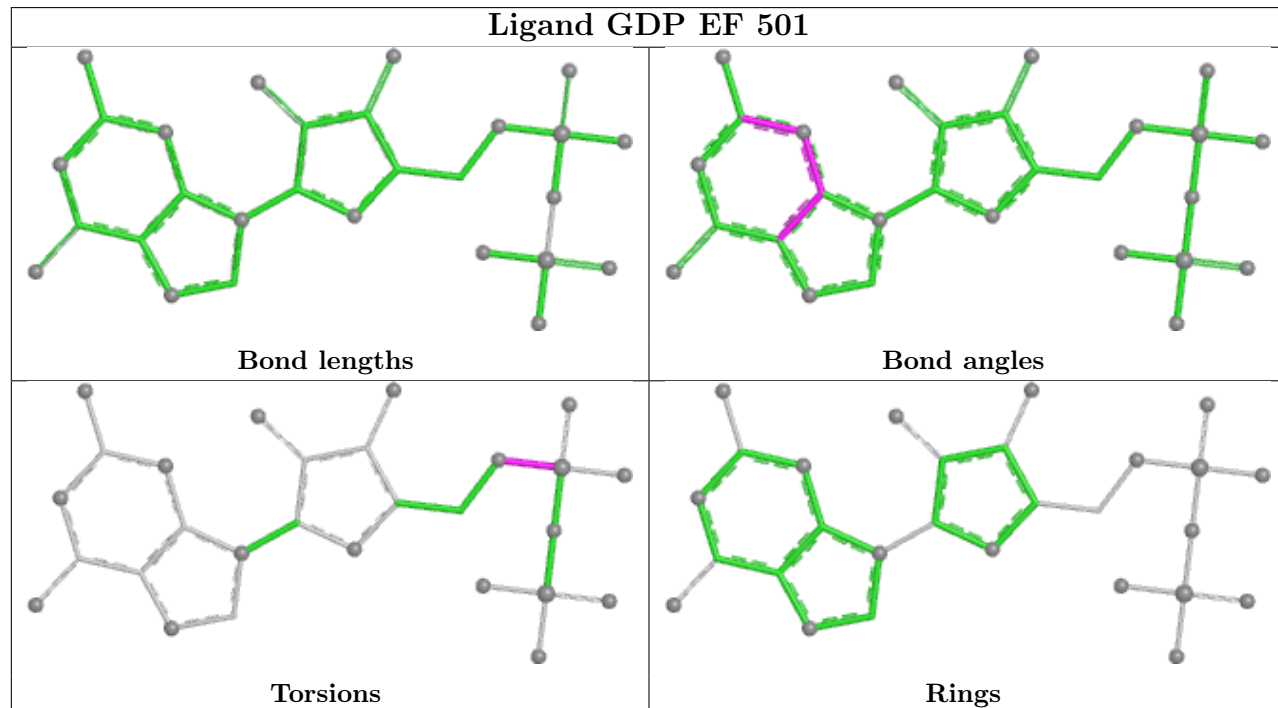


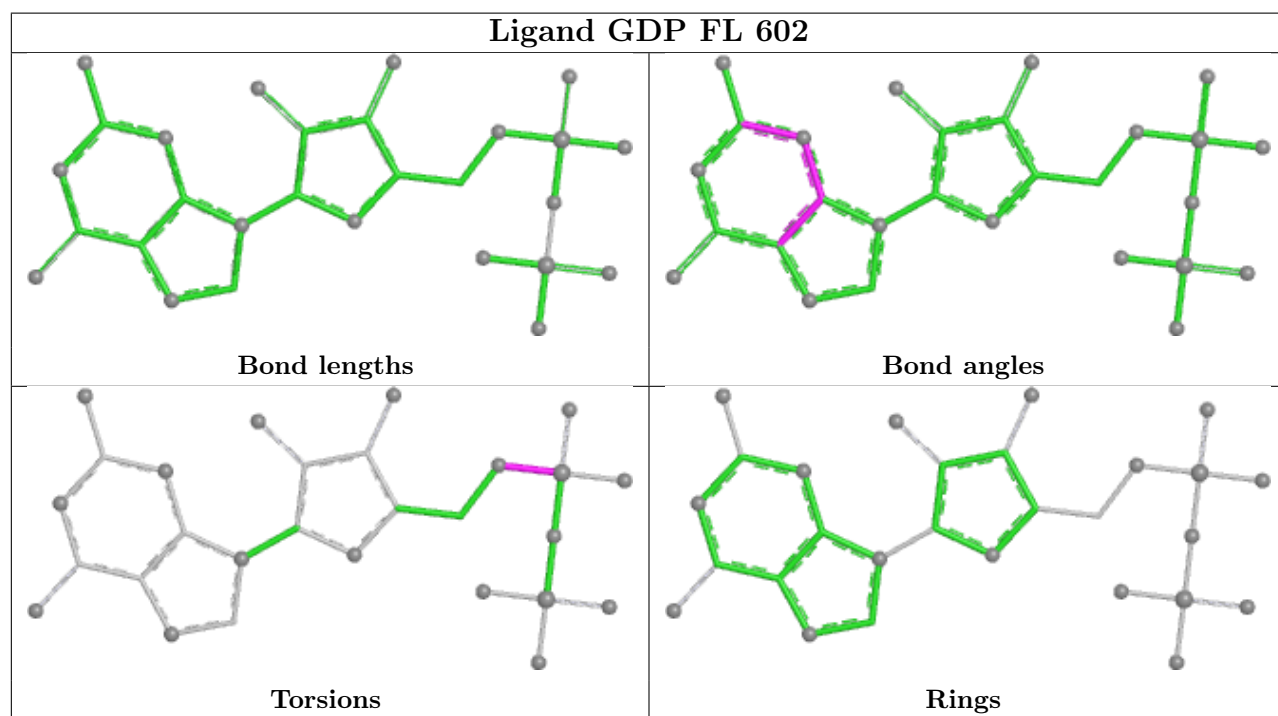
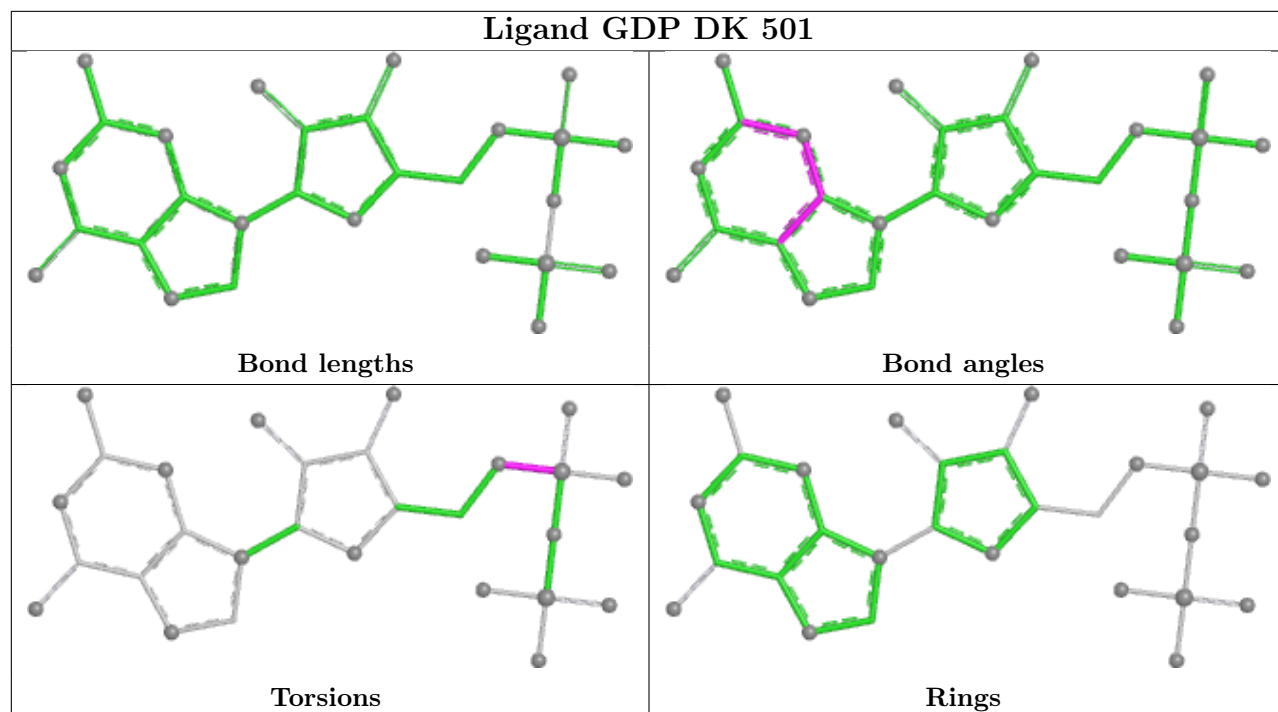


## Ligand GTP KN 602

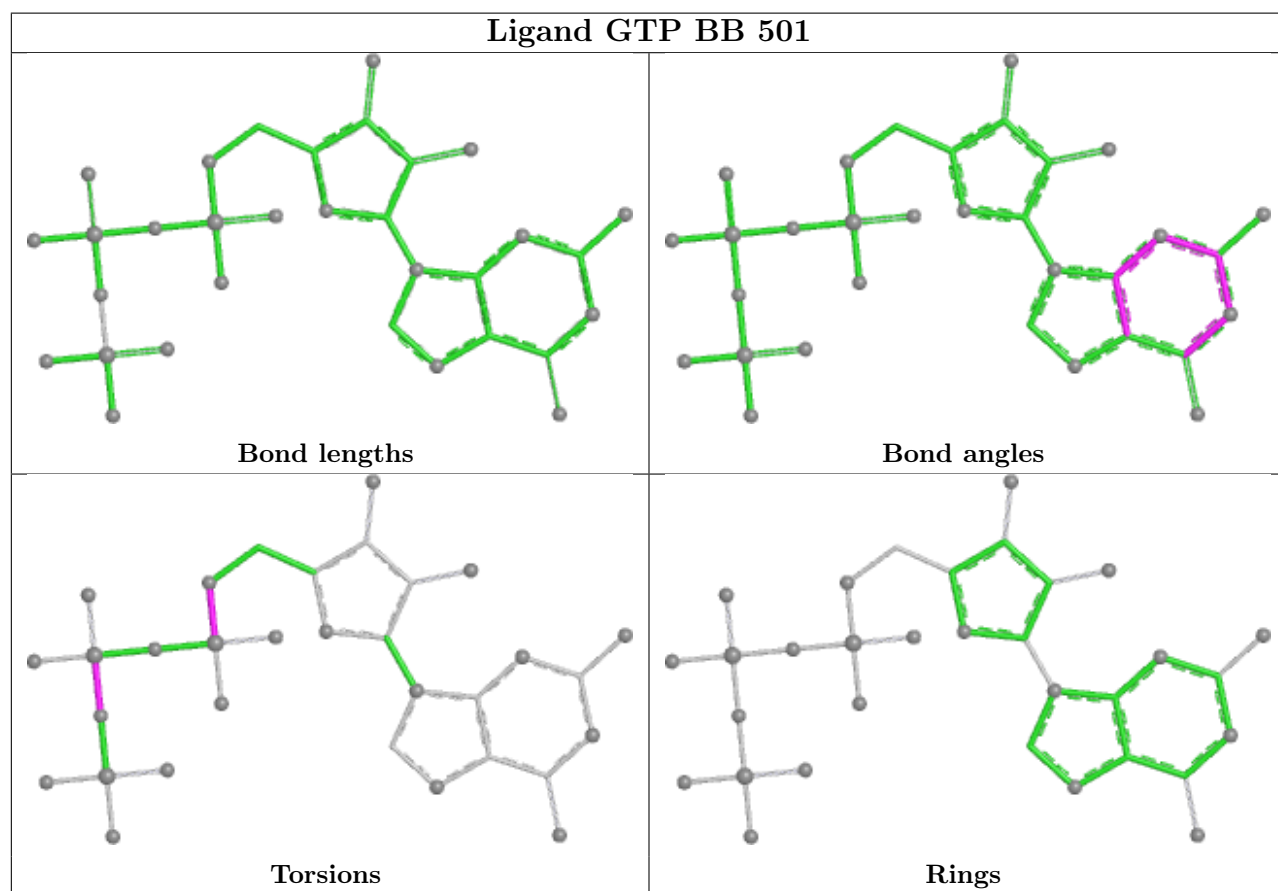
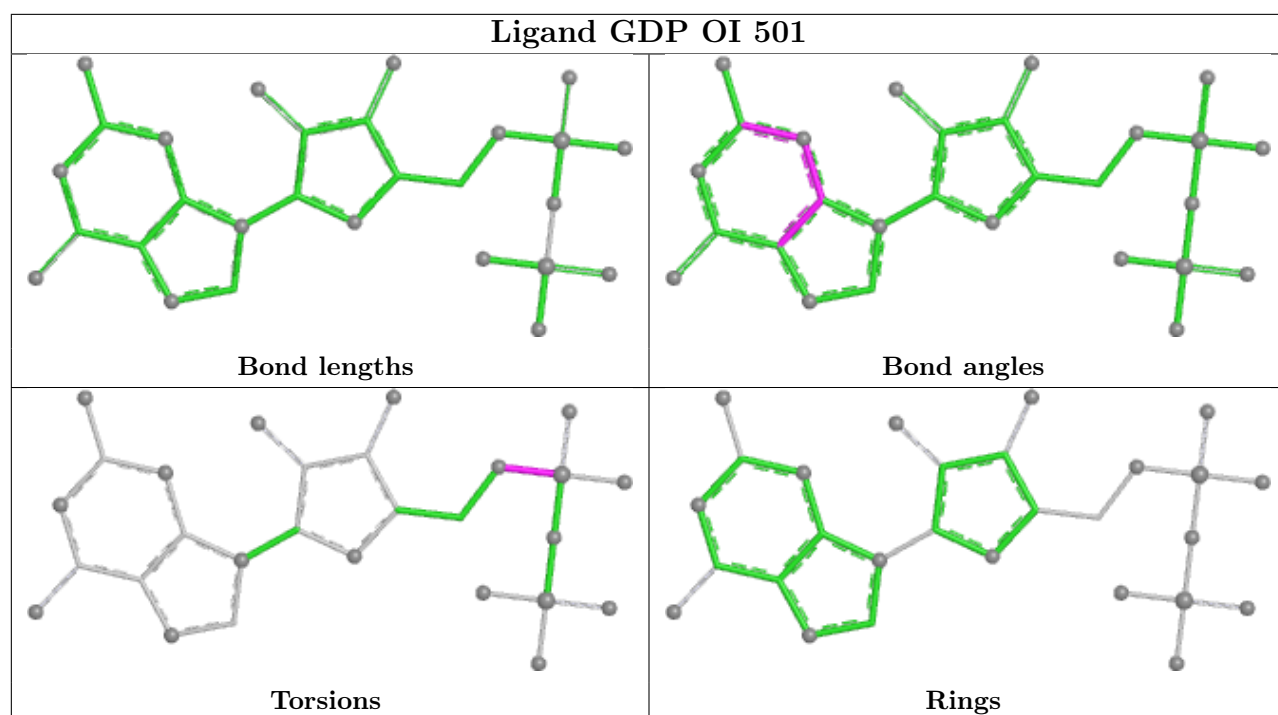


## Ligand GDP EF 501

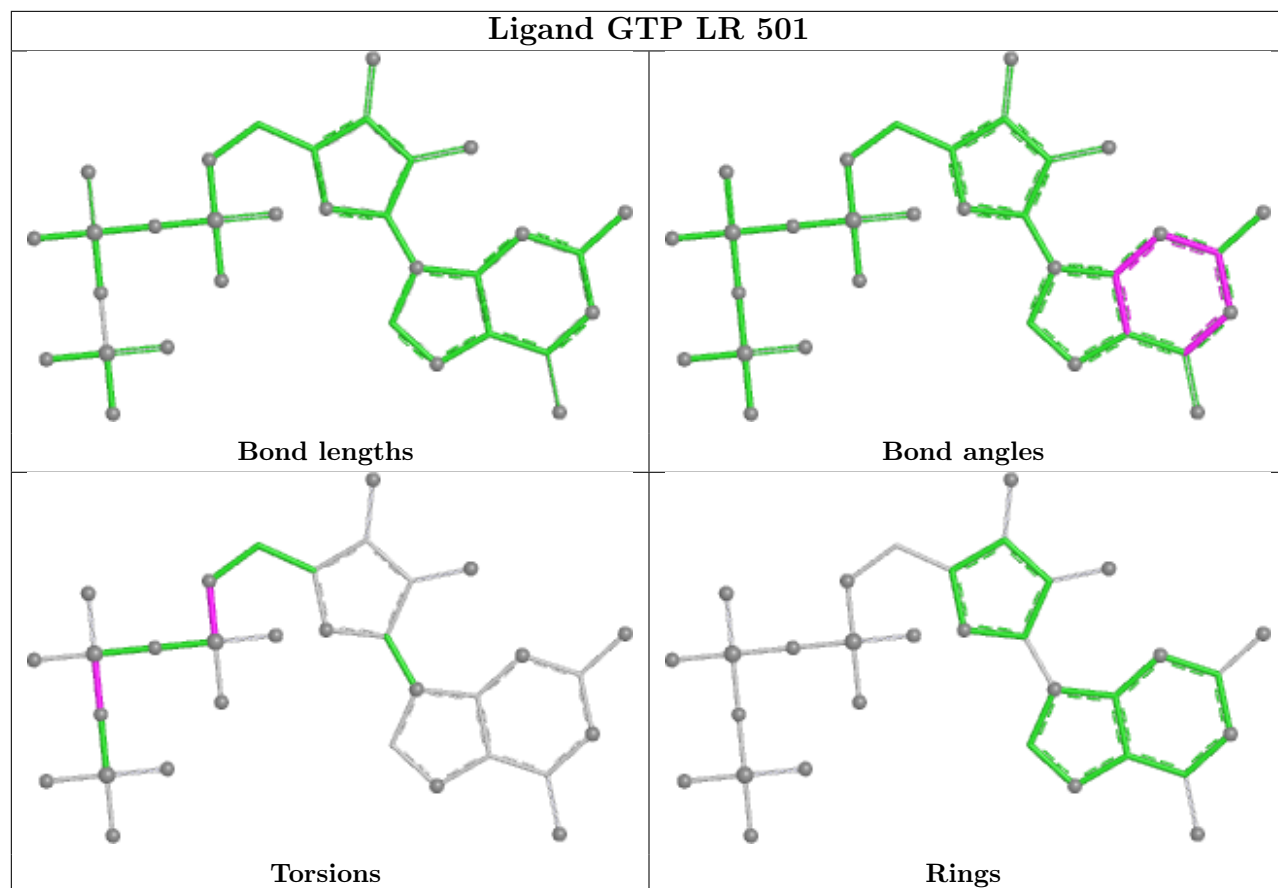




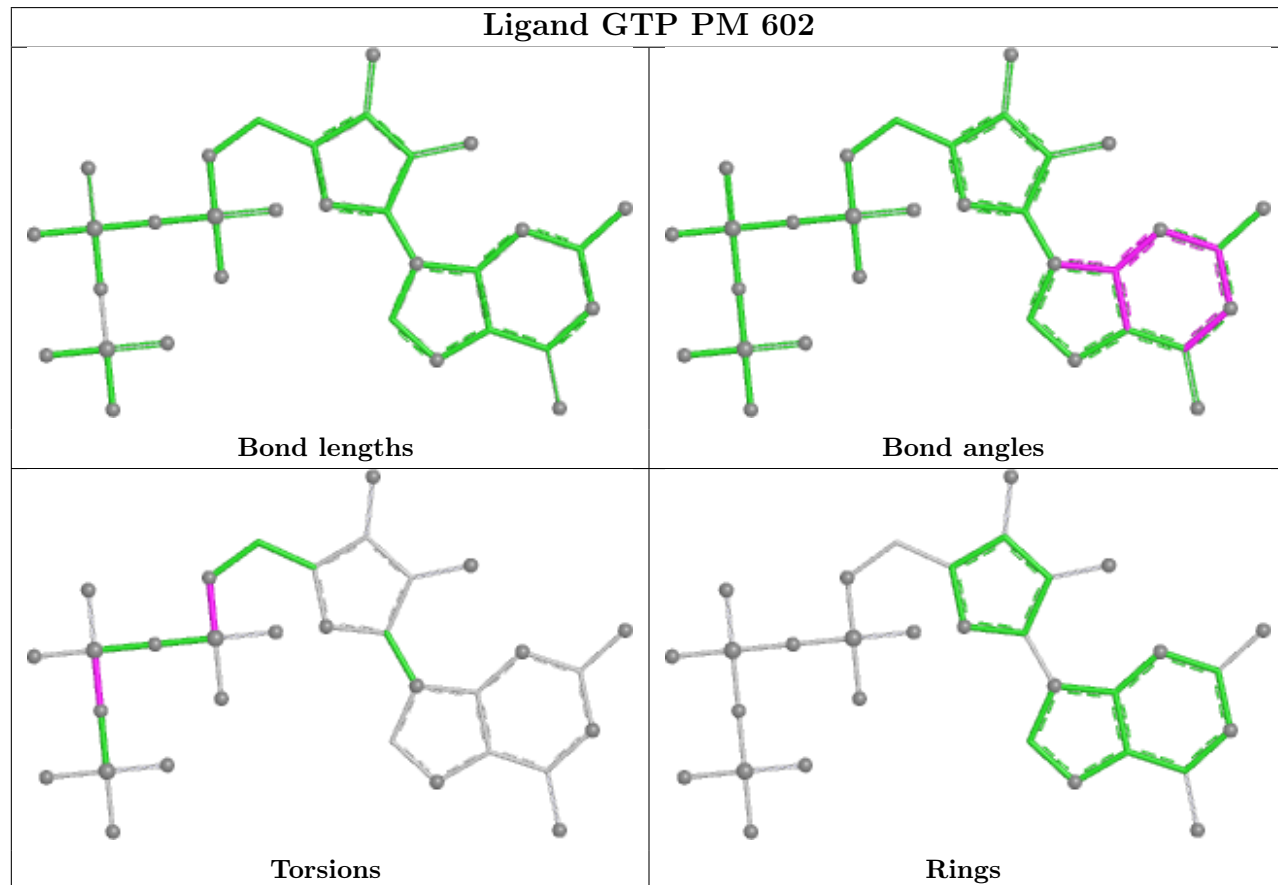


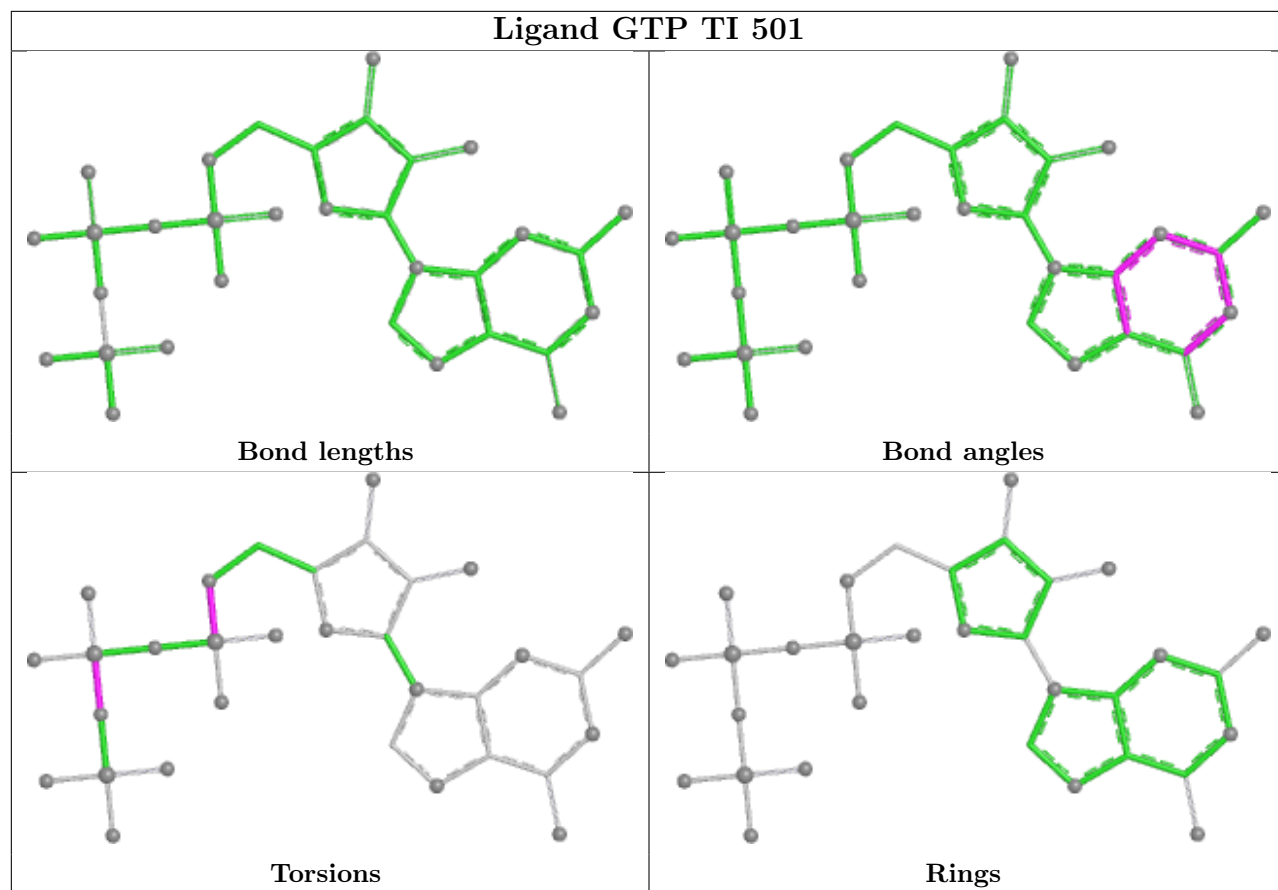


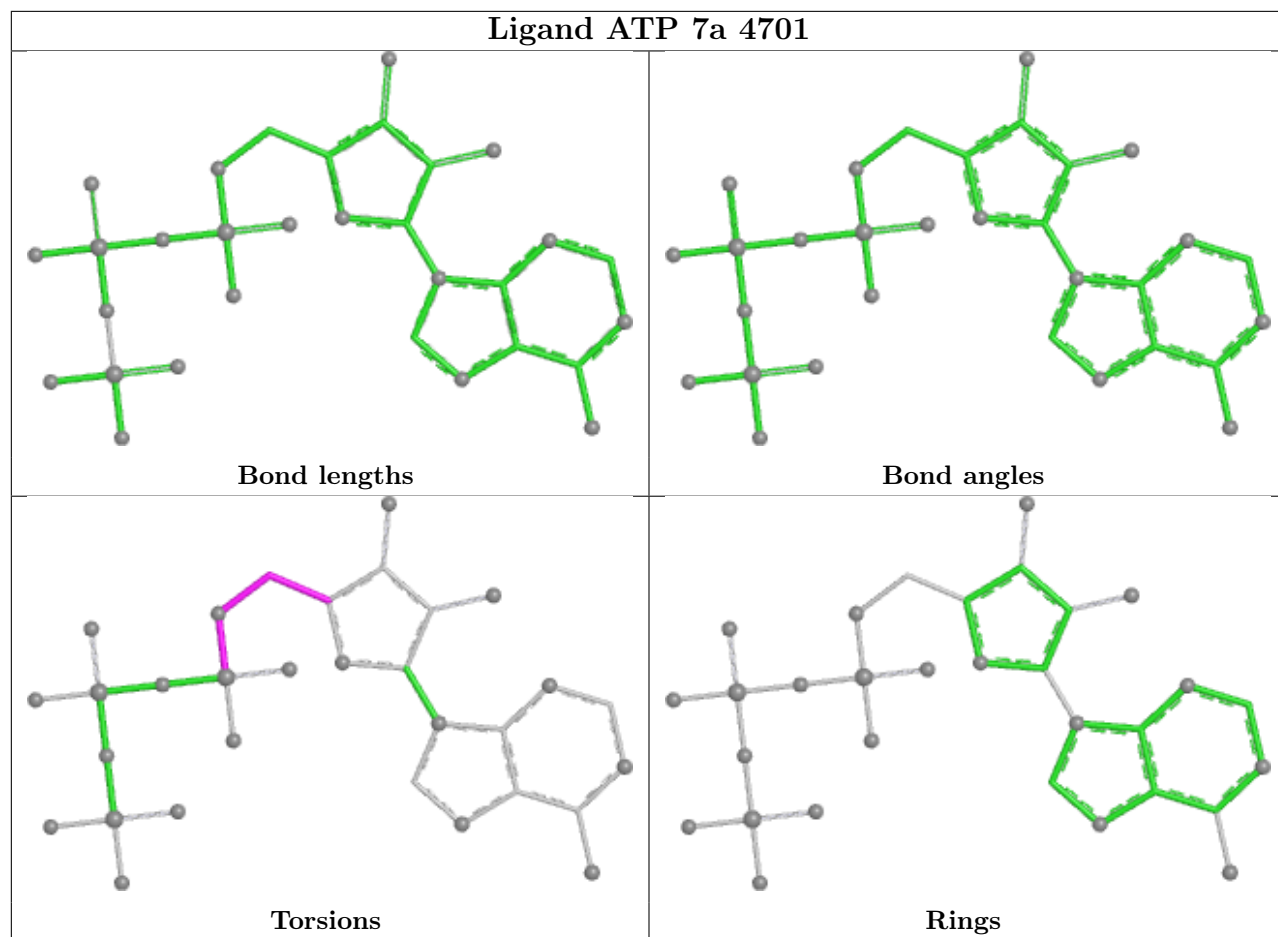
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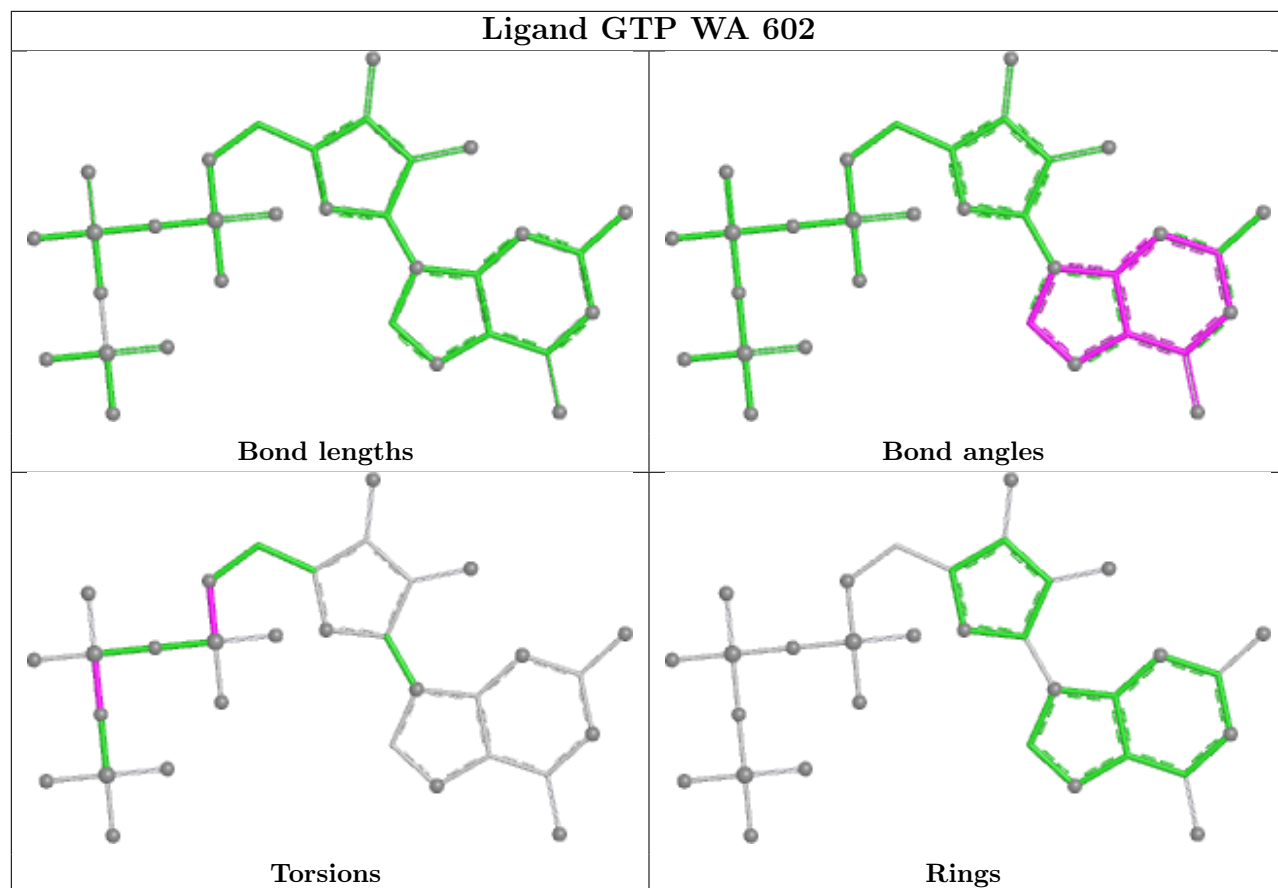
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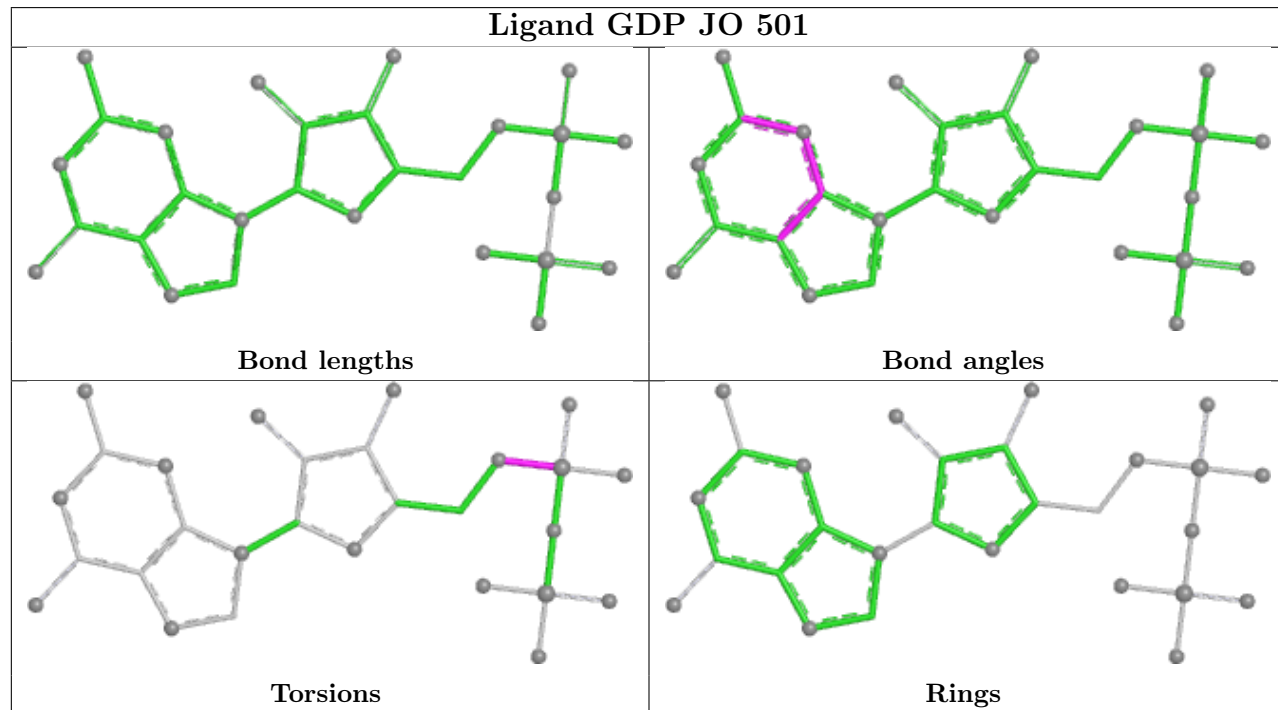




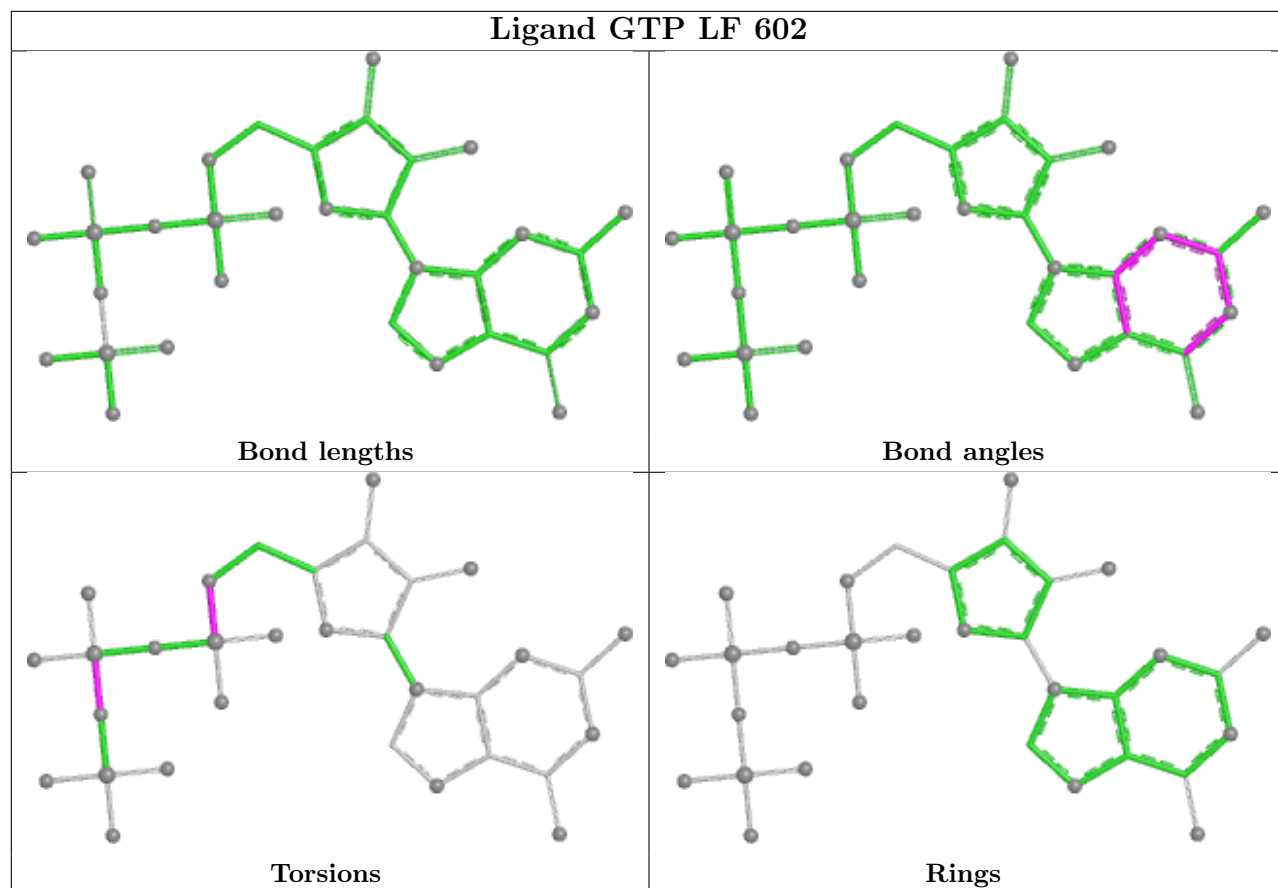
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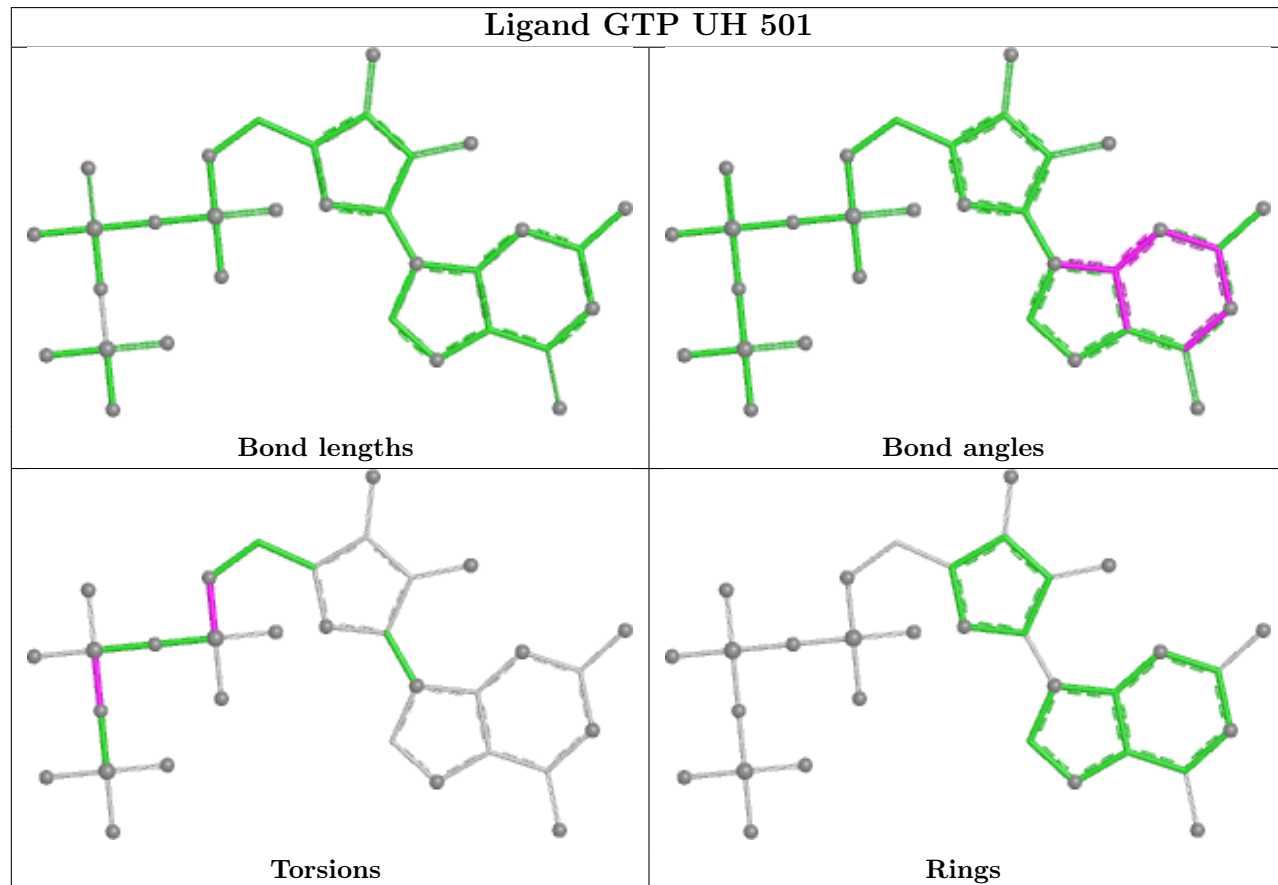
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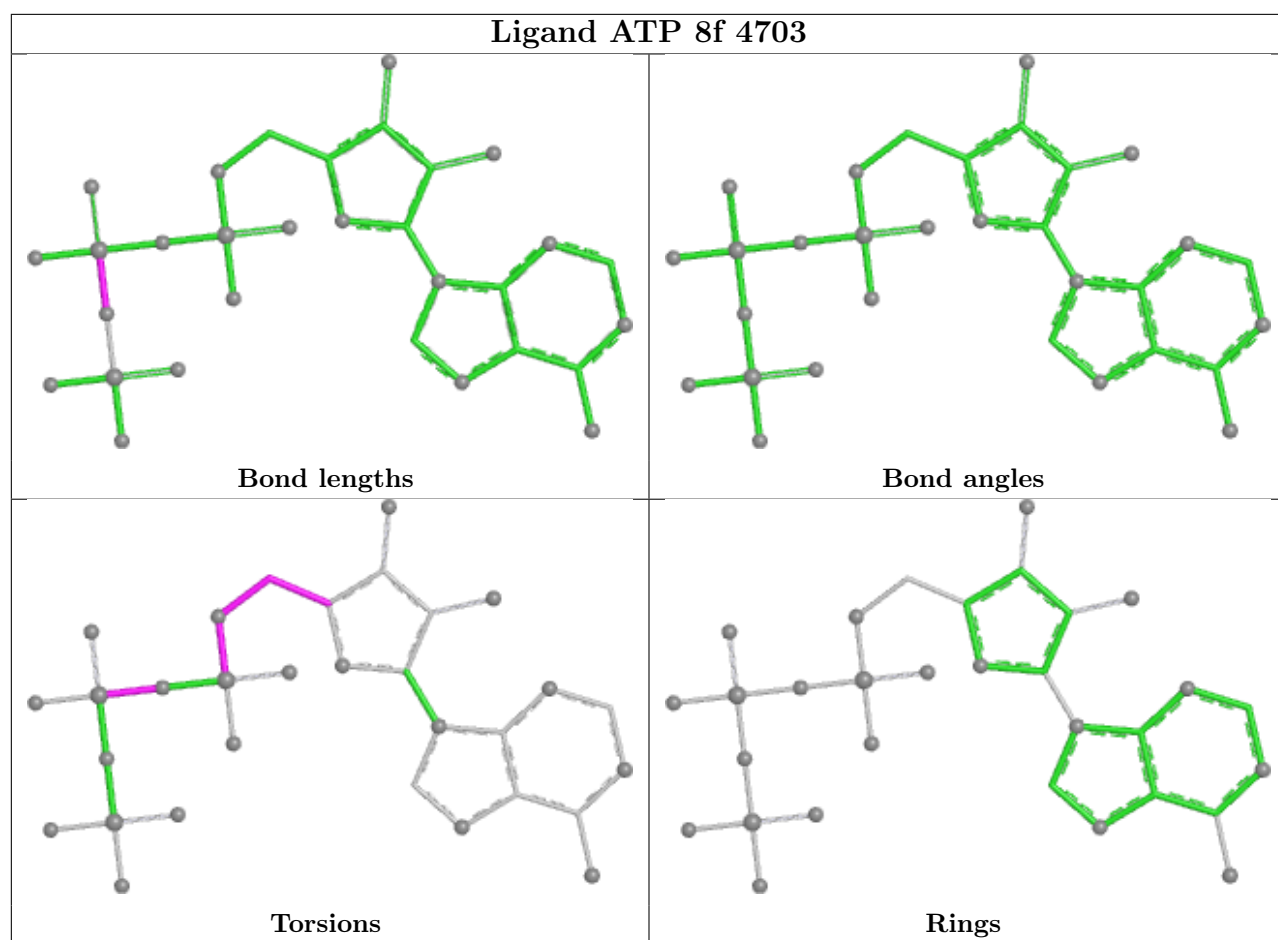


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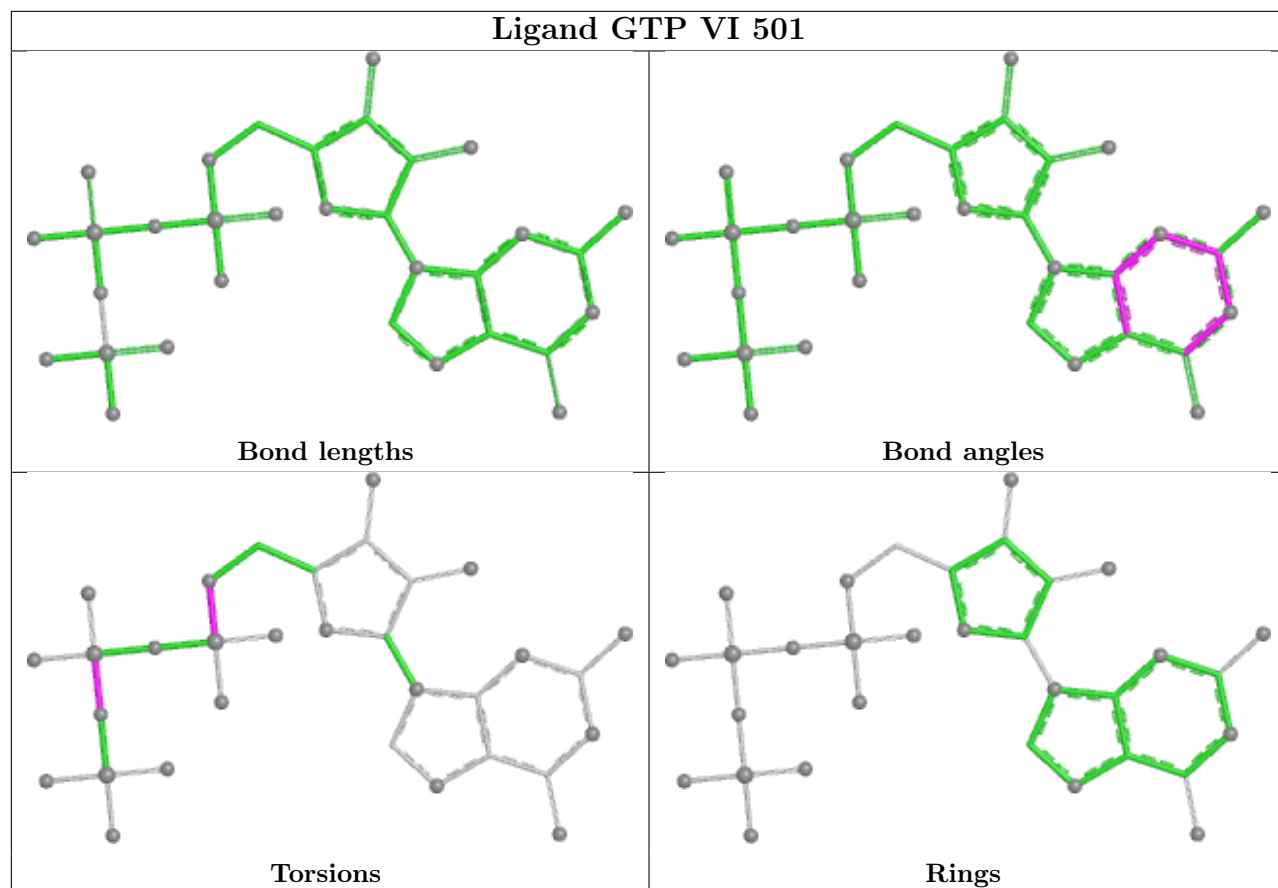


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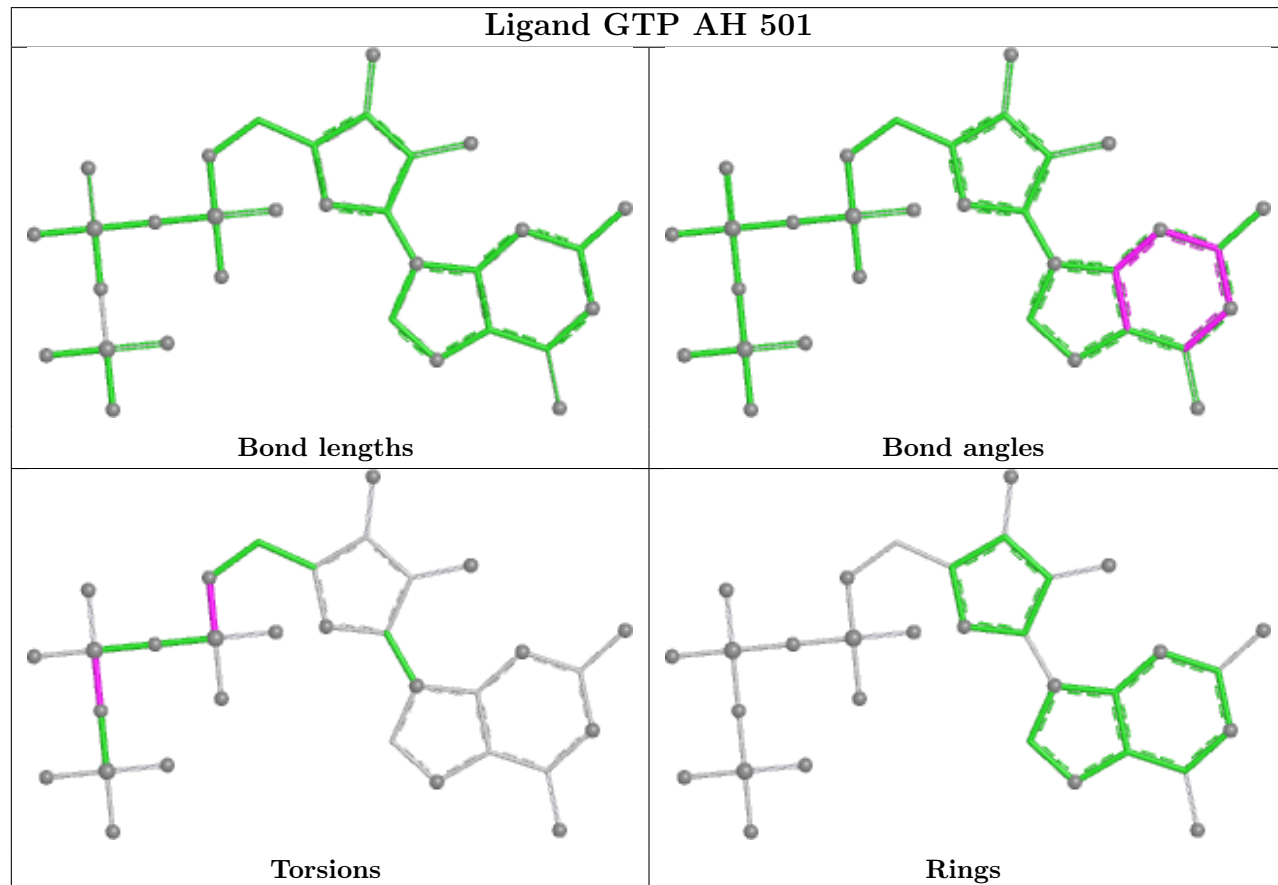




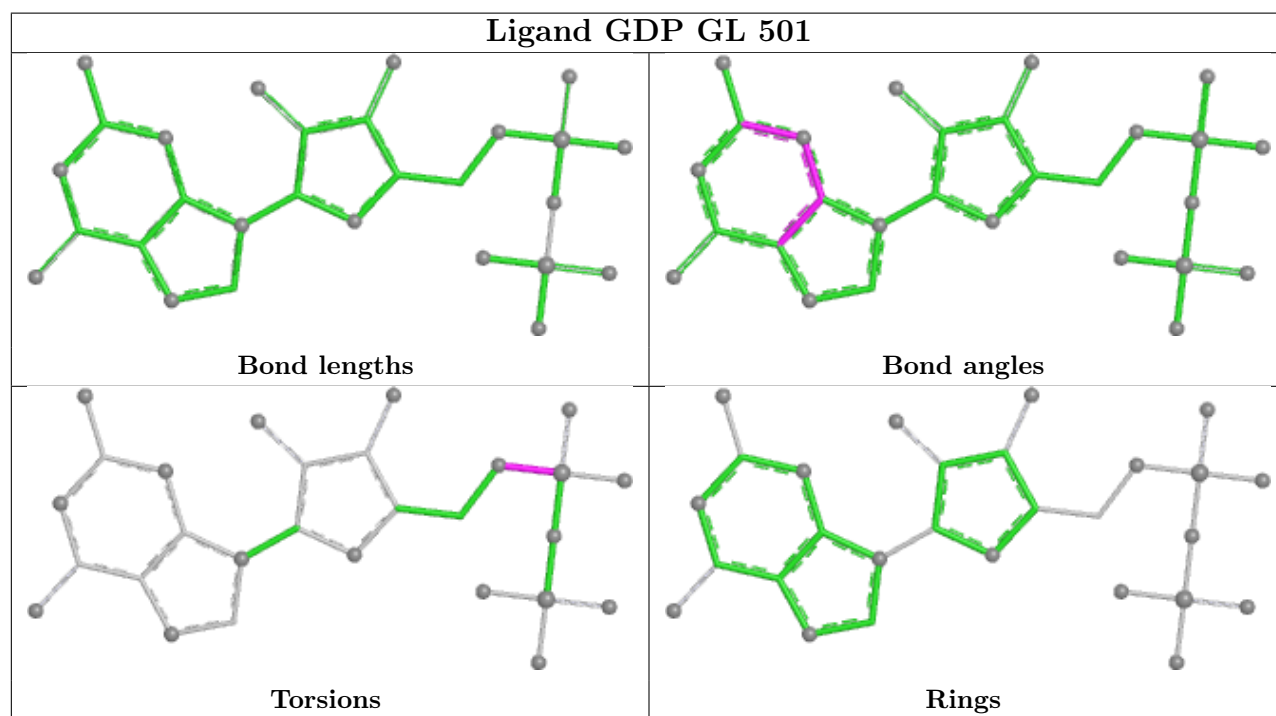
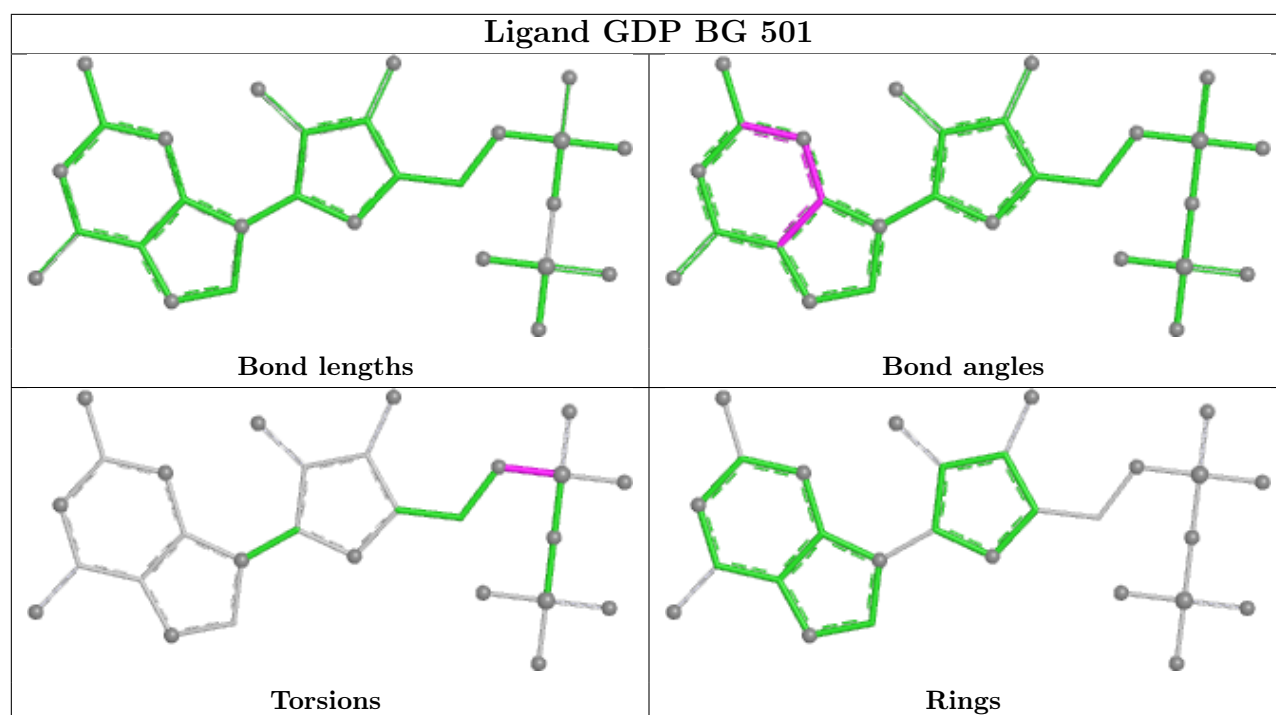
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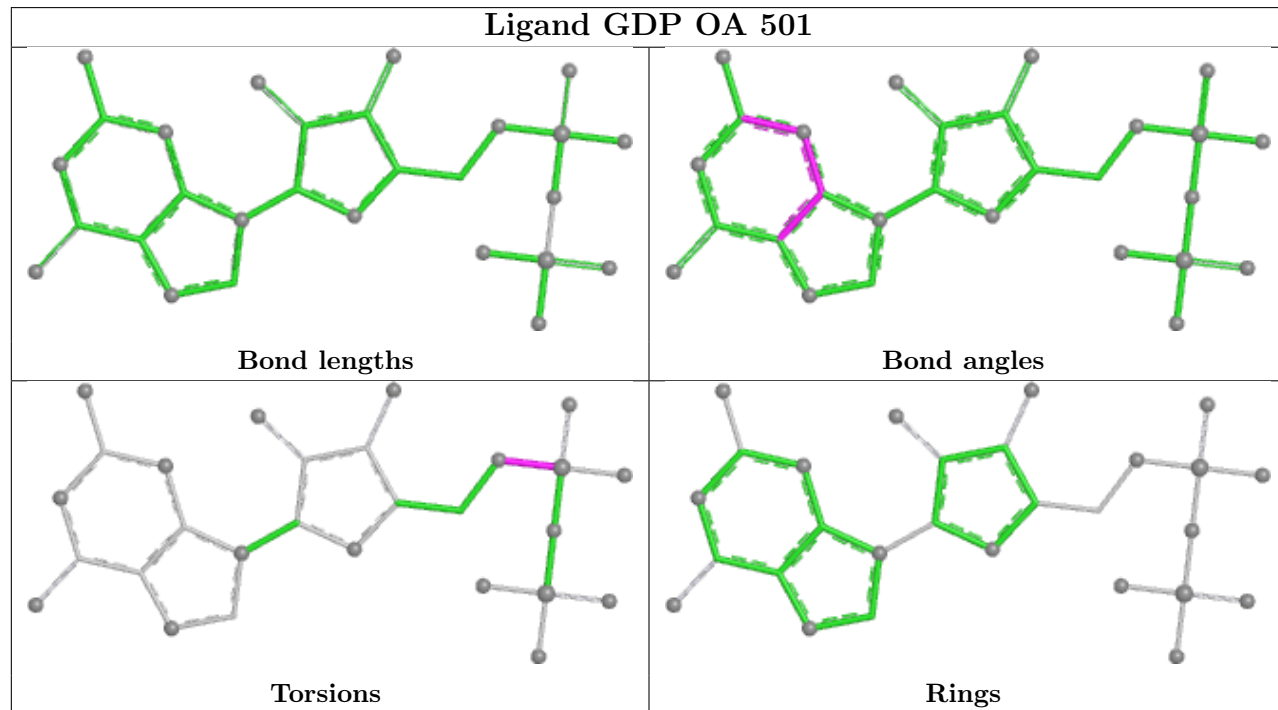
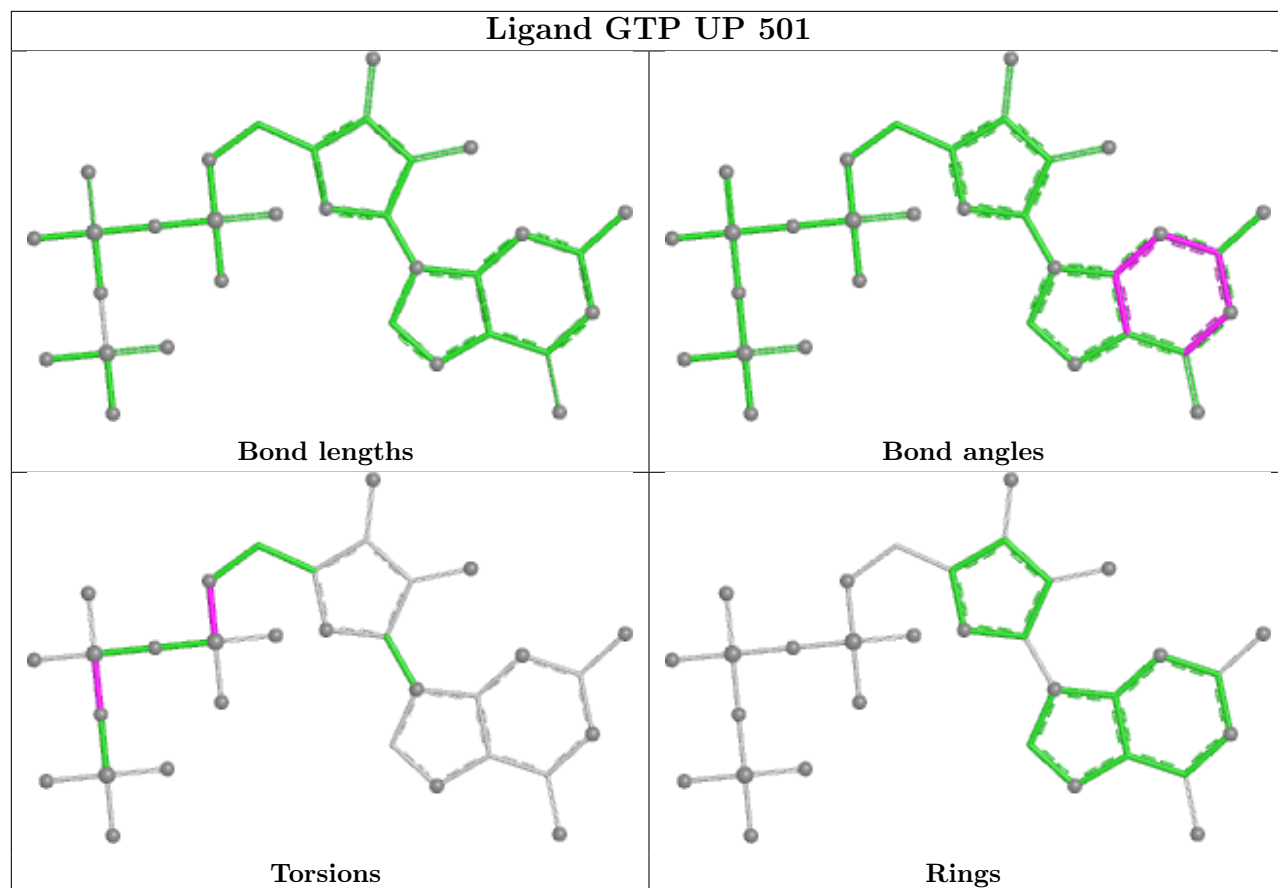


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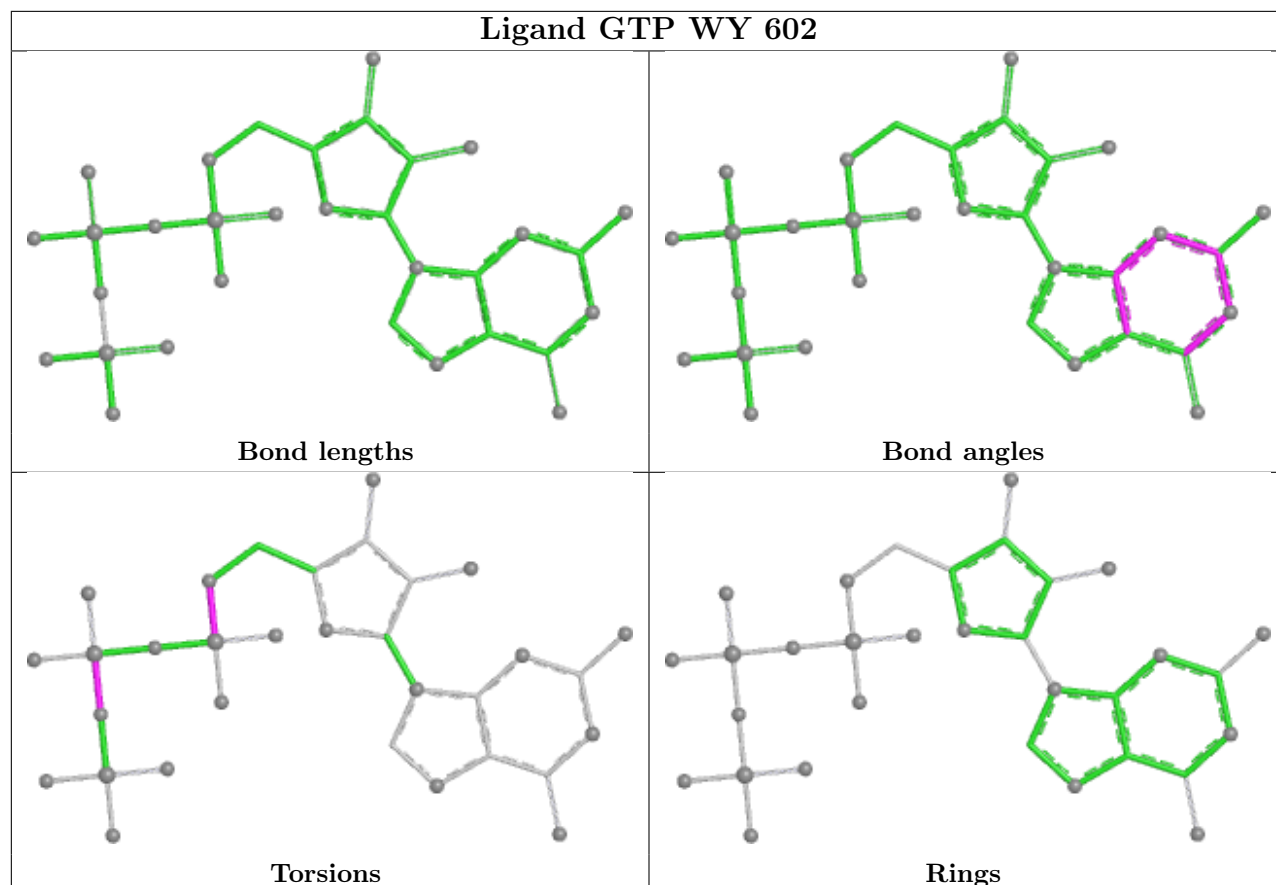




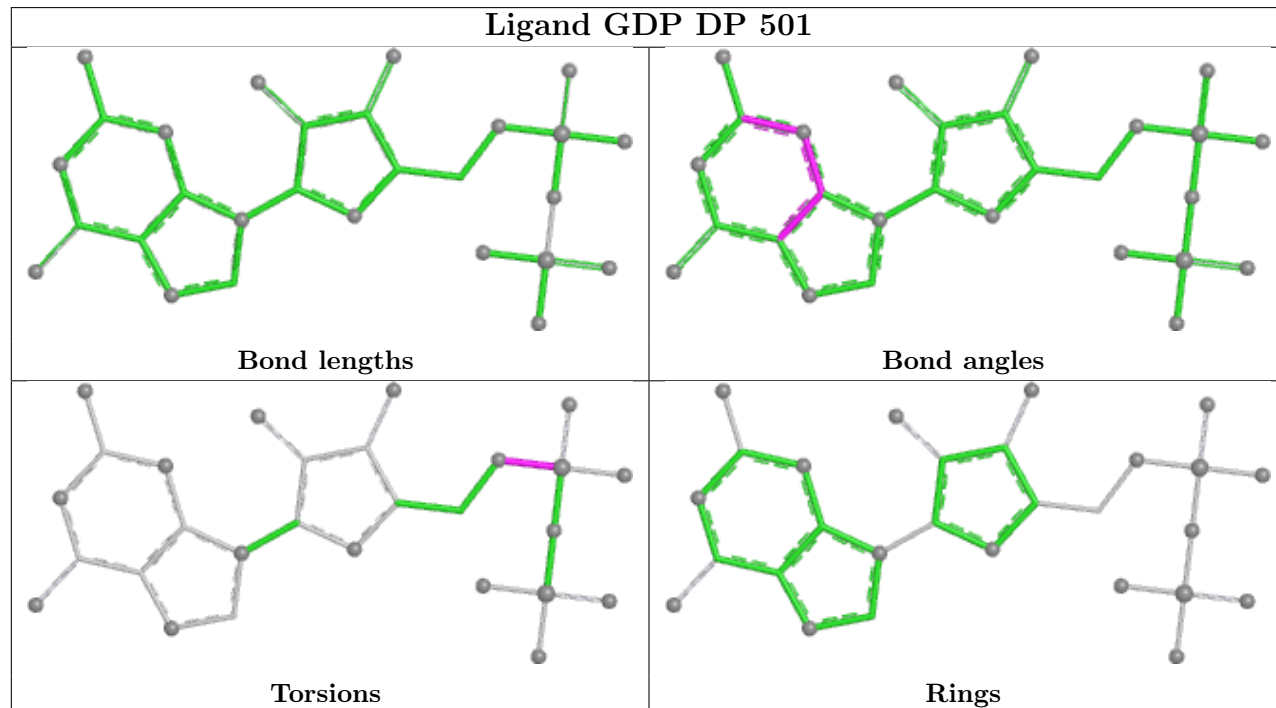


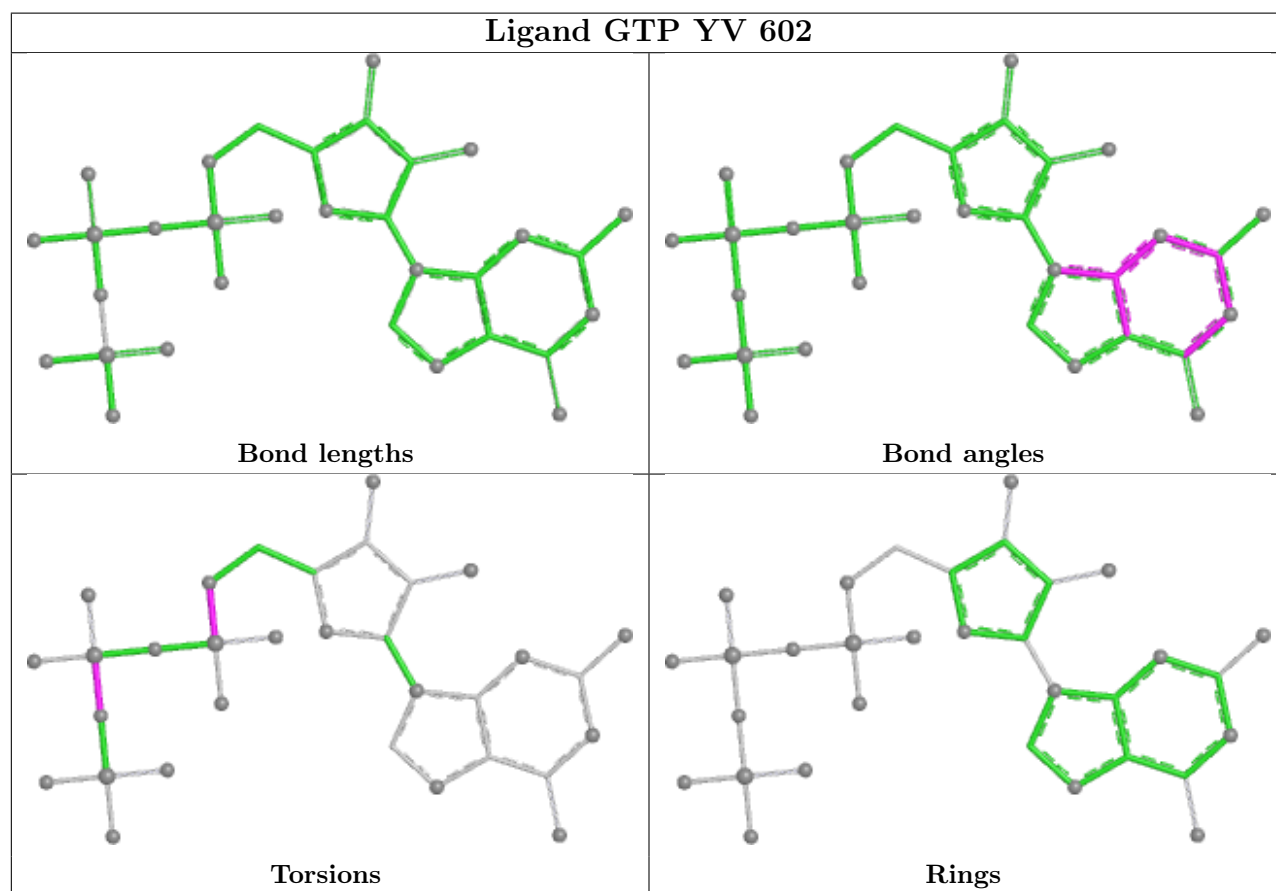
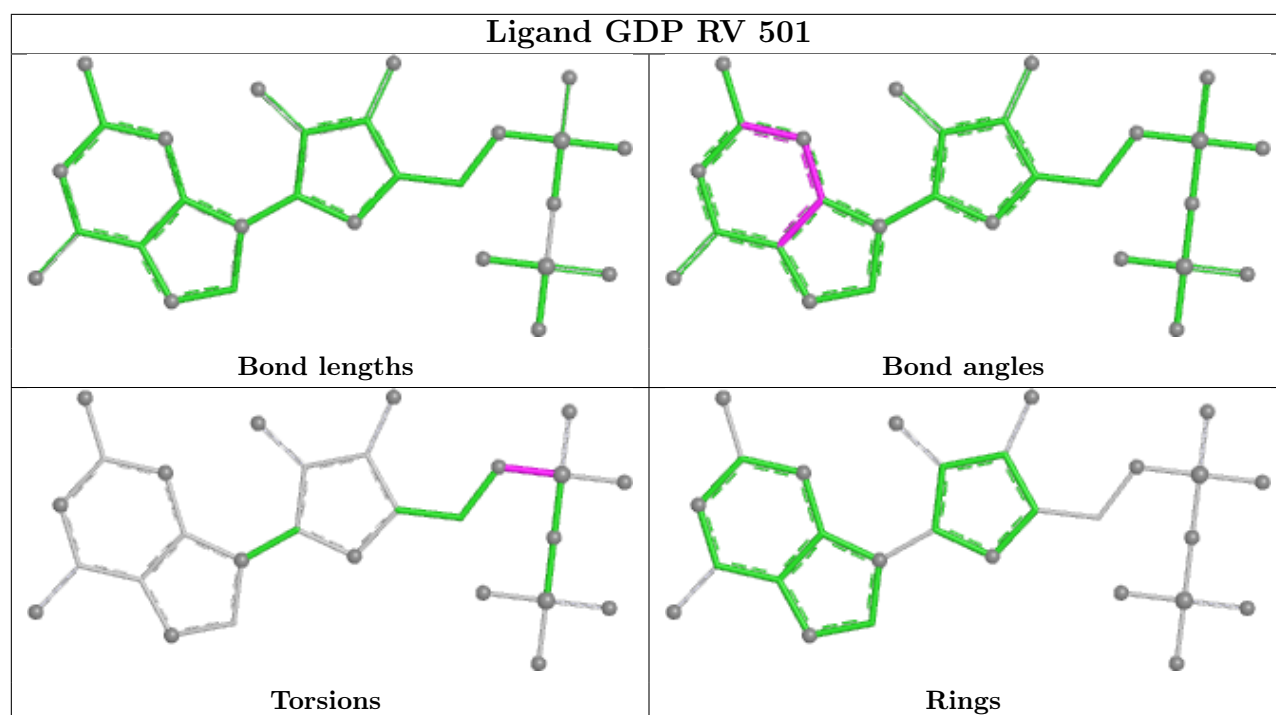


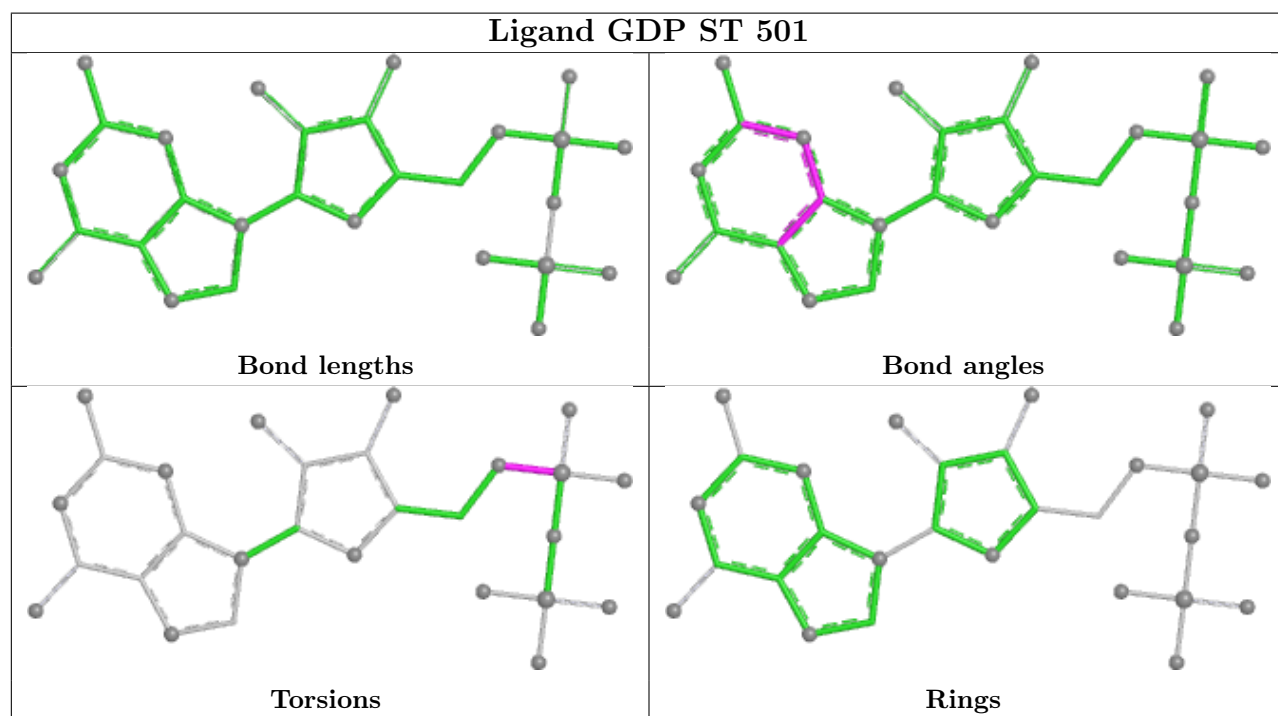
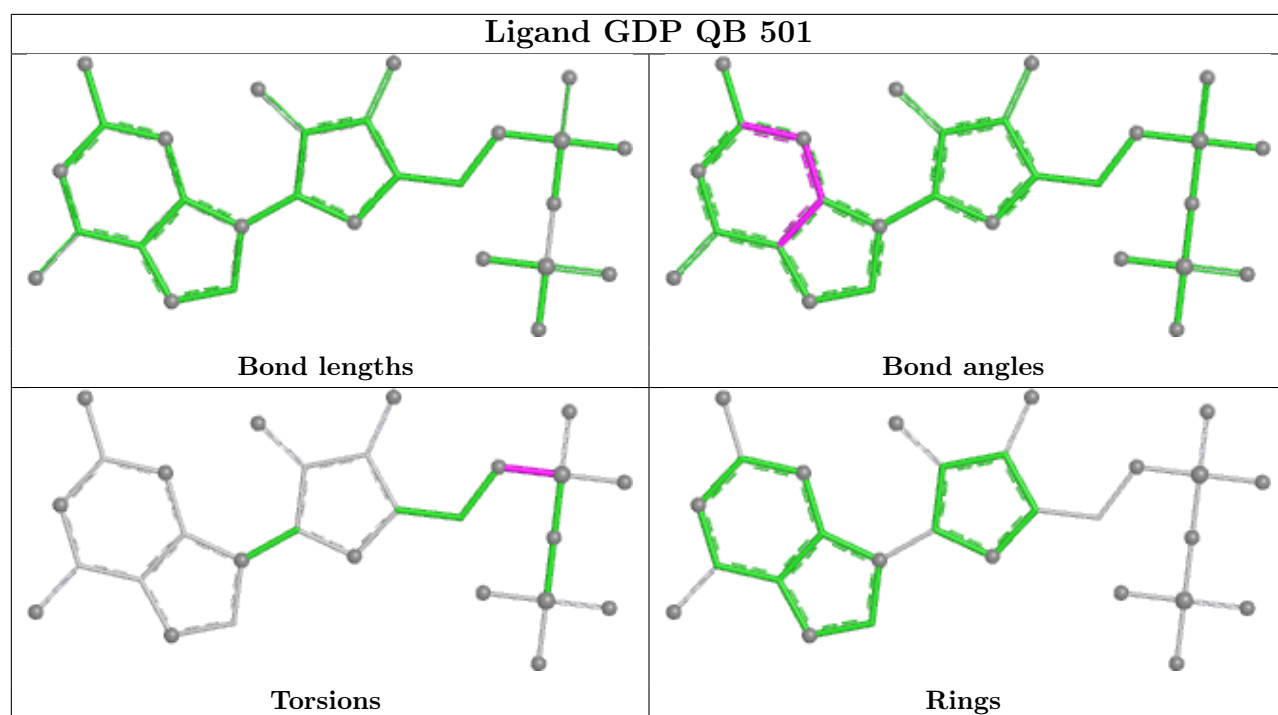
## Ligand GTP WY 602

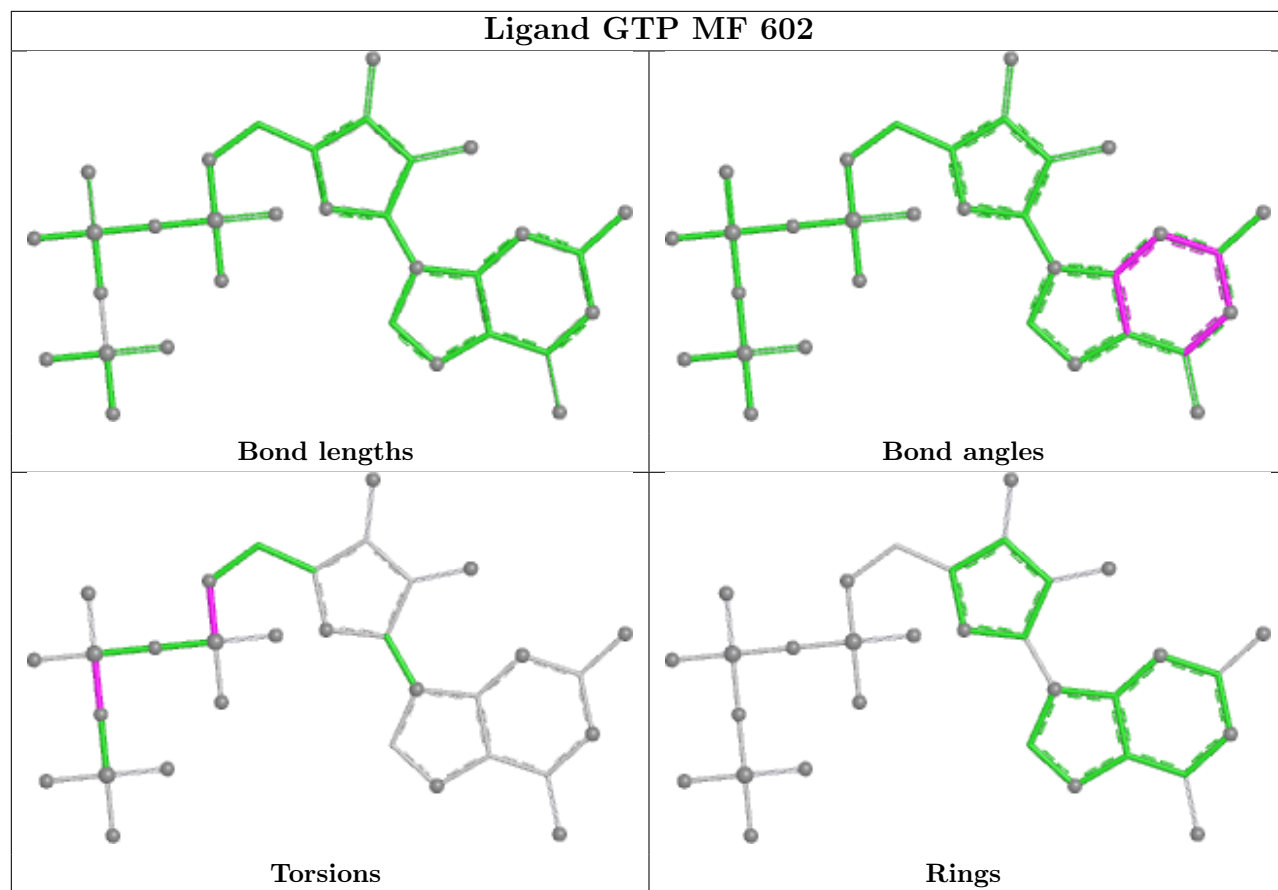


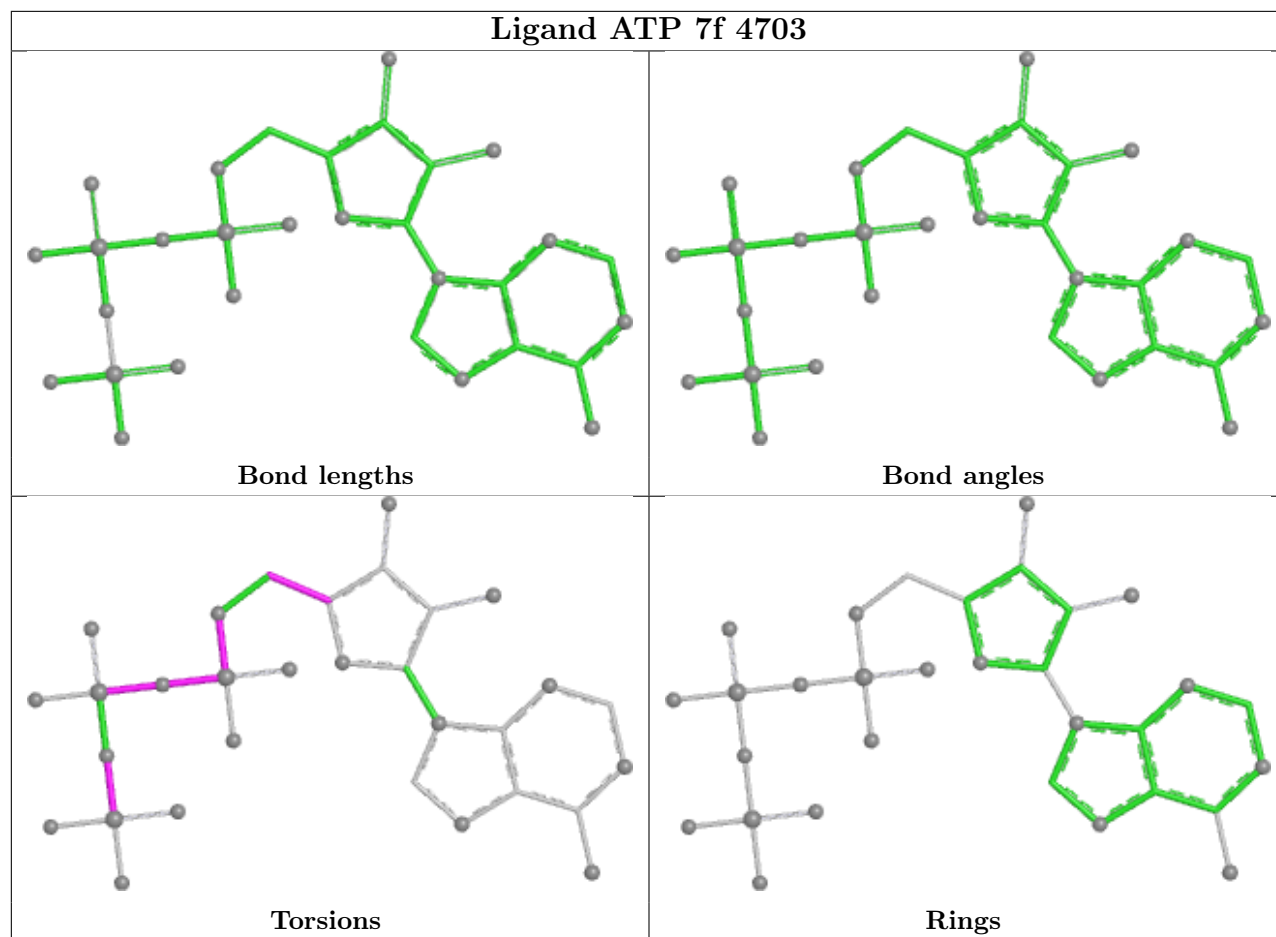
## Ligand GDP DP 501

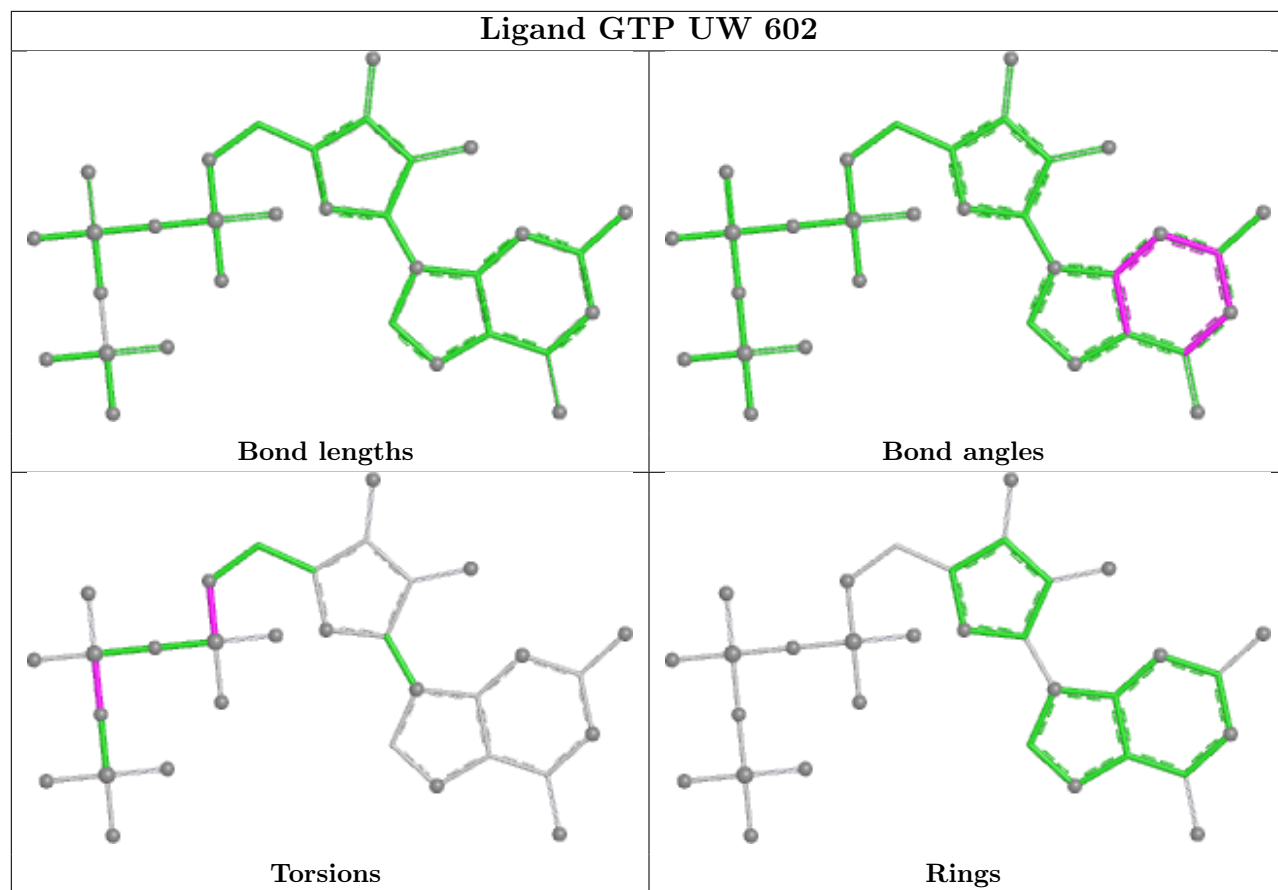




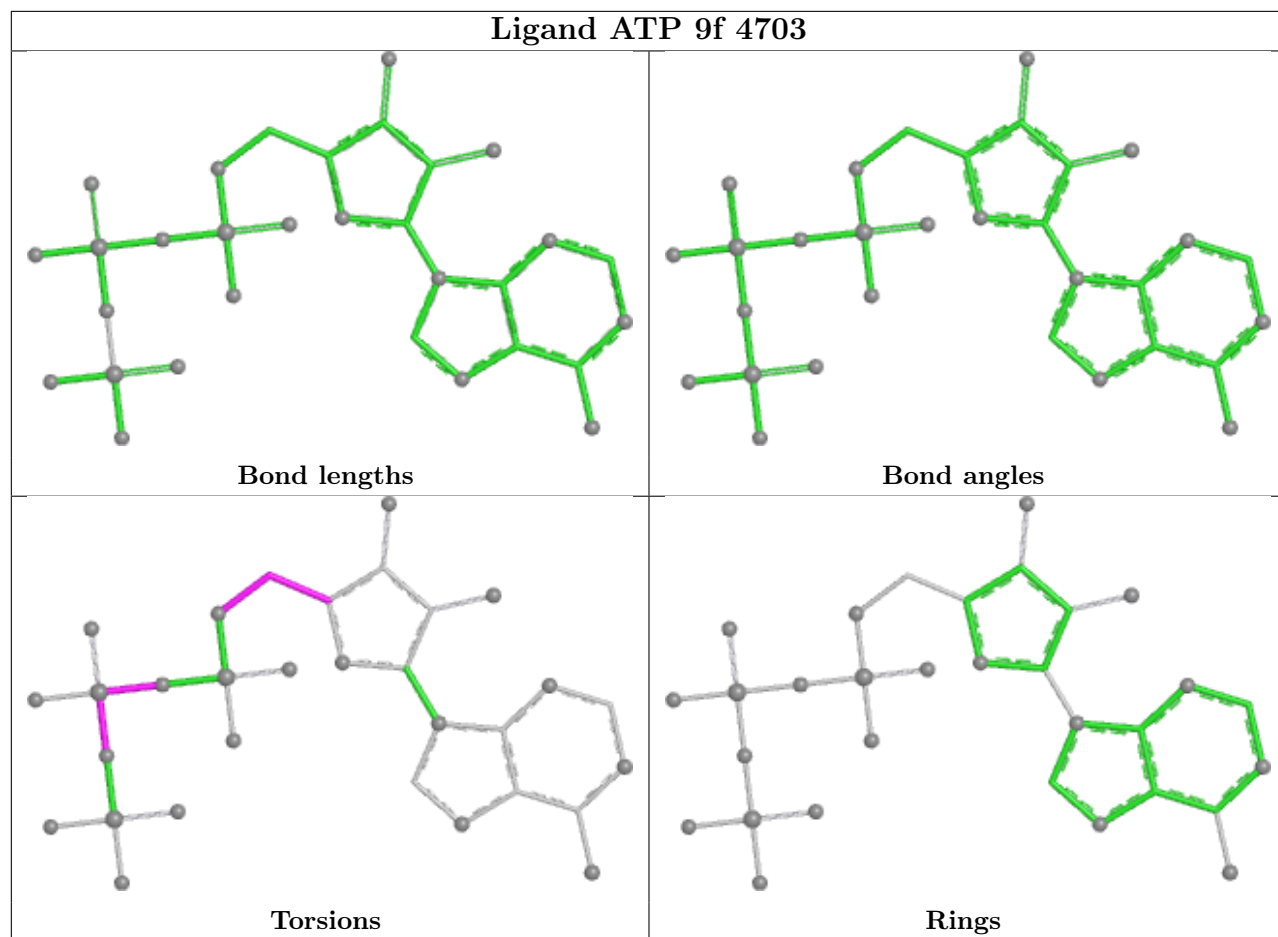




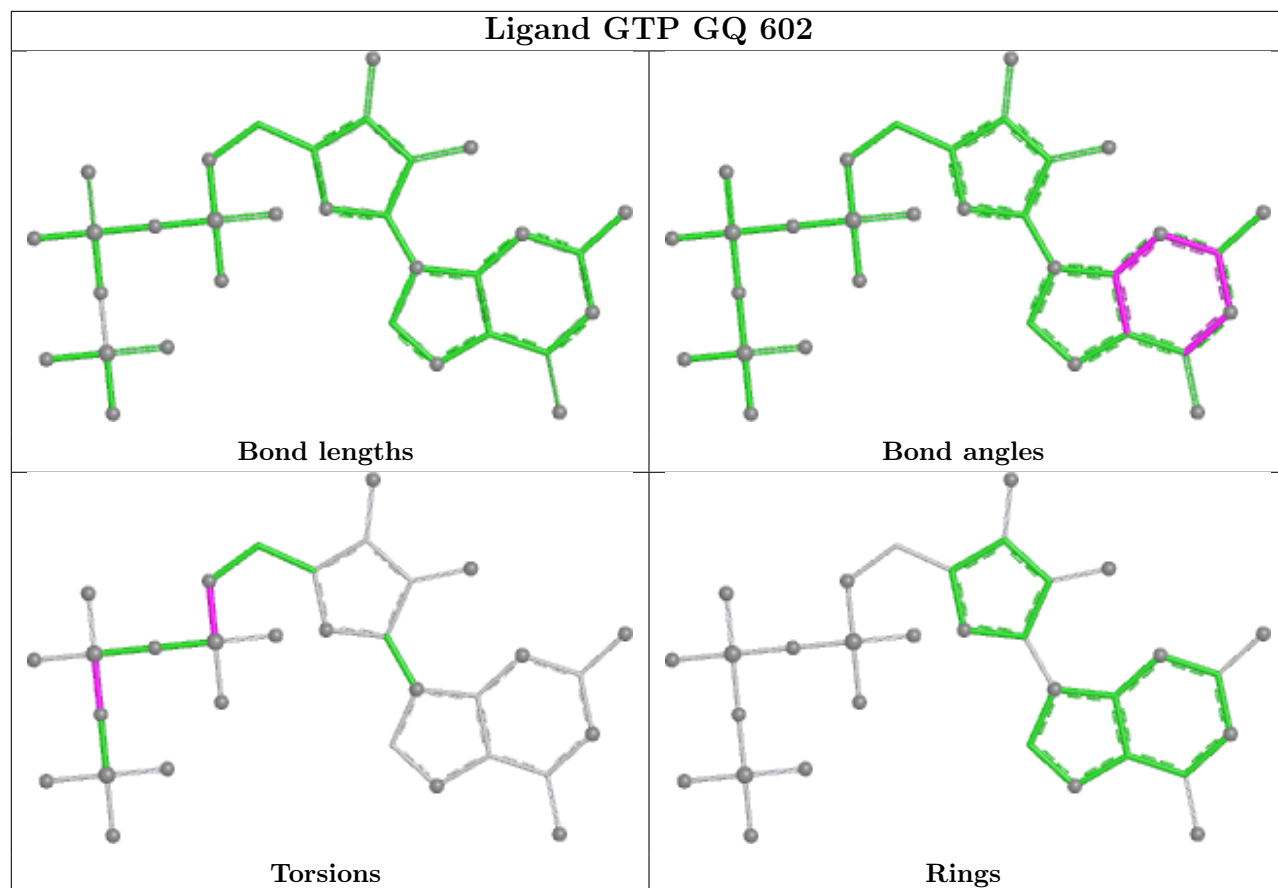




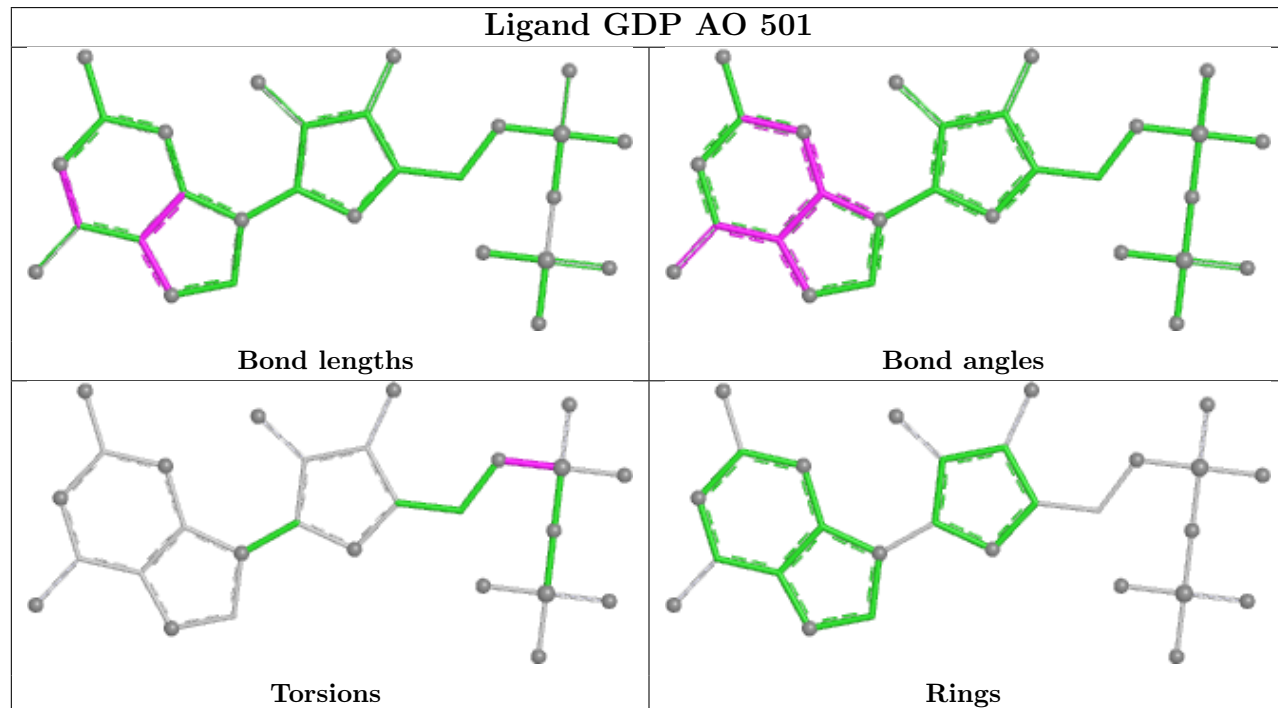


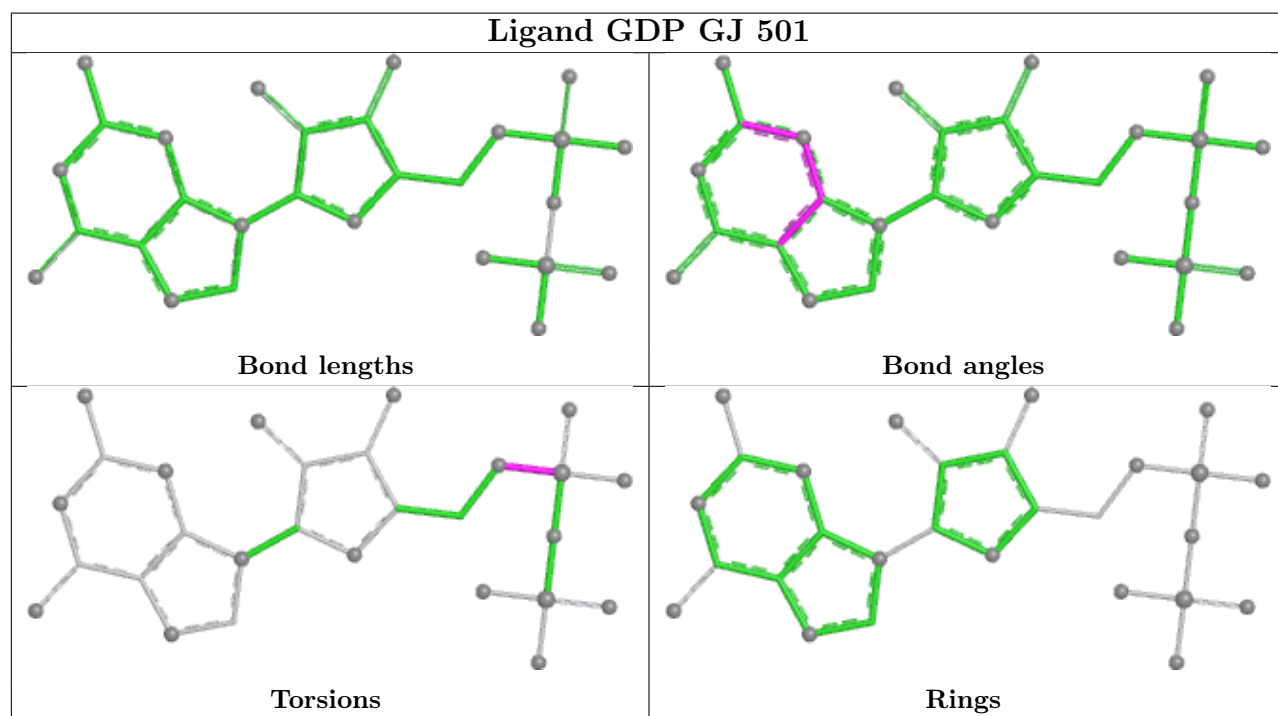
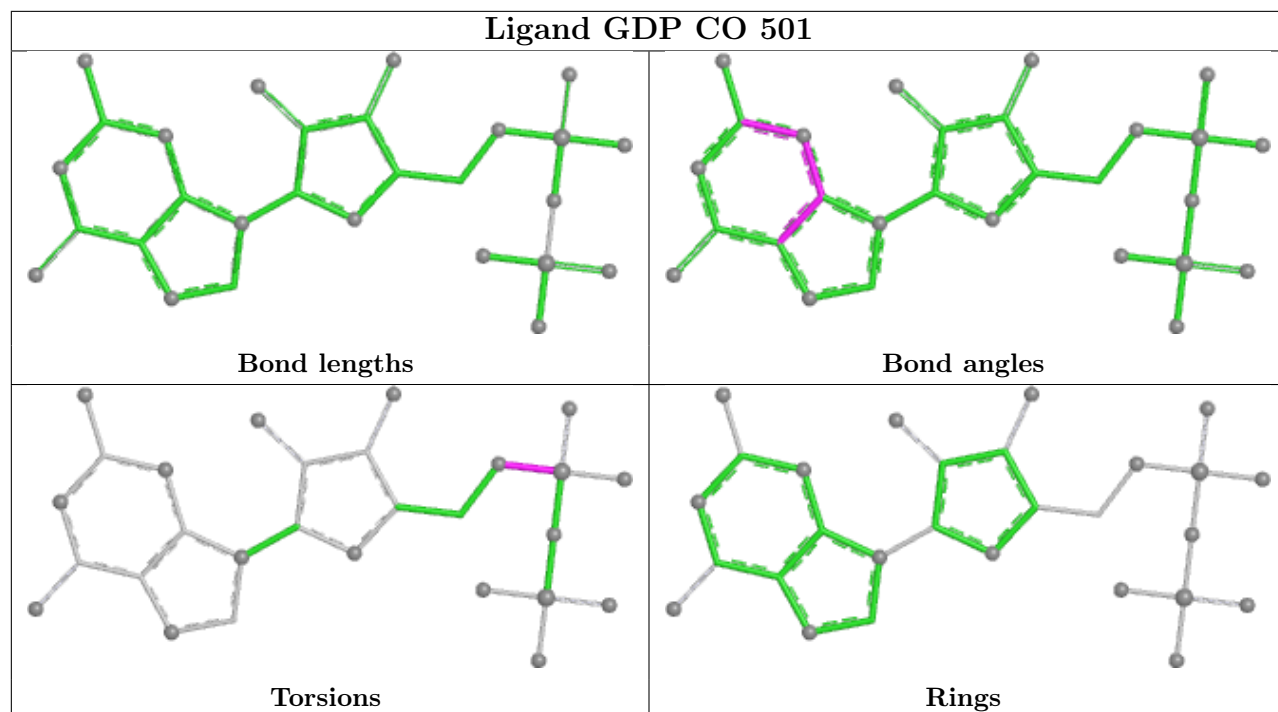


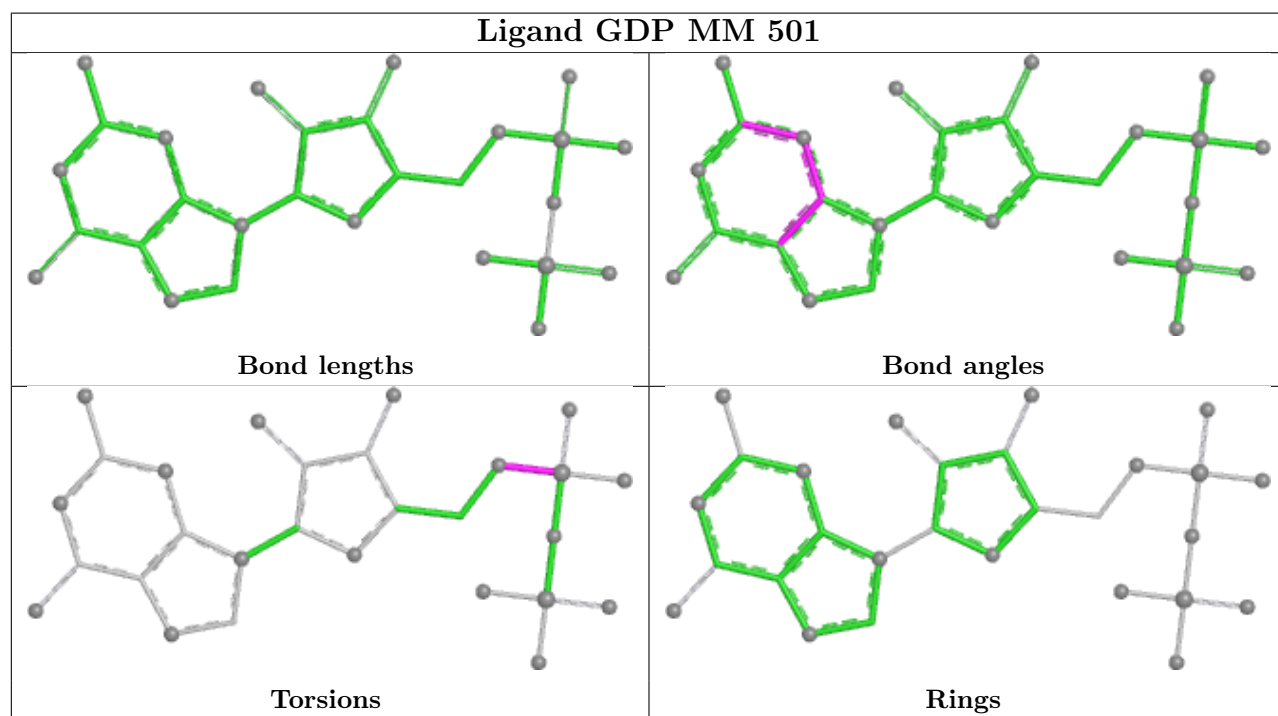
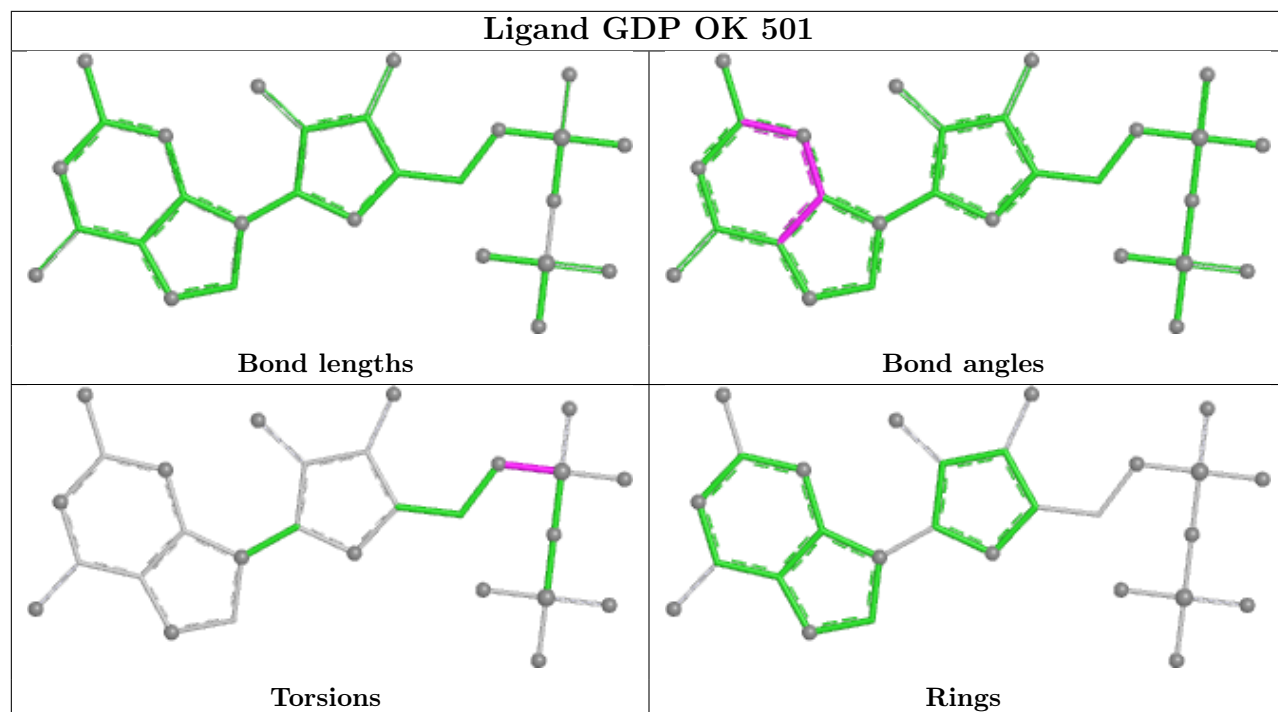
## Ligand GTP GQ 602

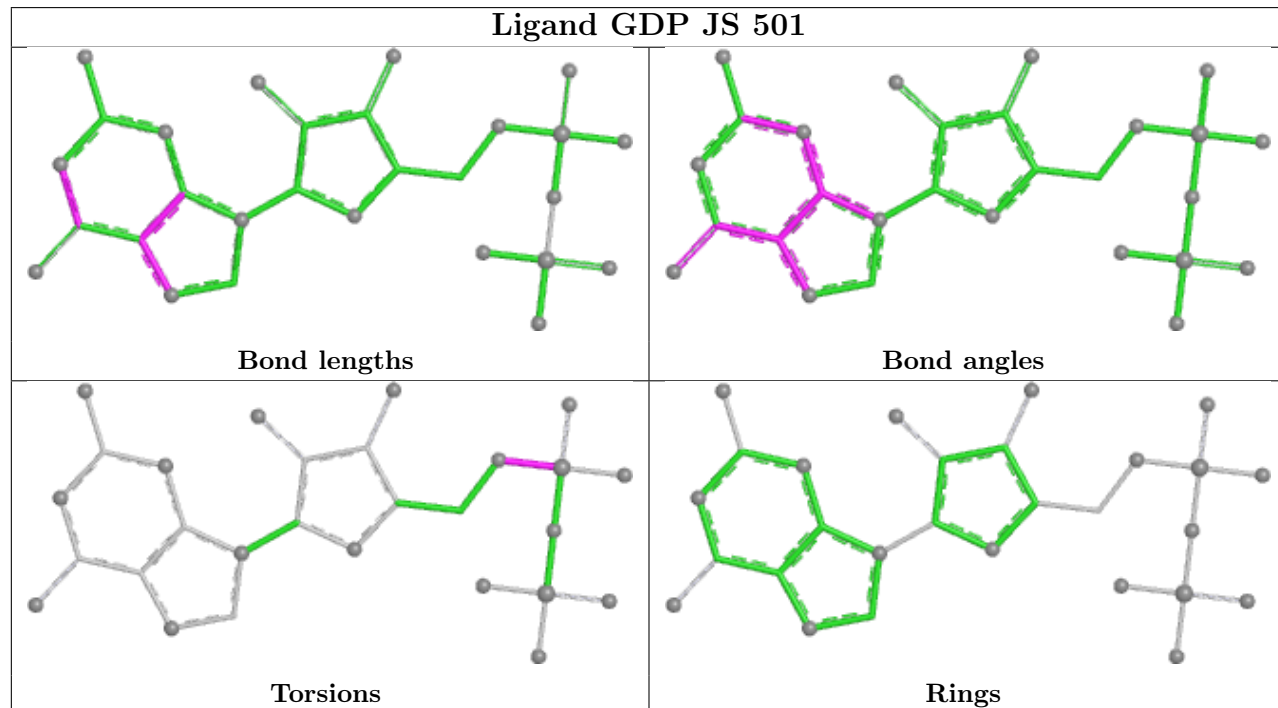
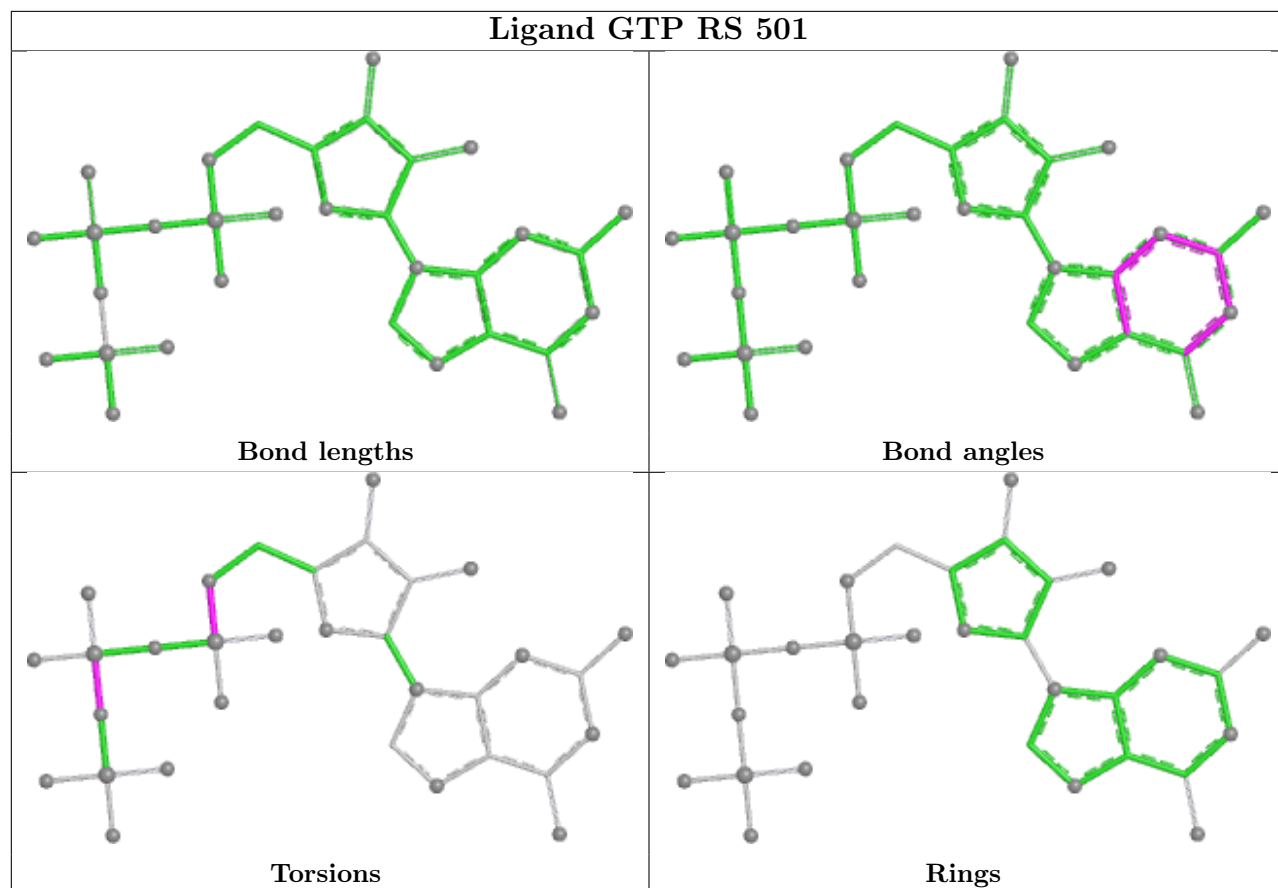


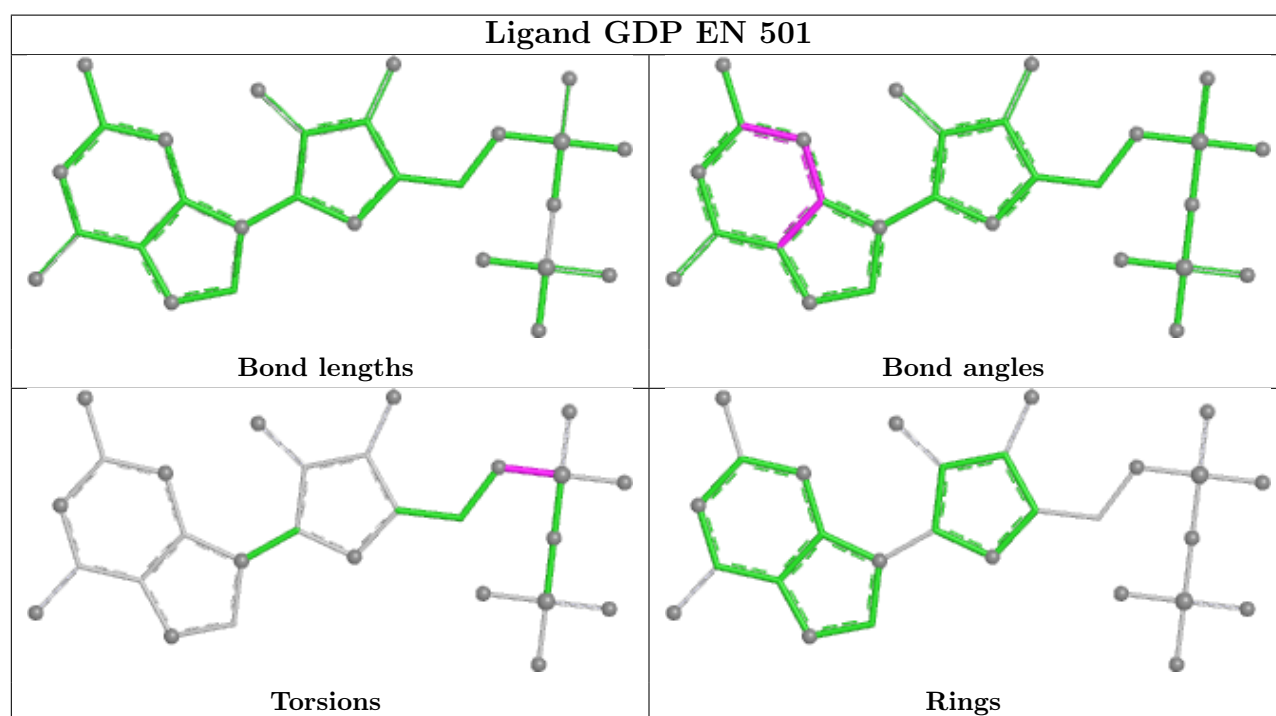
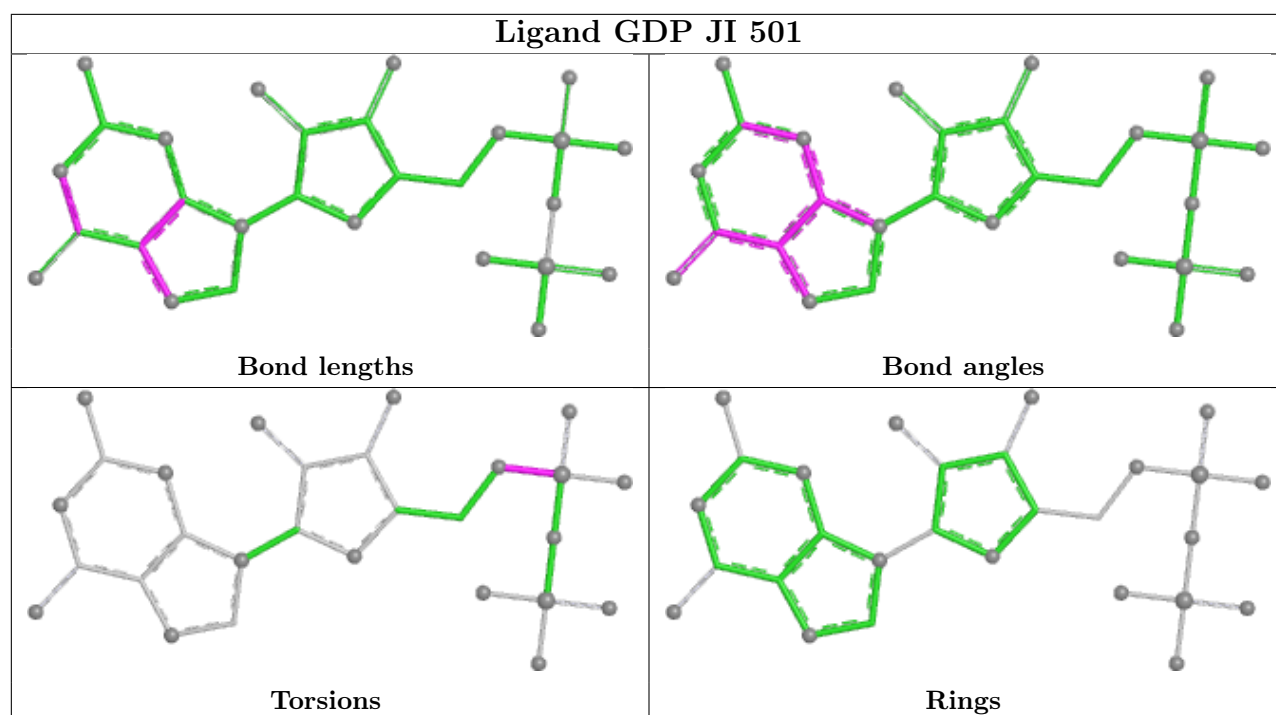
## Ligand GDP AO 501

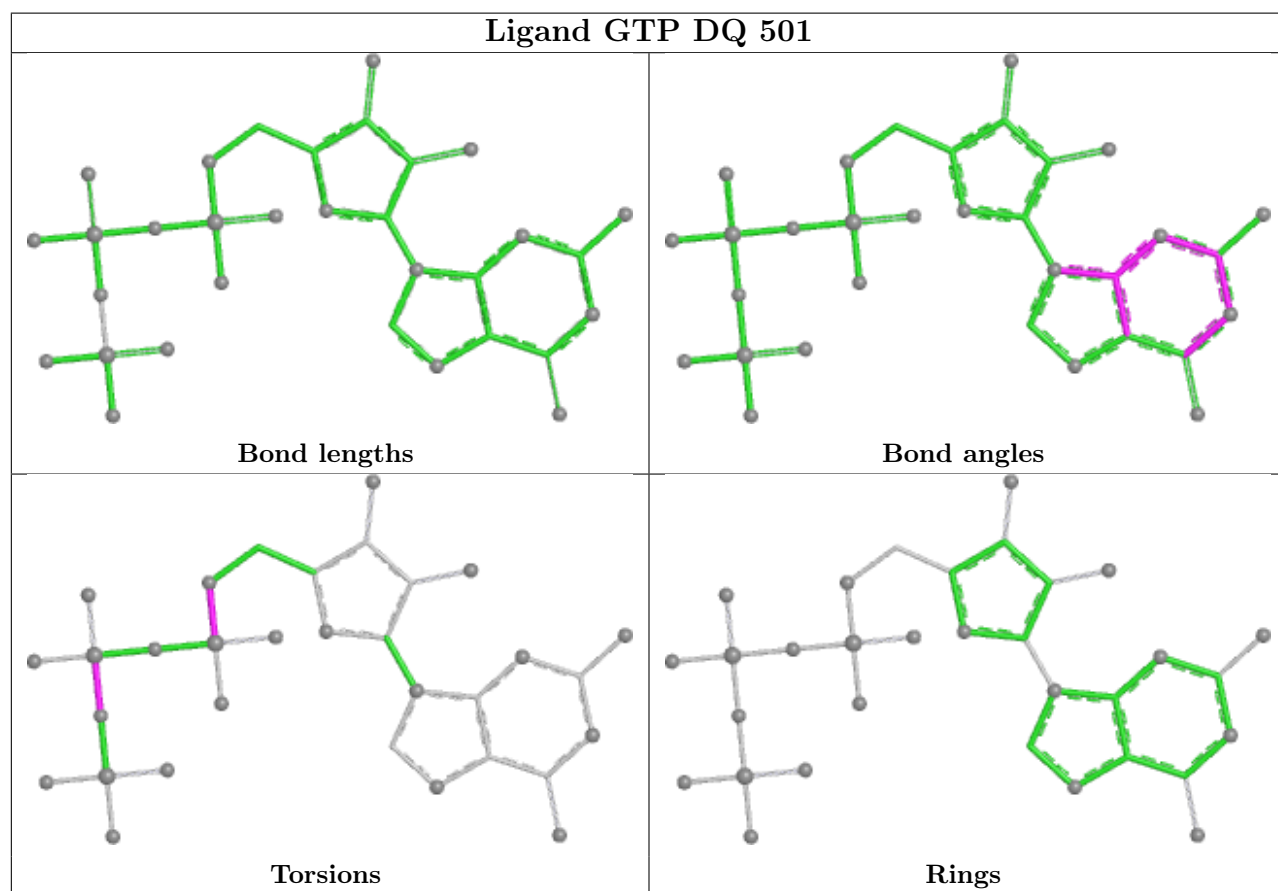
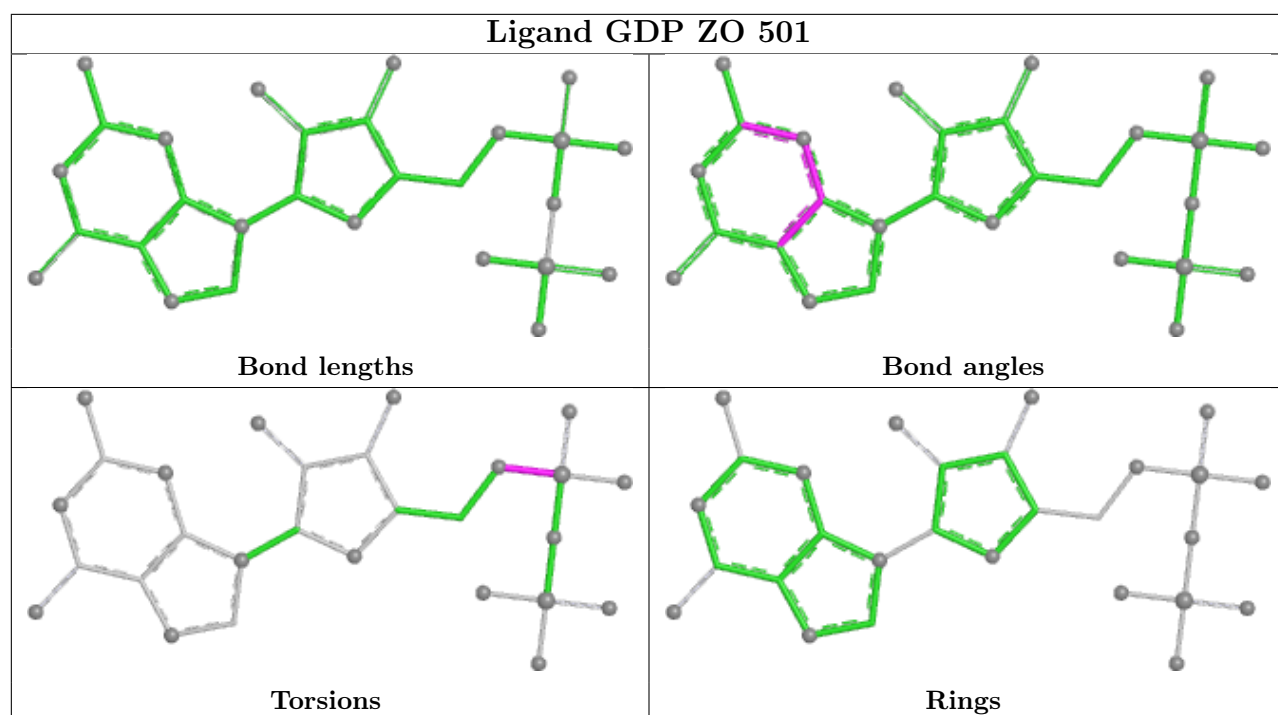




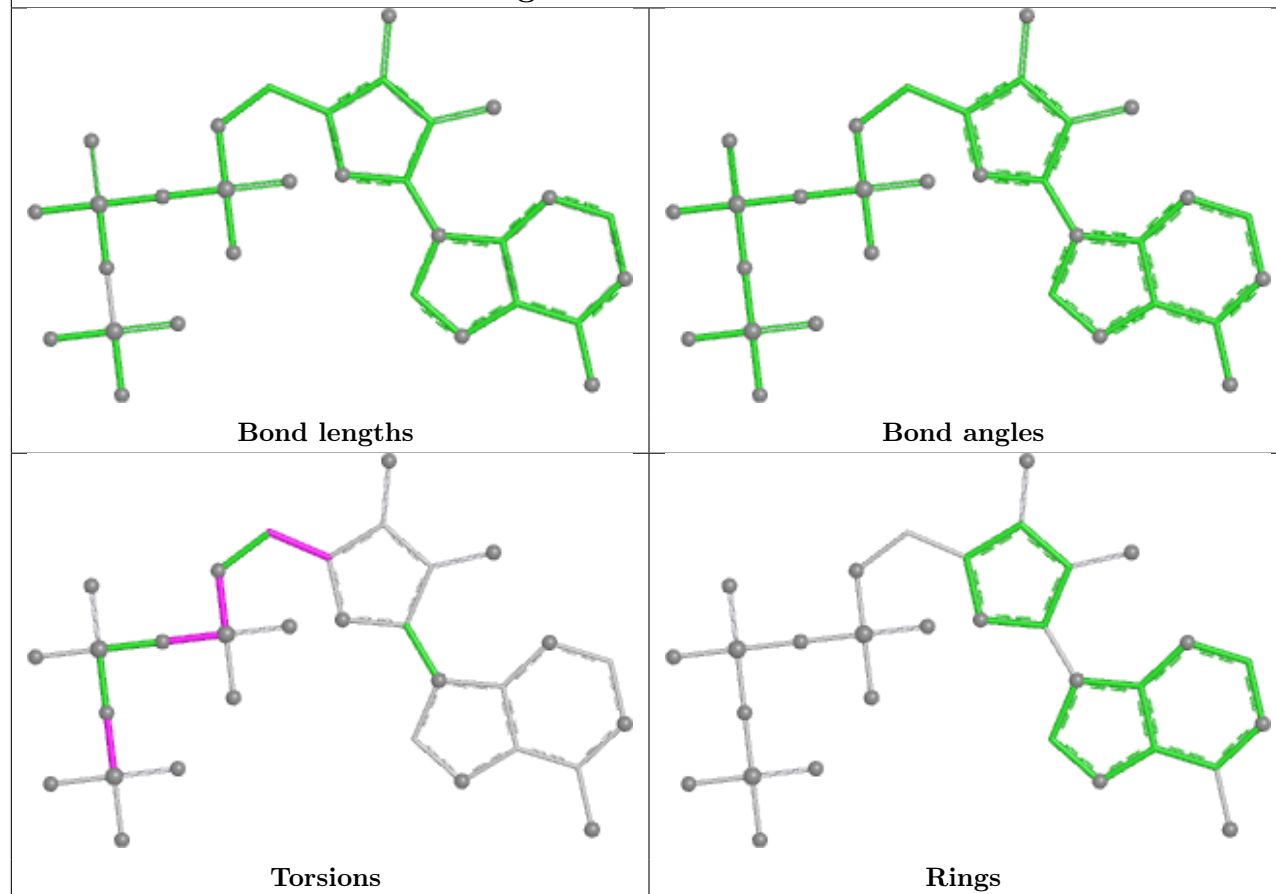




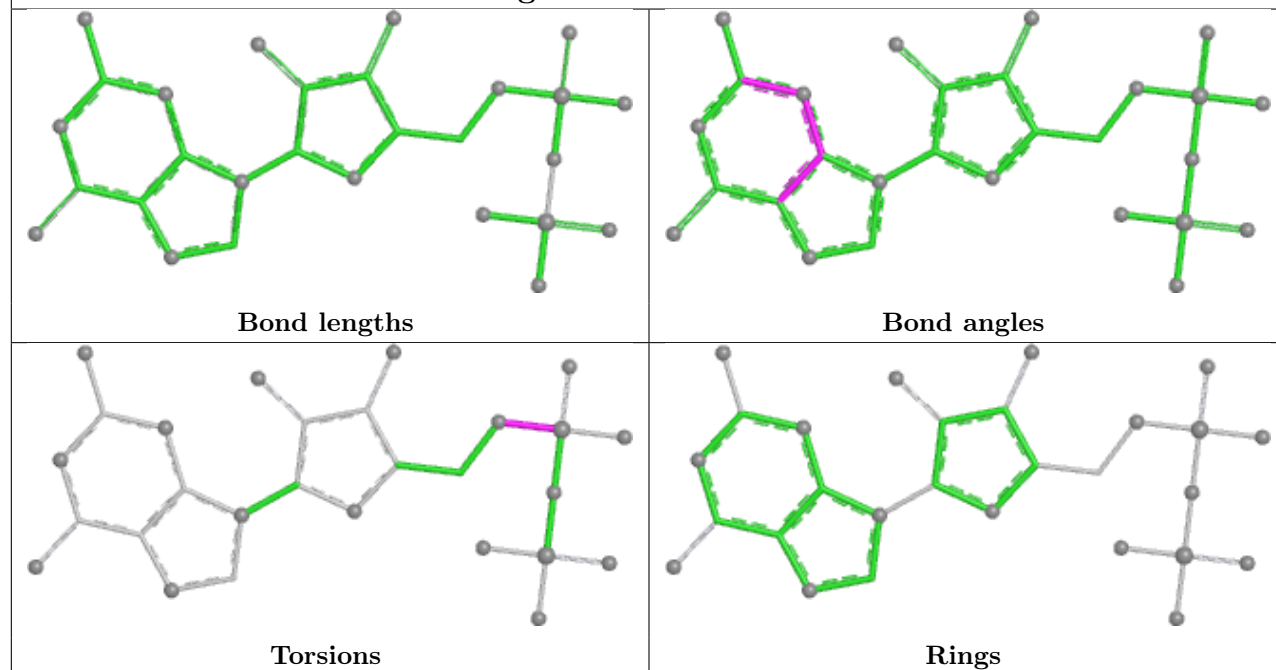




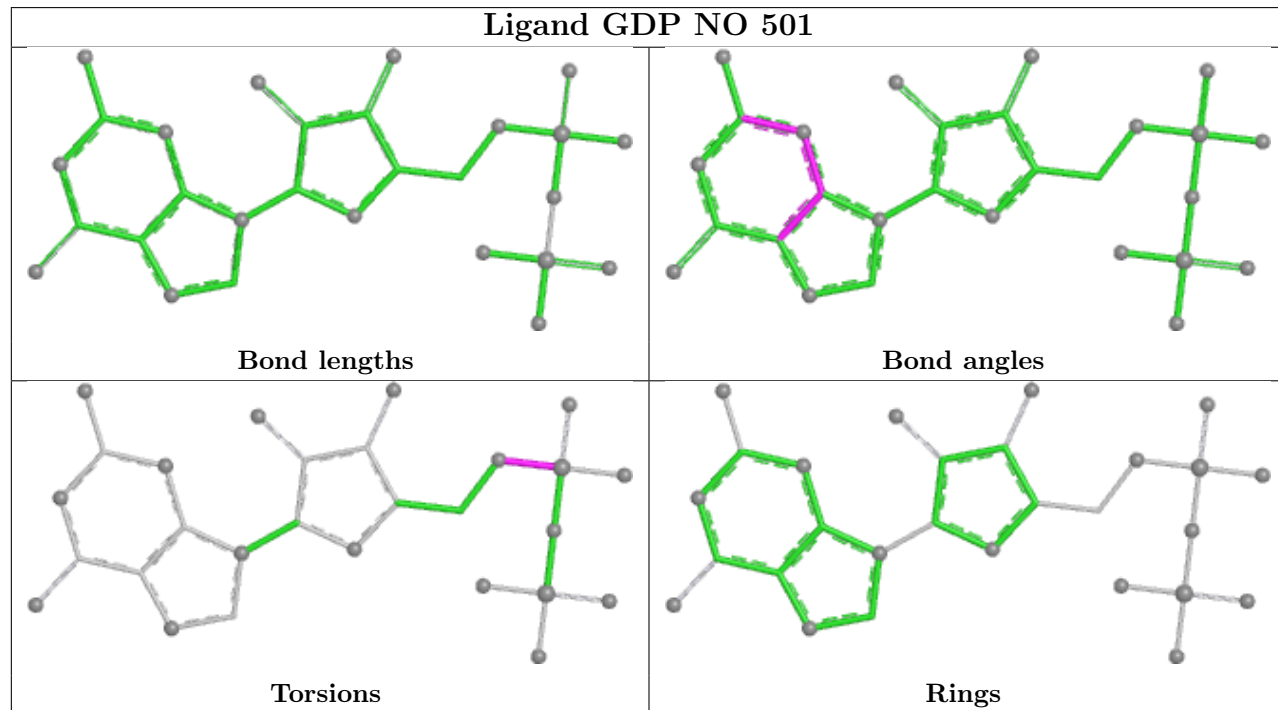
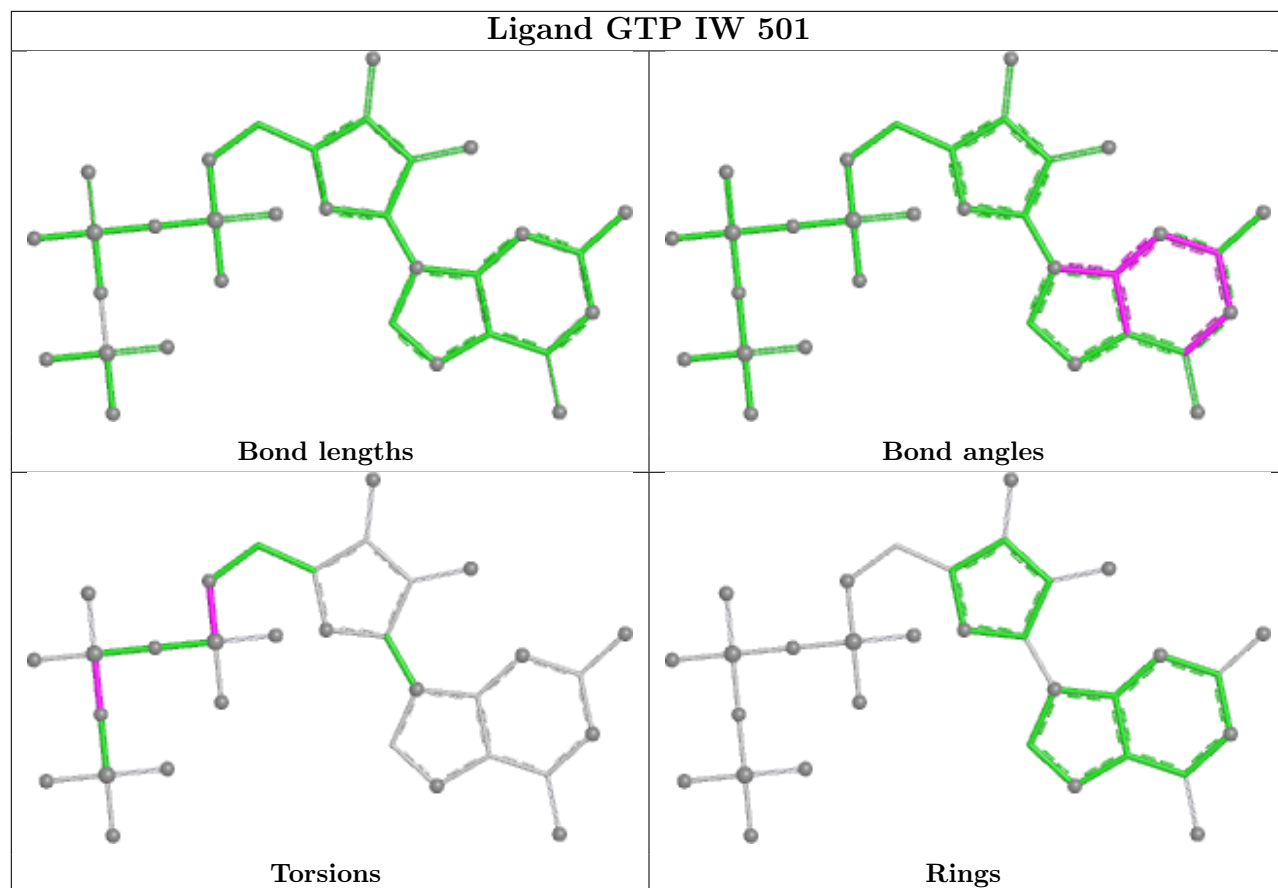
## Ligand ATP 7b 4703



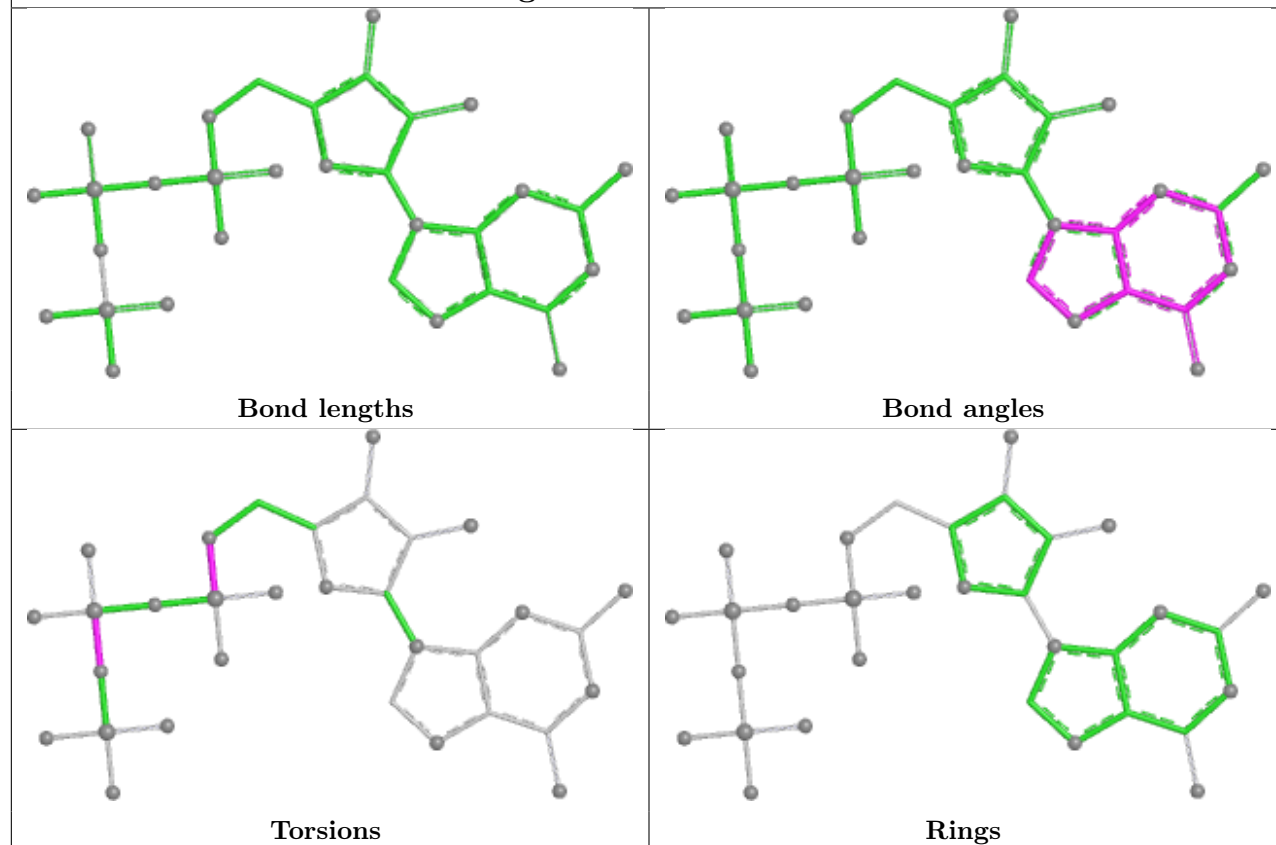
## Ligand GDP PA 501



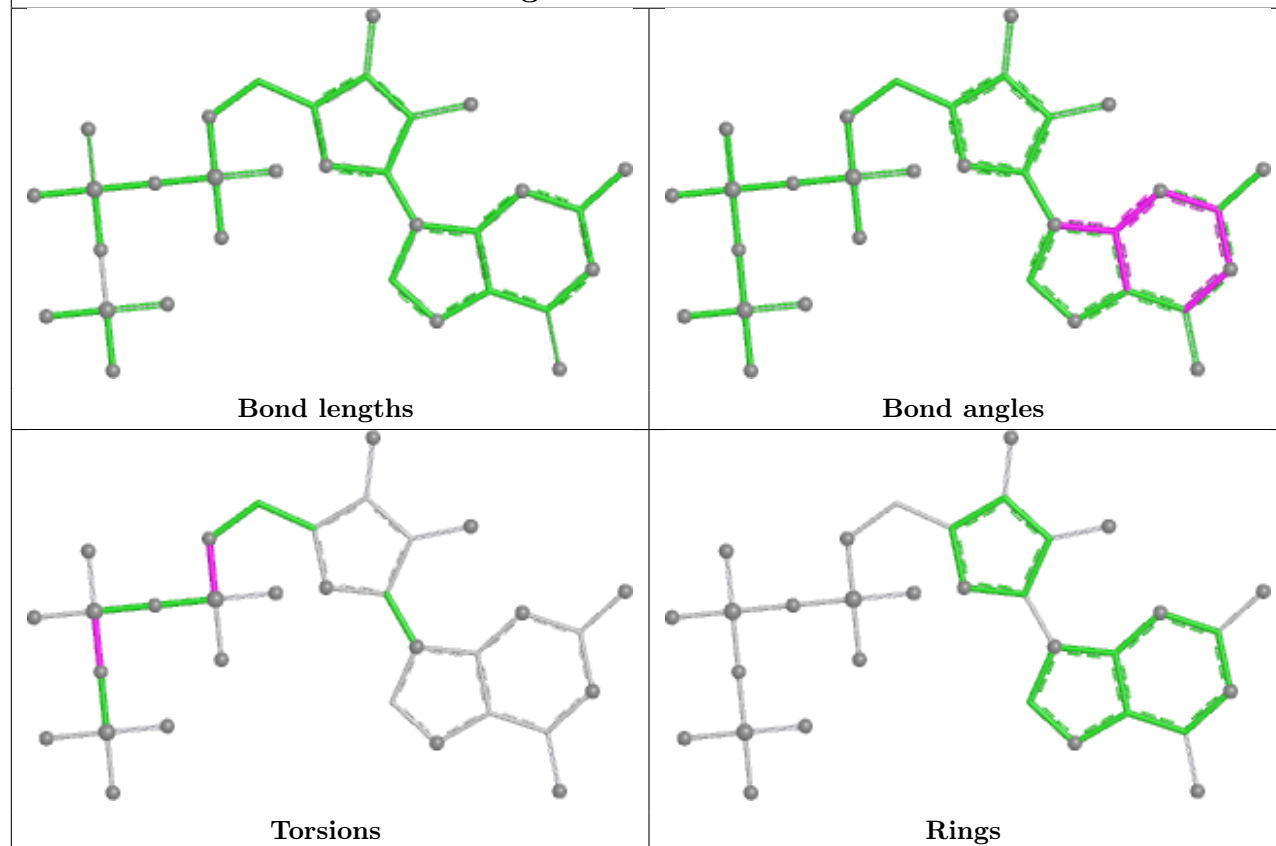




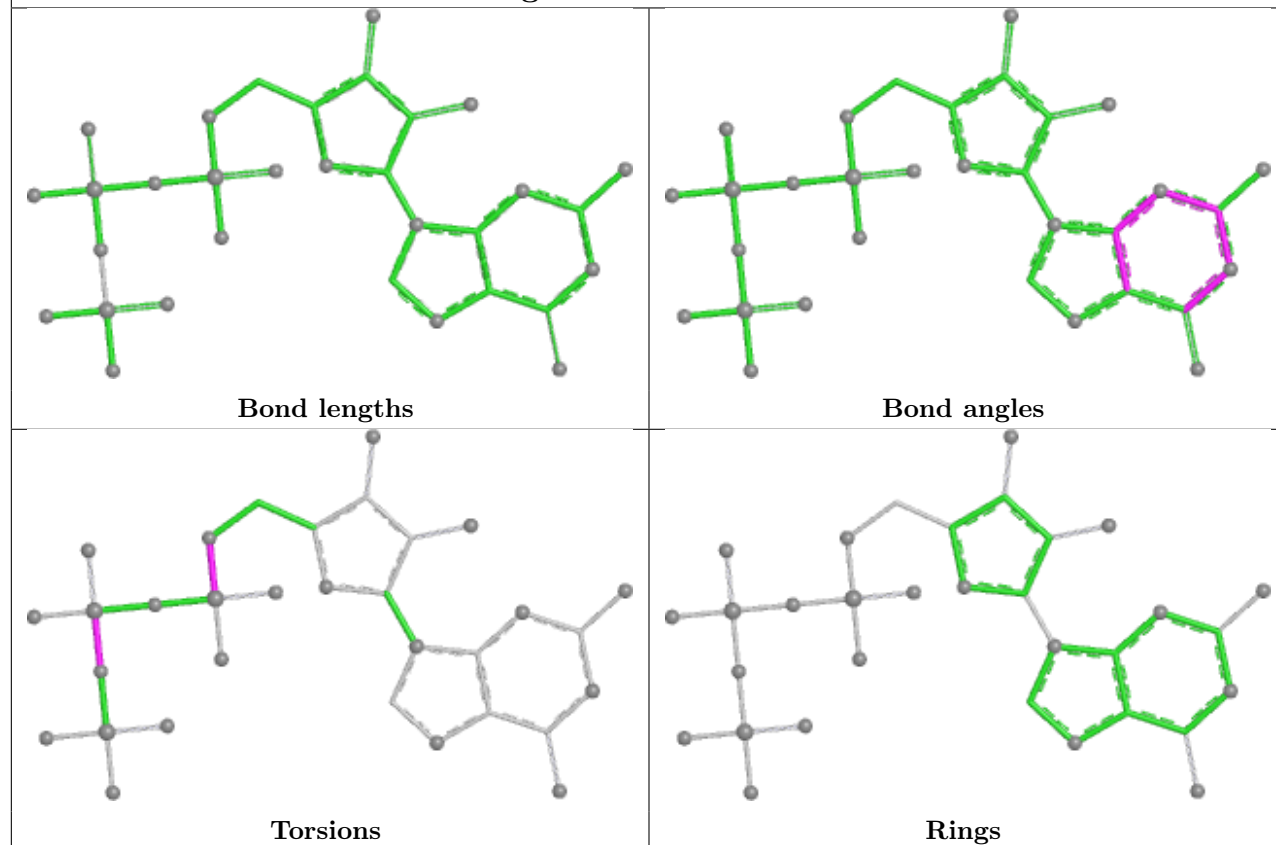
## Ligand GTP PC 602



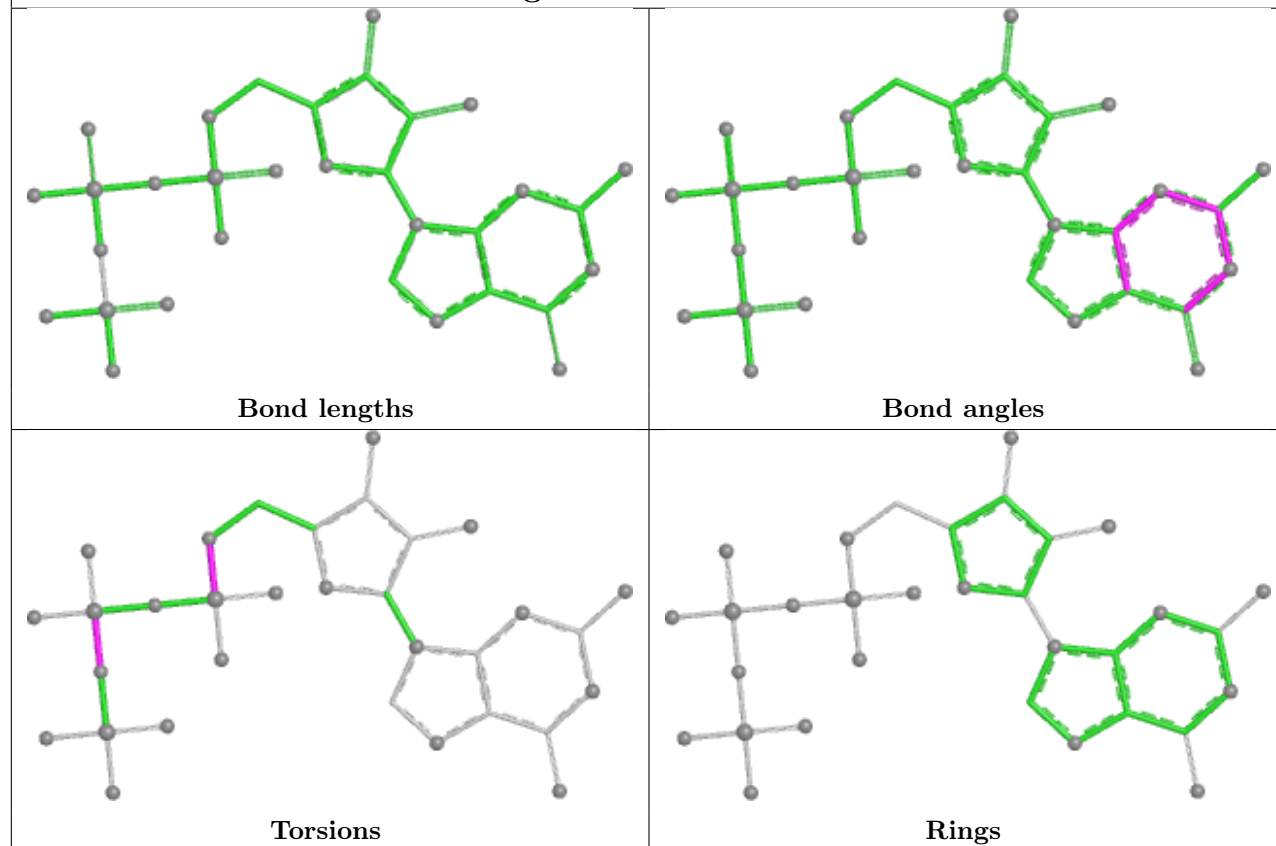
## Ligand GTP FA 602



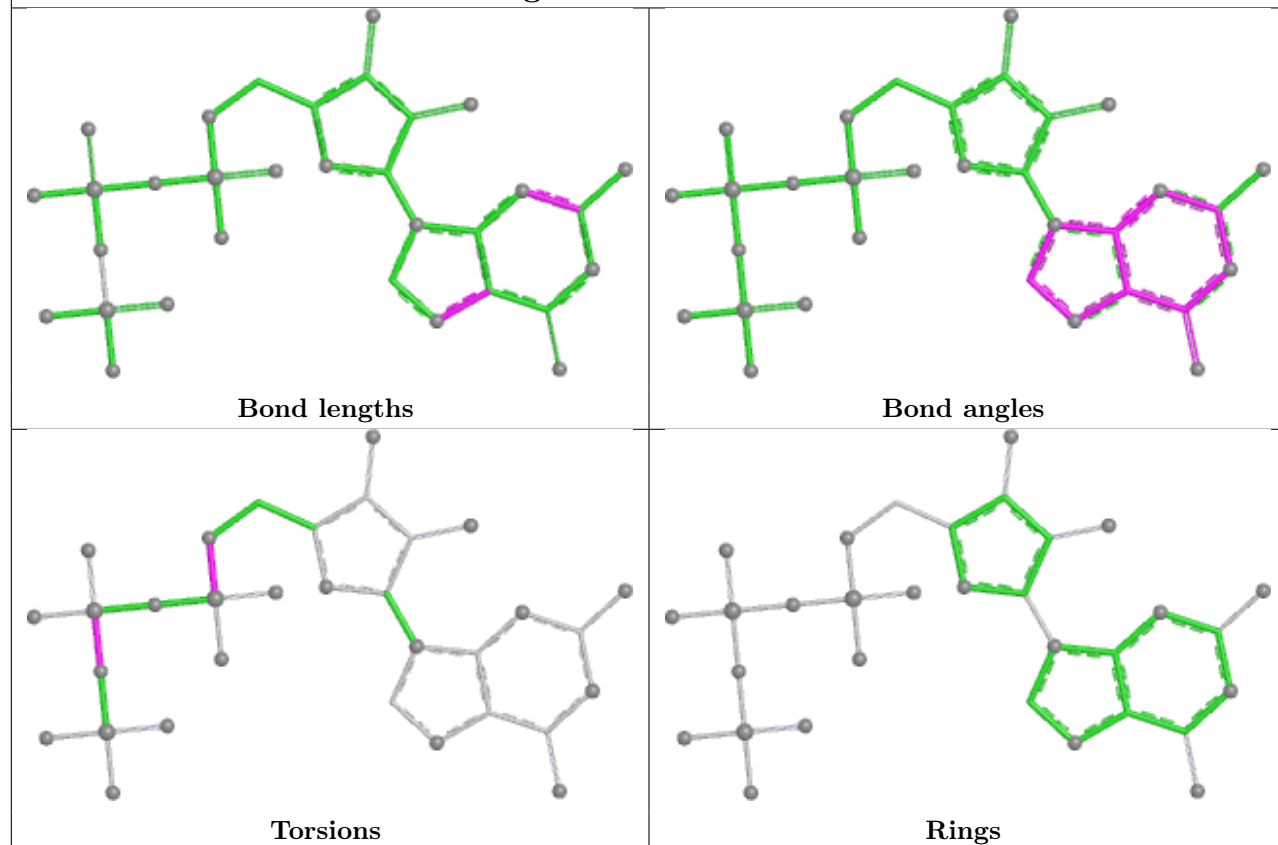
## Ligand GTP CJ 501



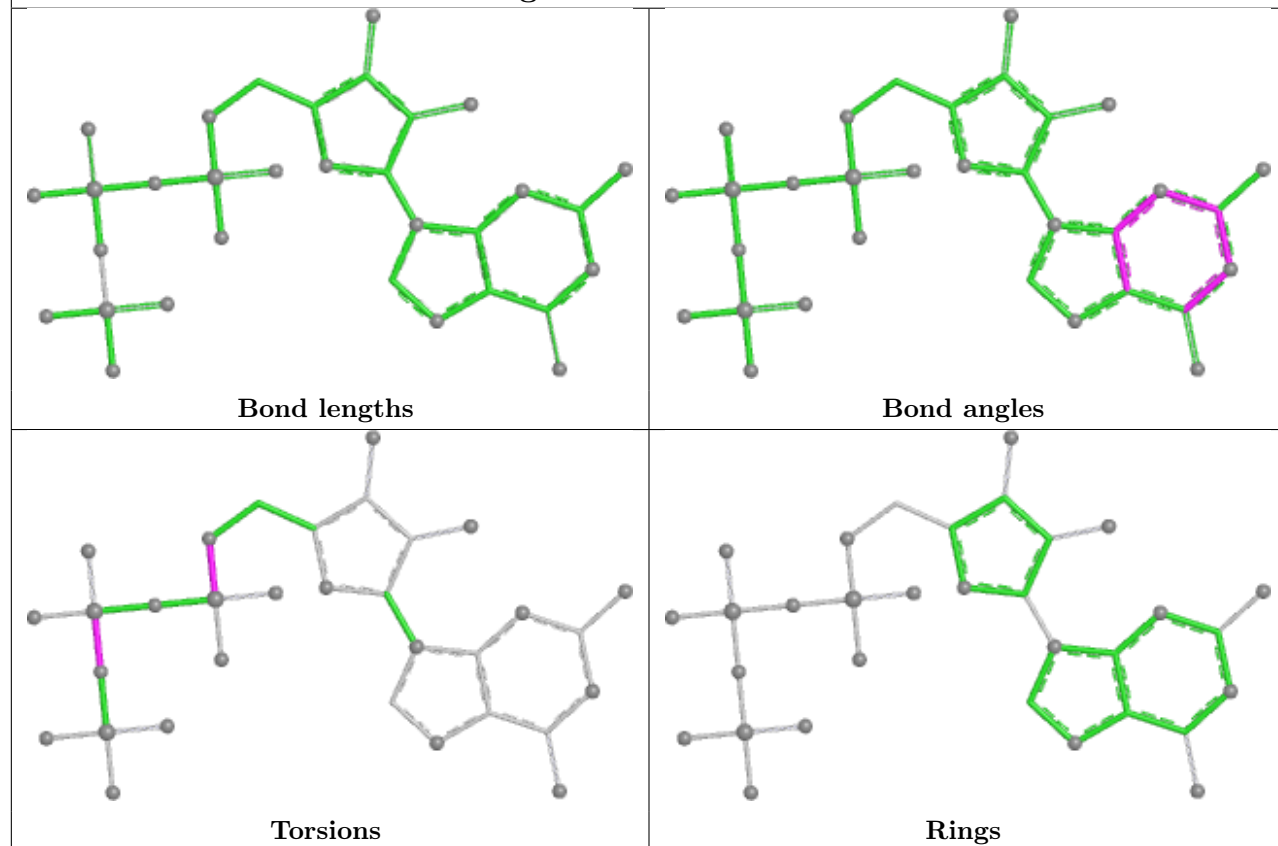
## Ligand GTP LJ 501

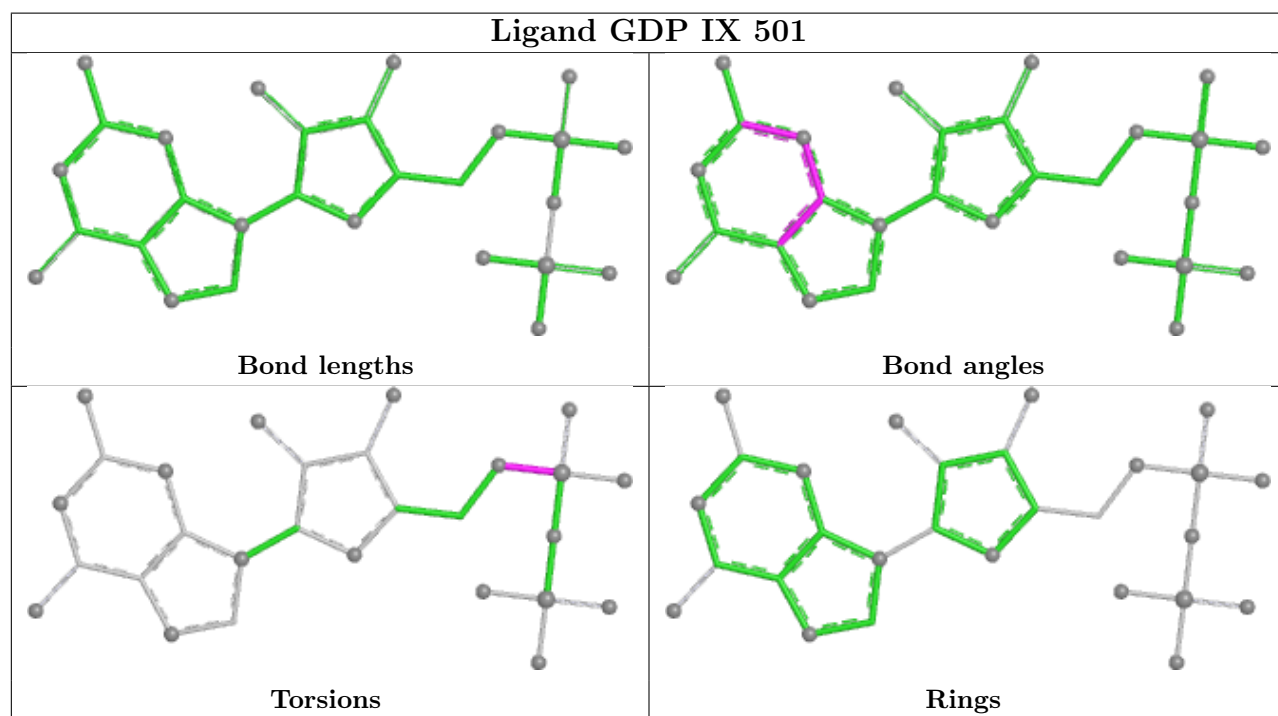
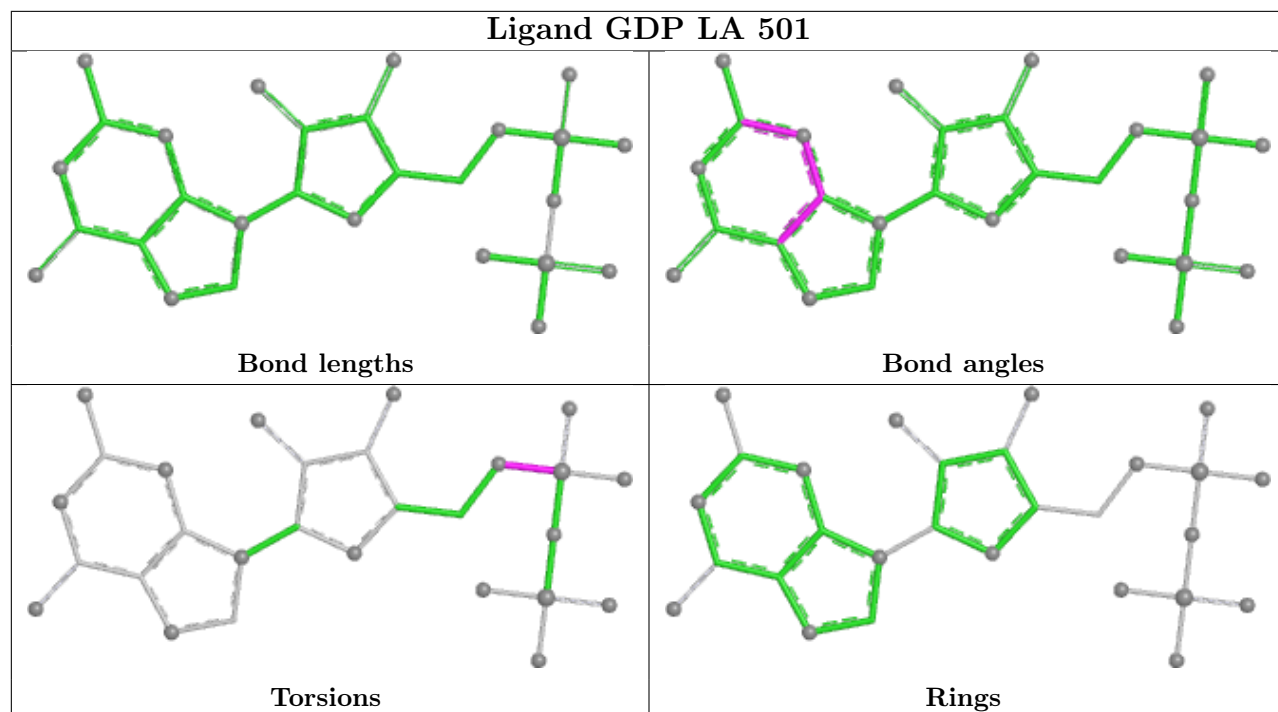


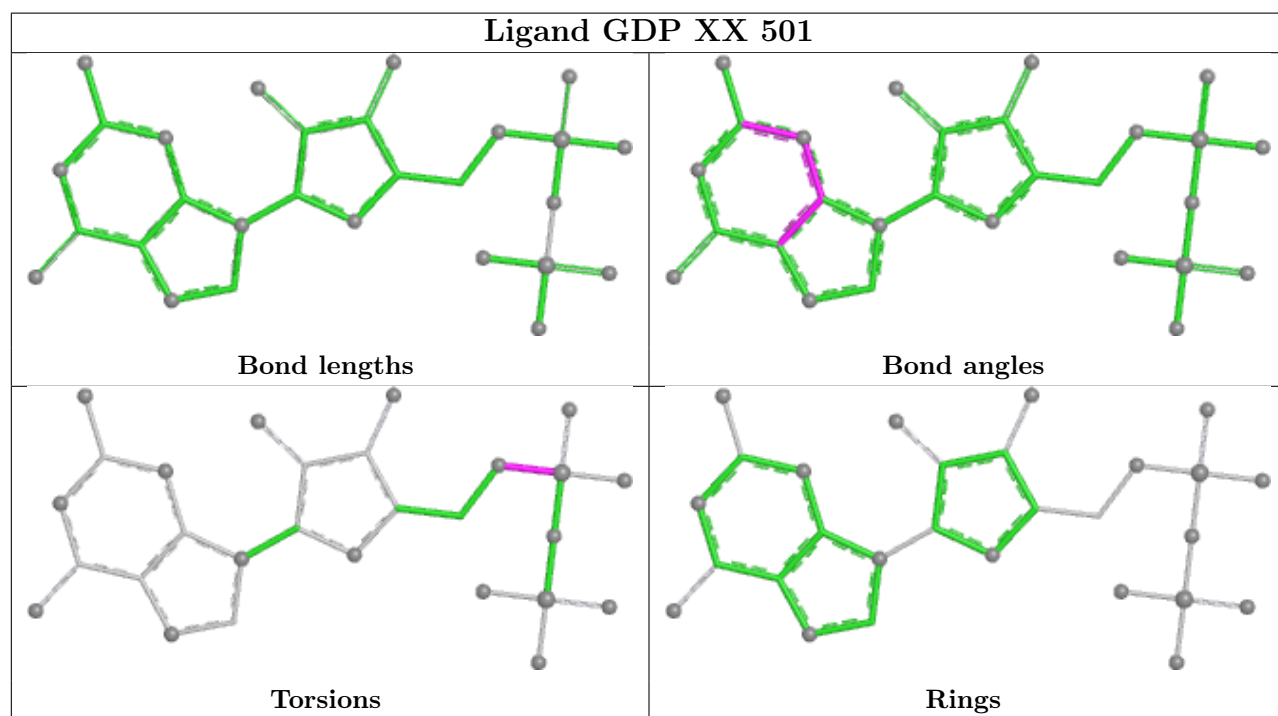
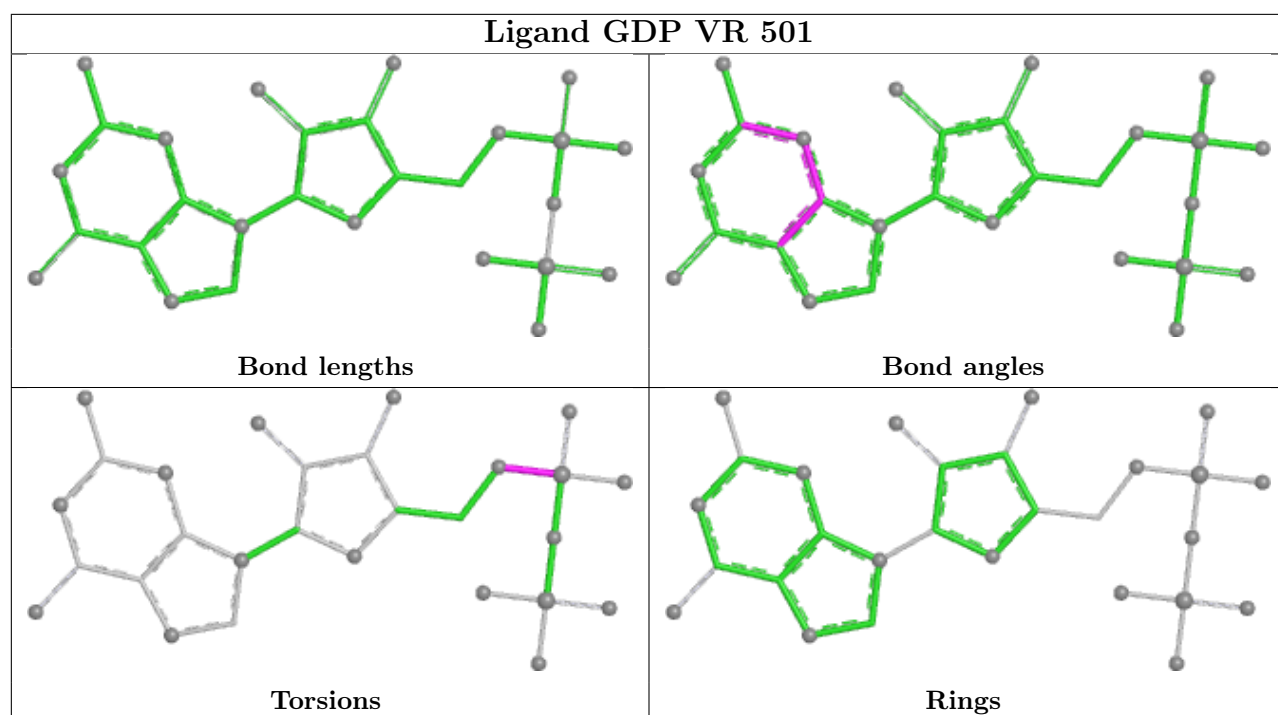
## Ligand GTP IU 501

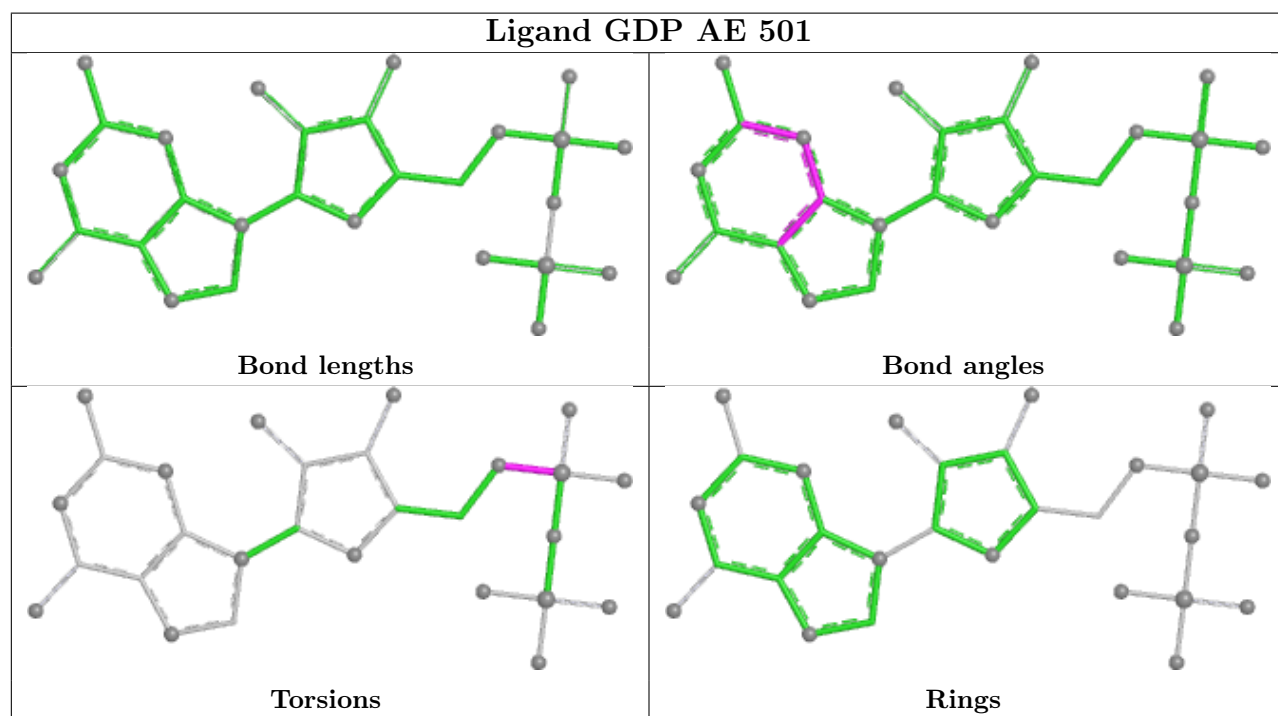
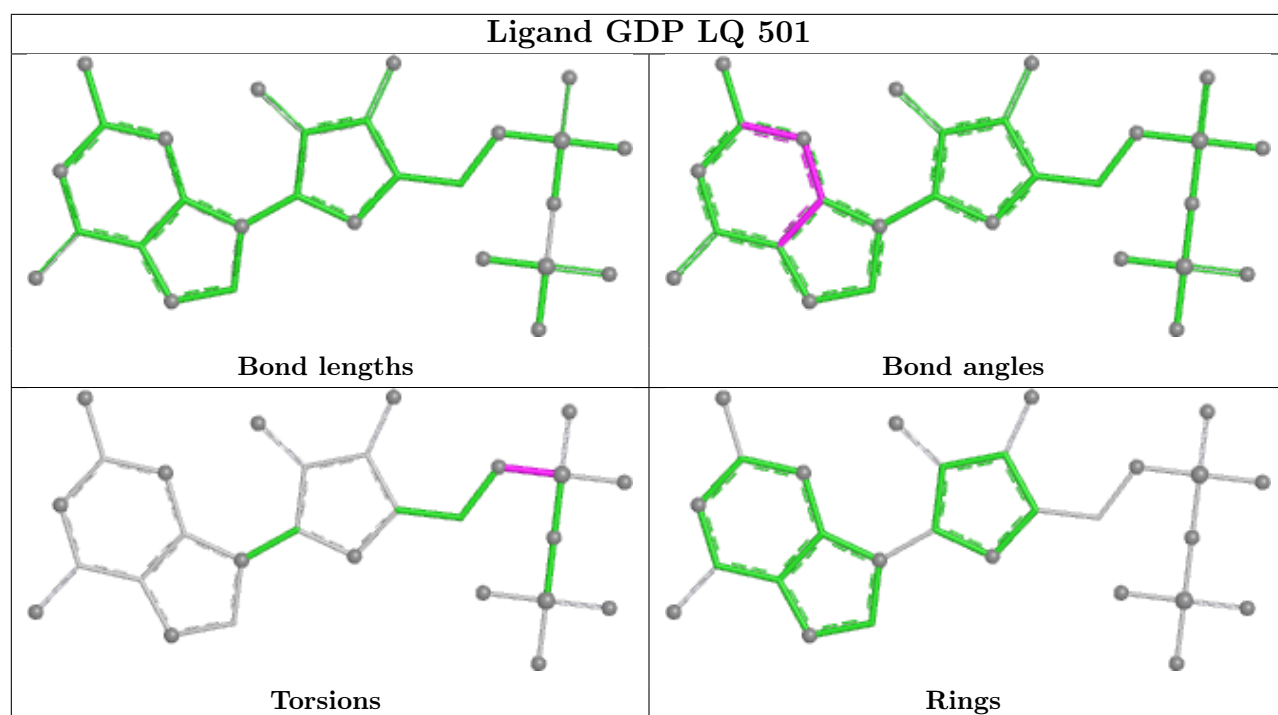


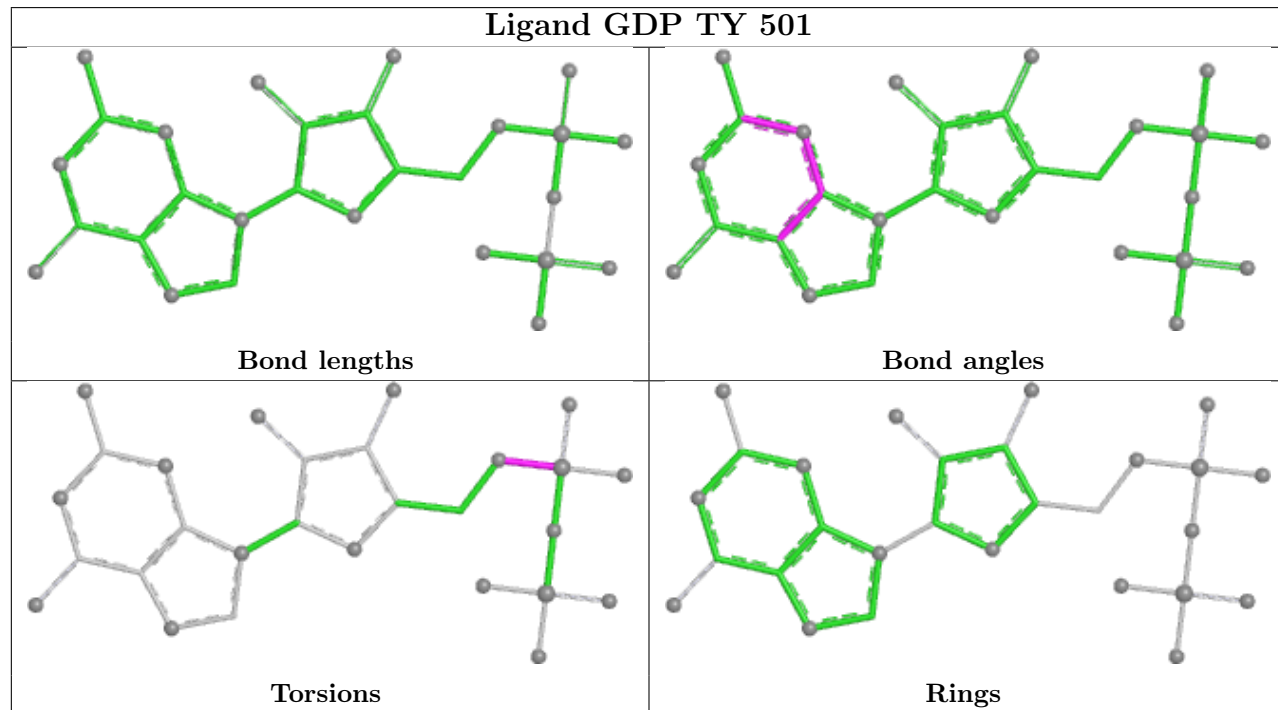
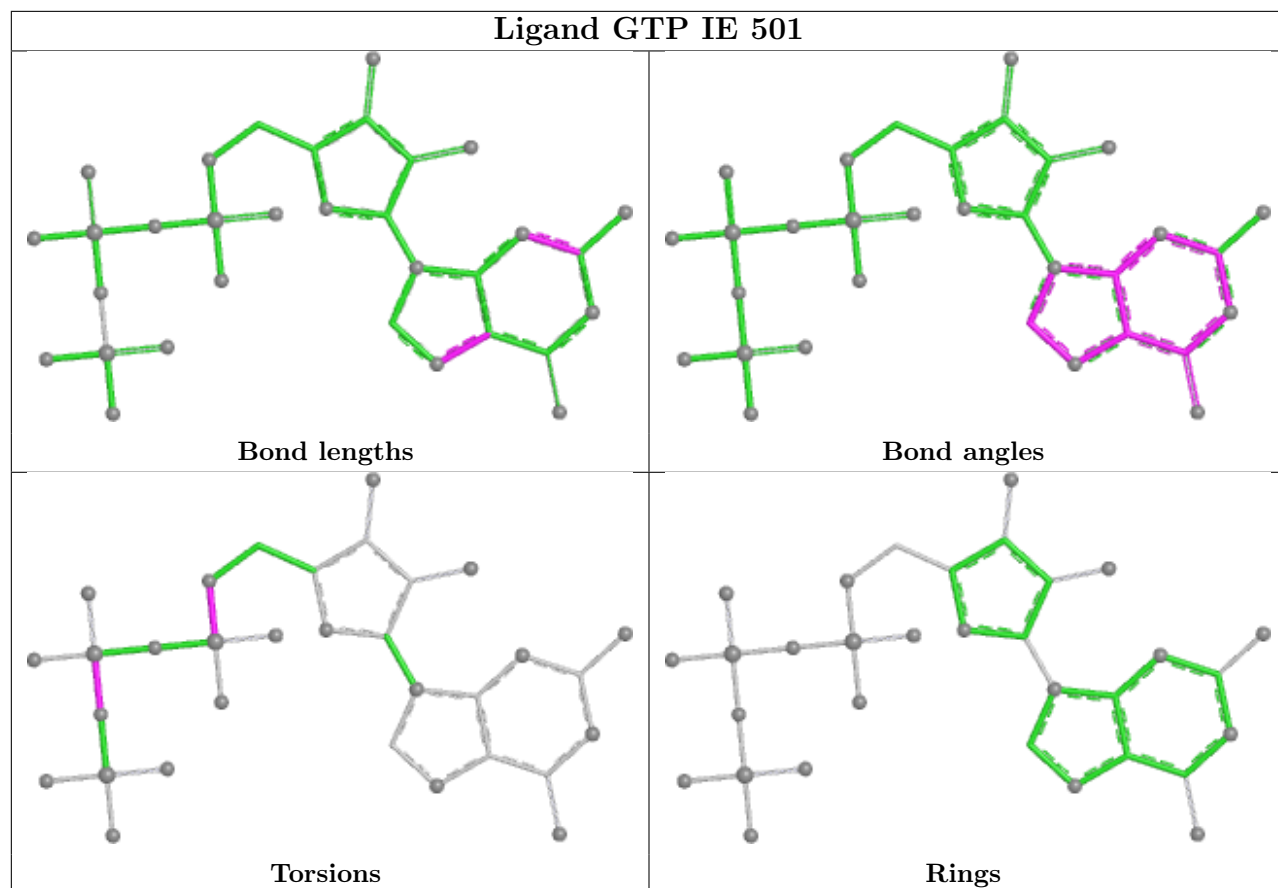
## Ligand GTP HS 501





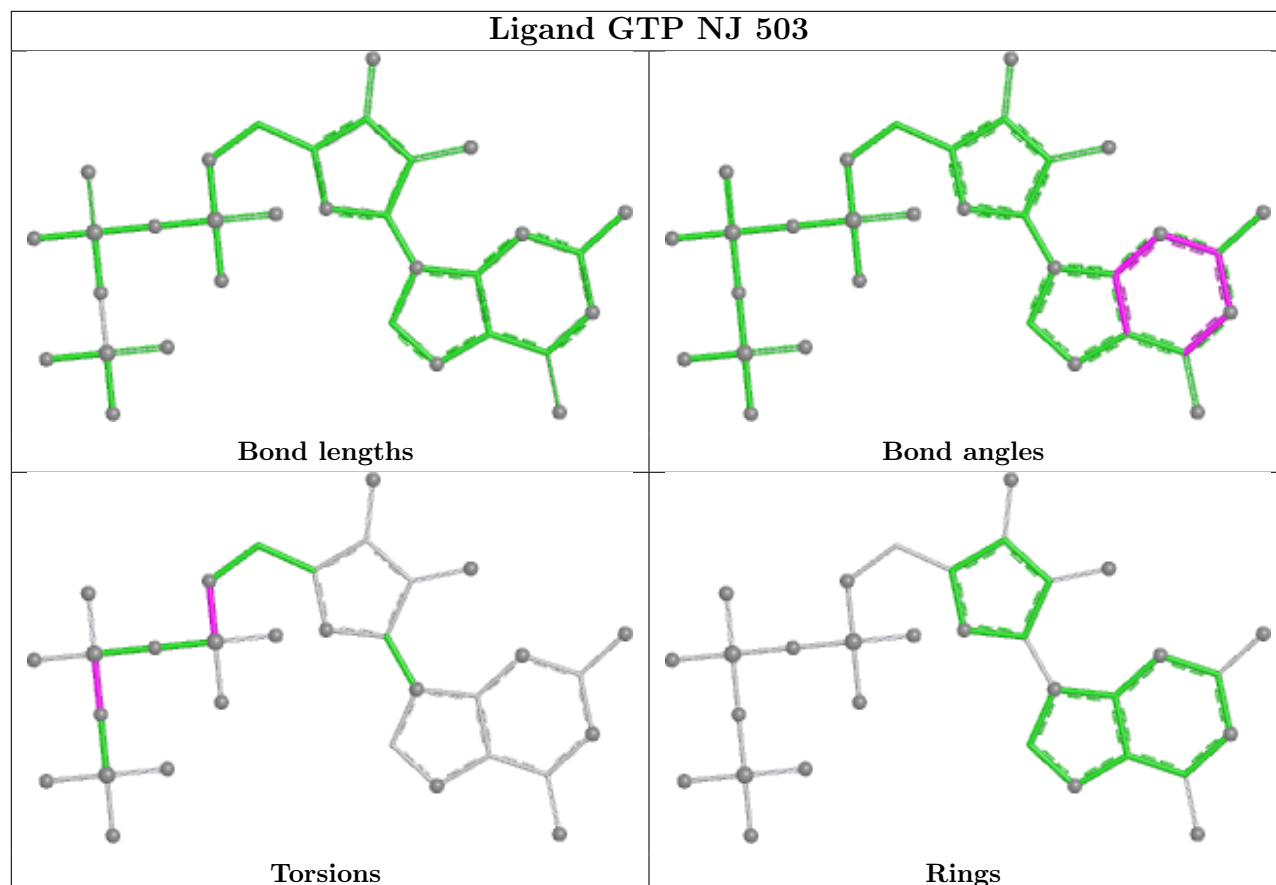




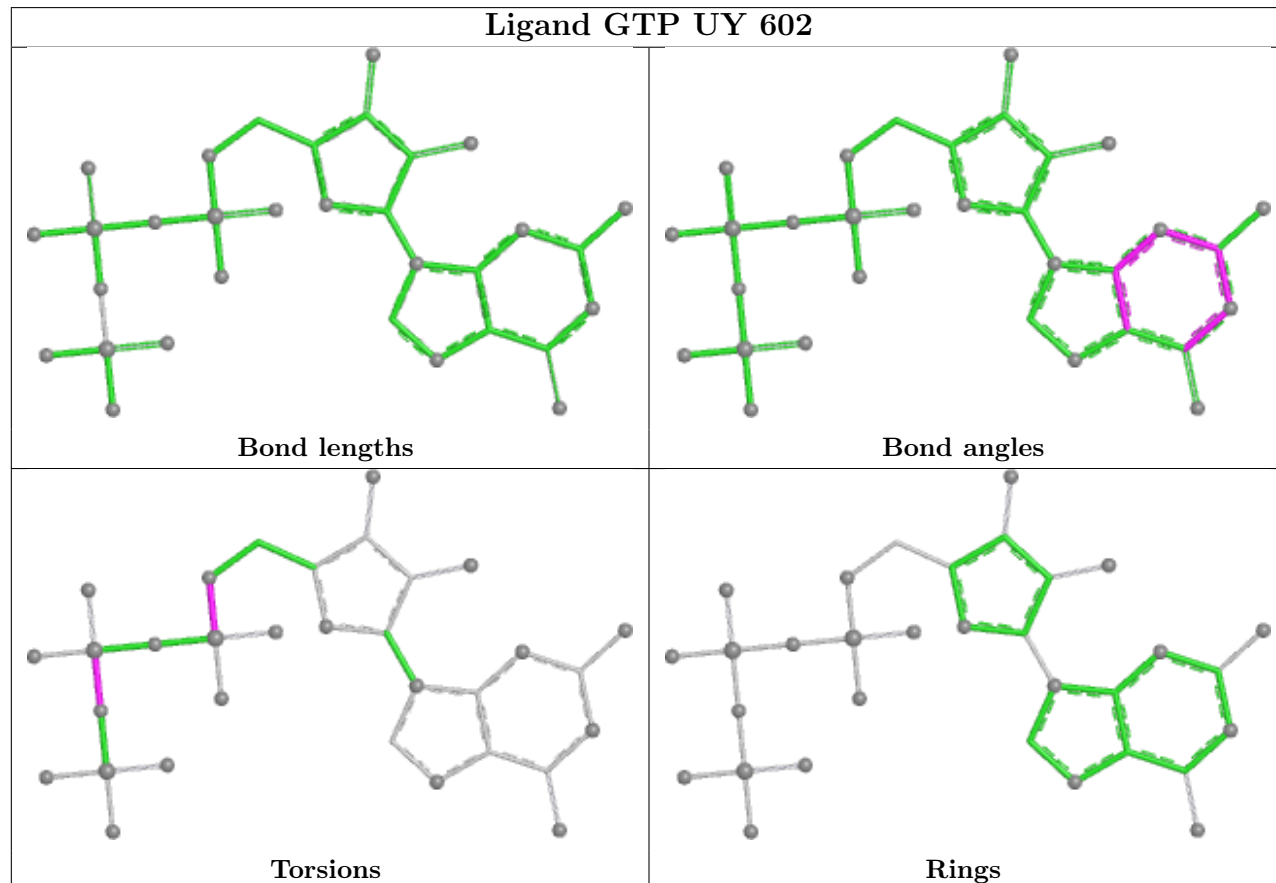




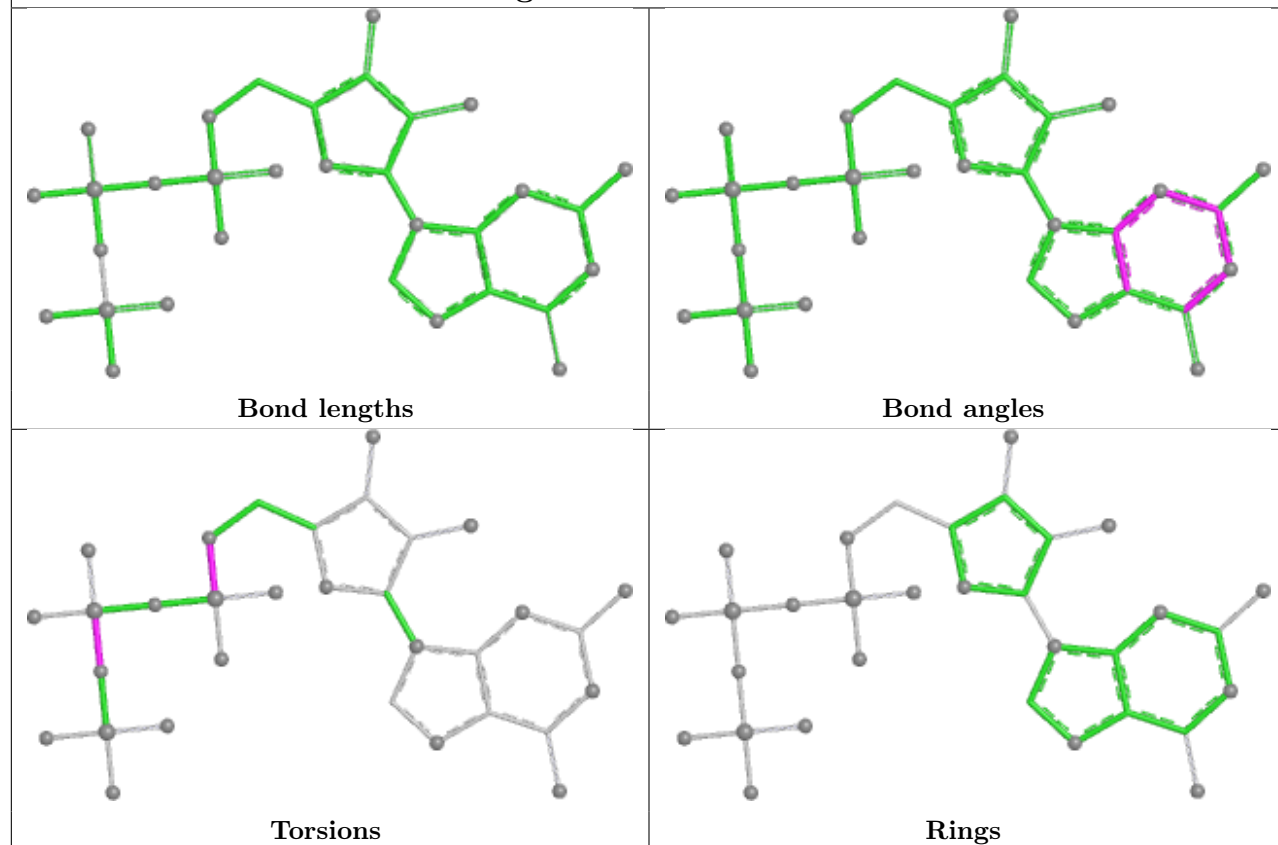
## Ligand GTP NJ 503



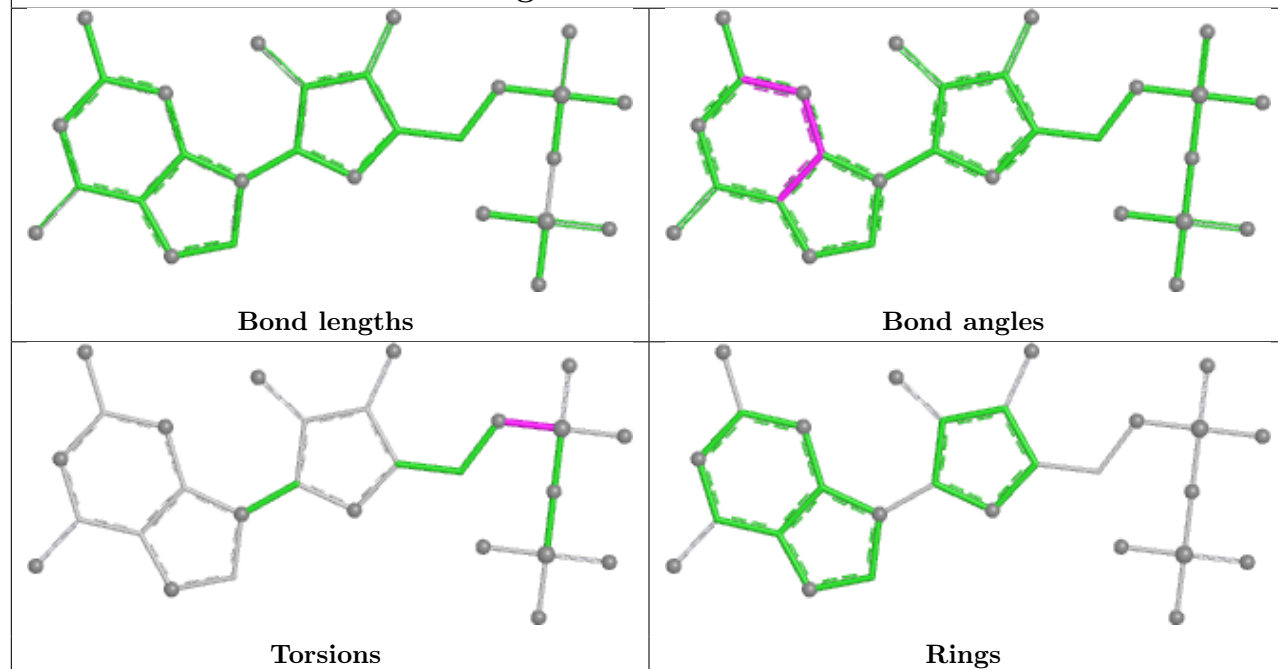
## Ligand GTP UY 602

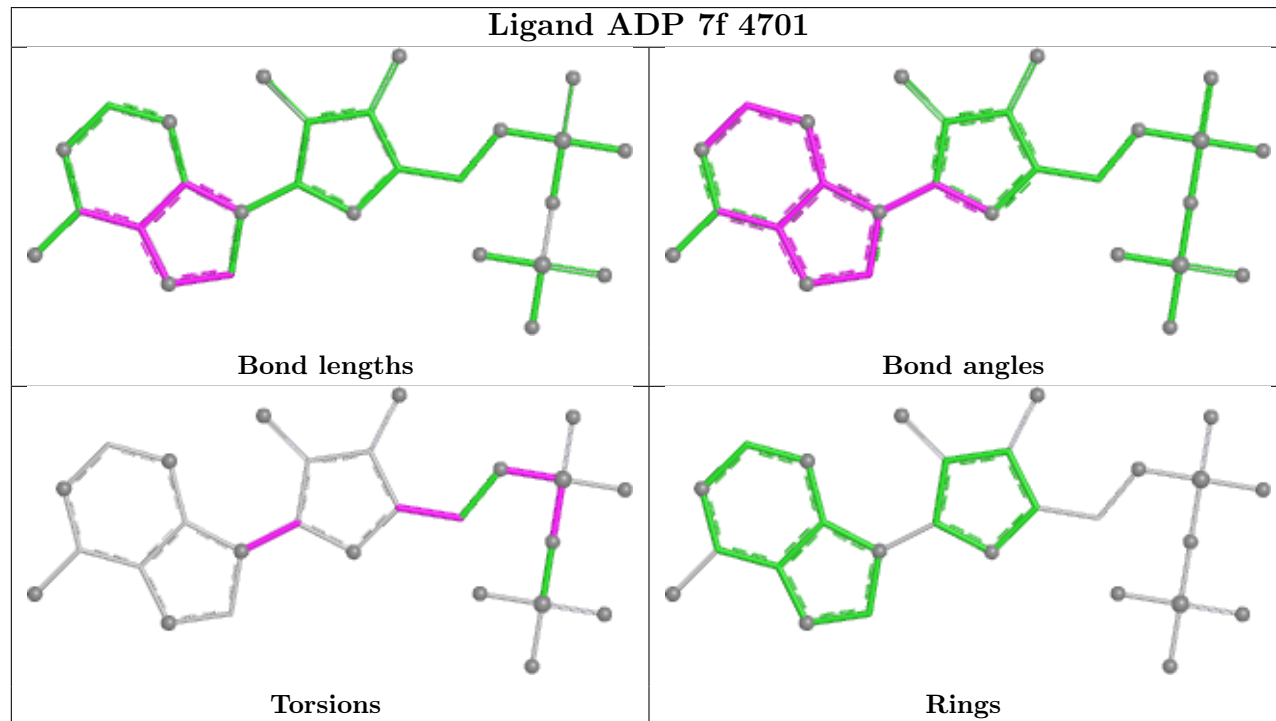
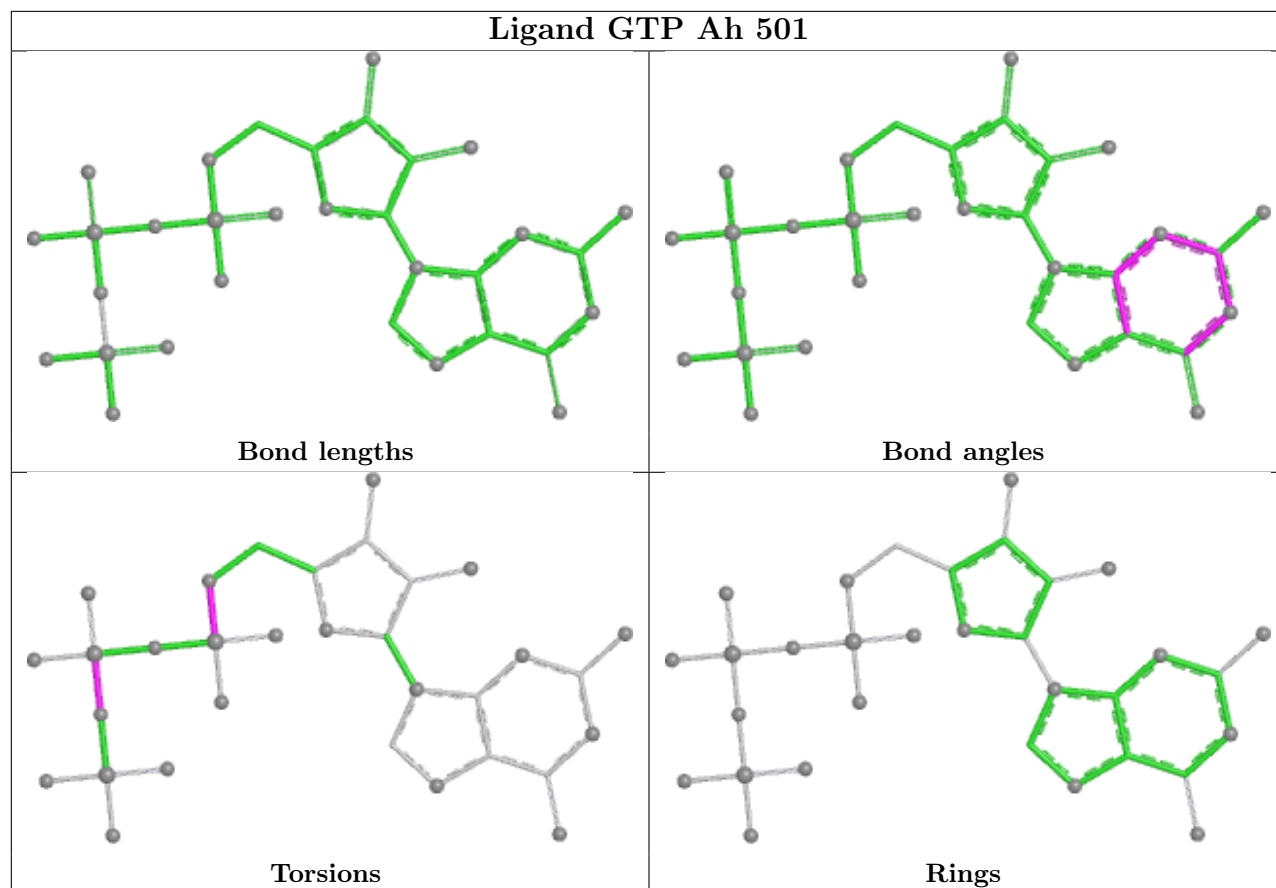


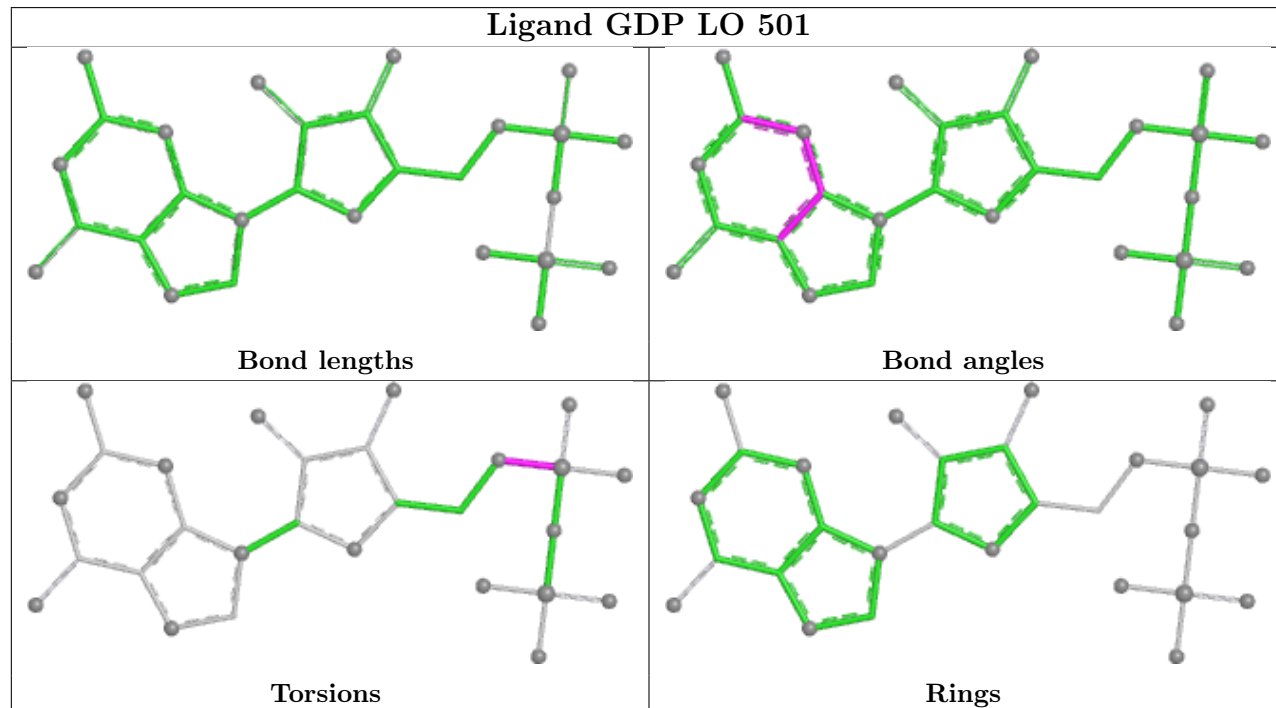
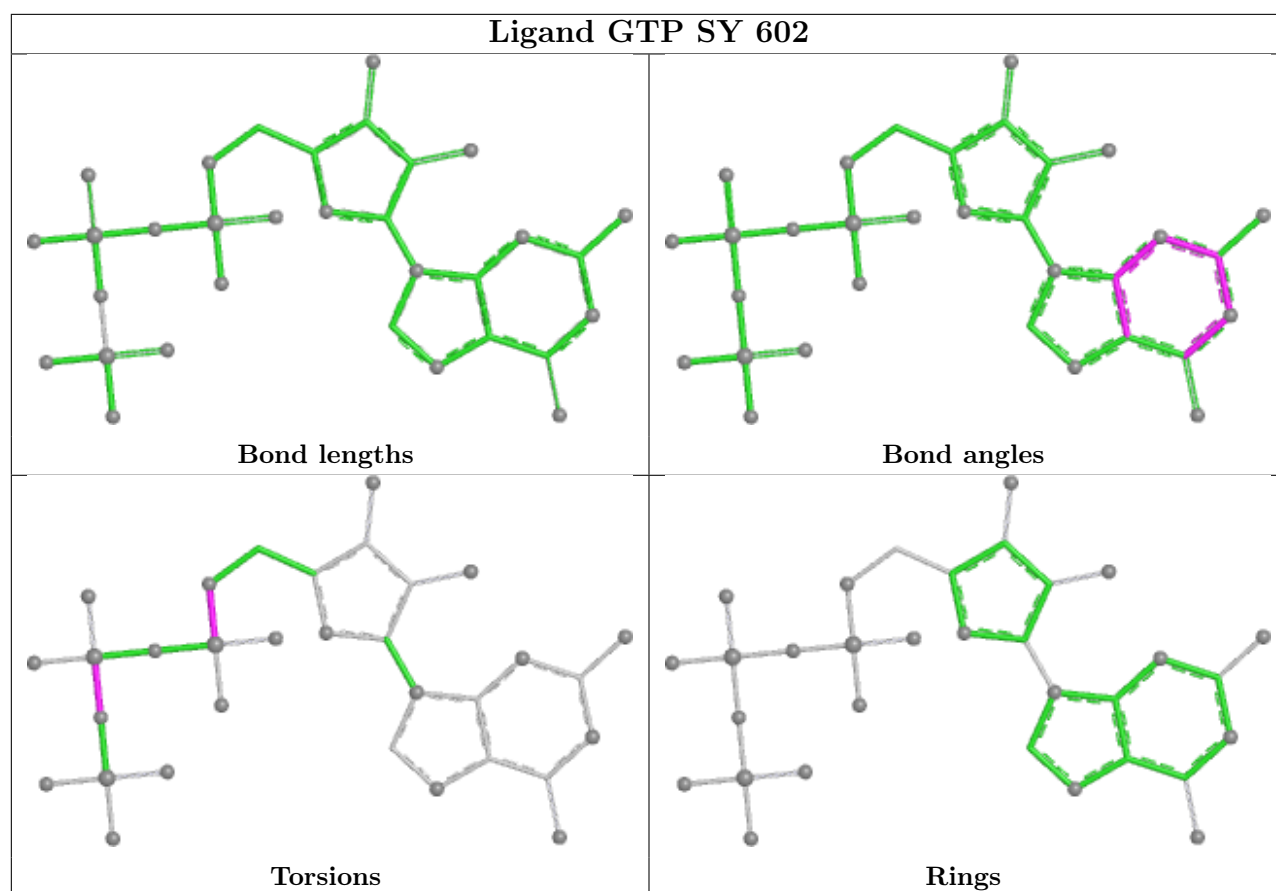
## Ligand GTP AN 501



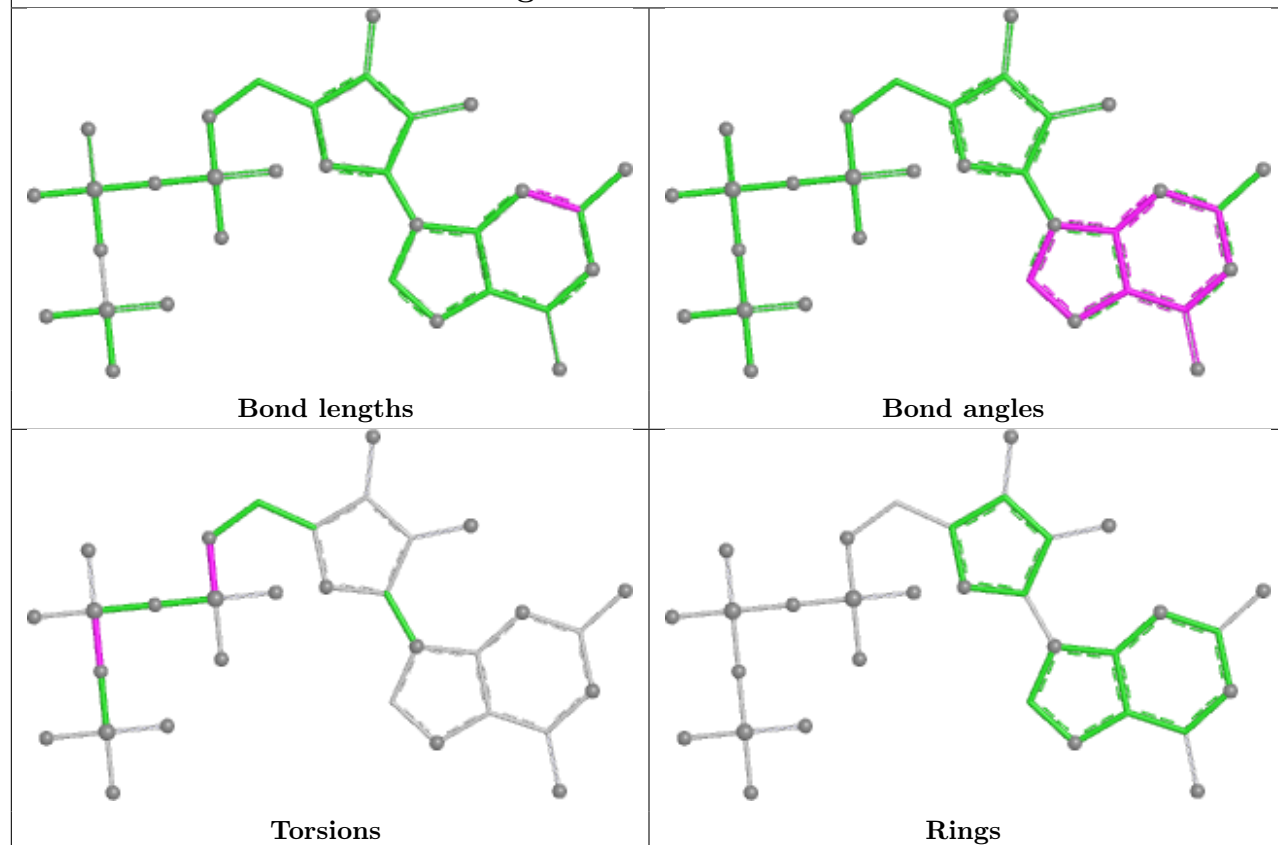
## Ligand GDP KE 501



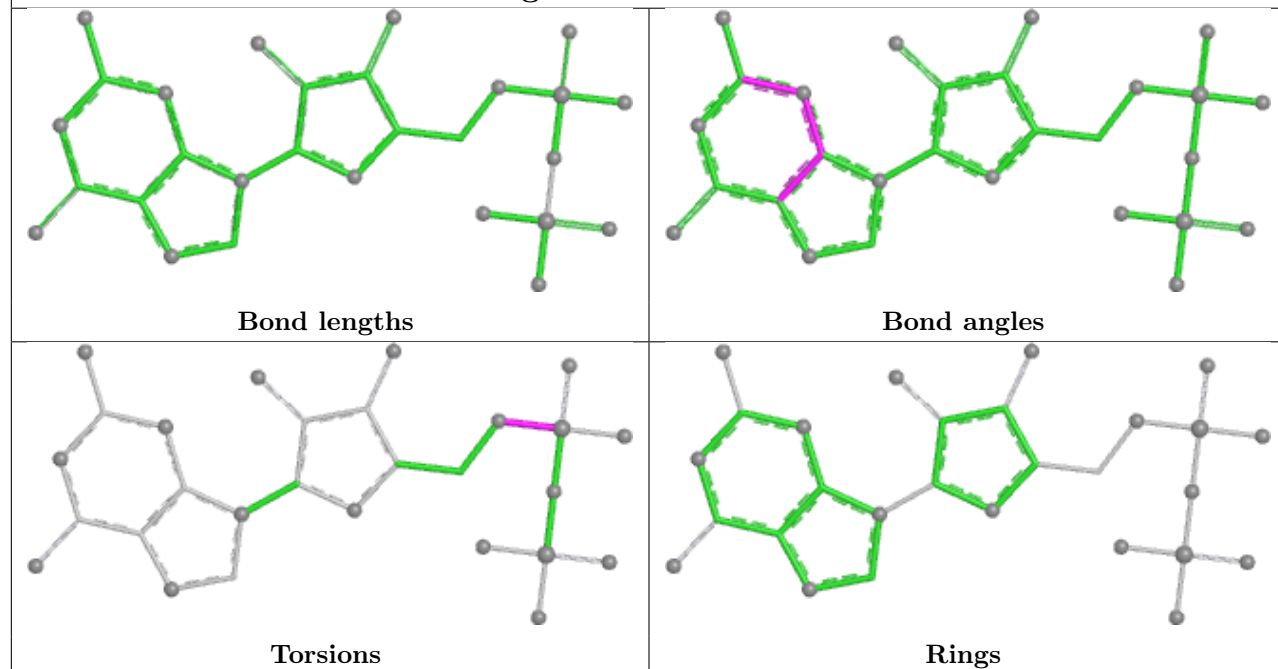




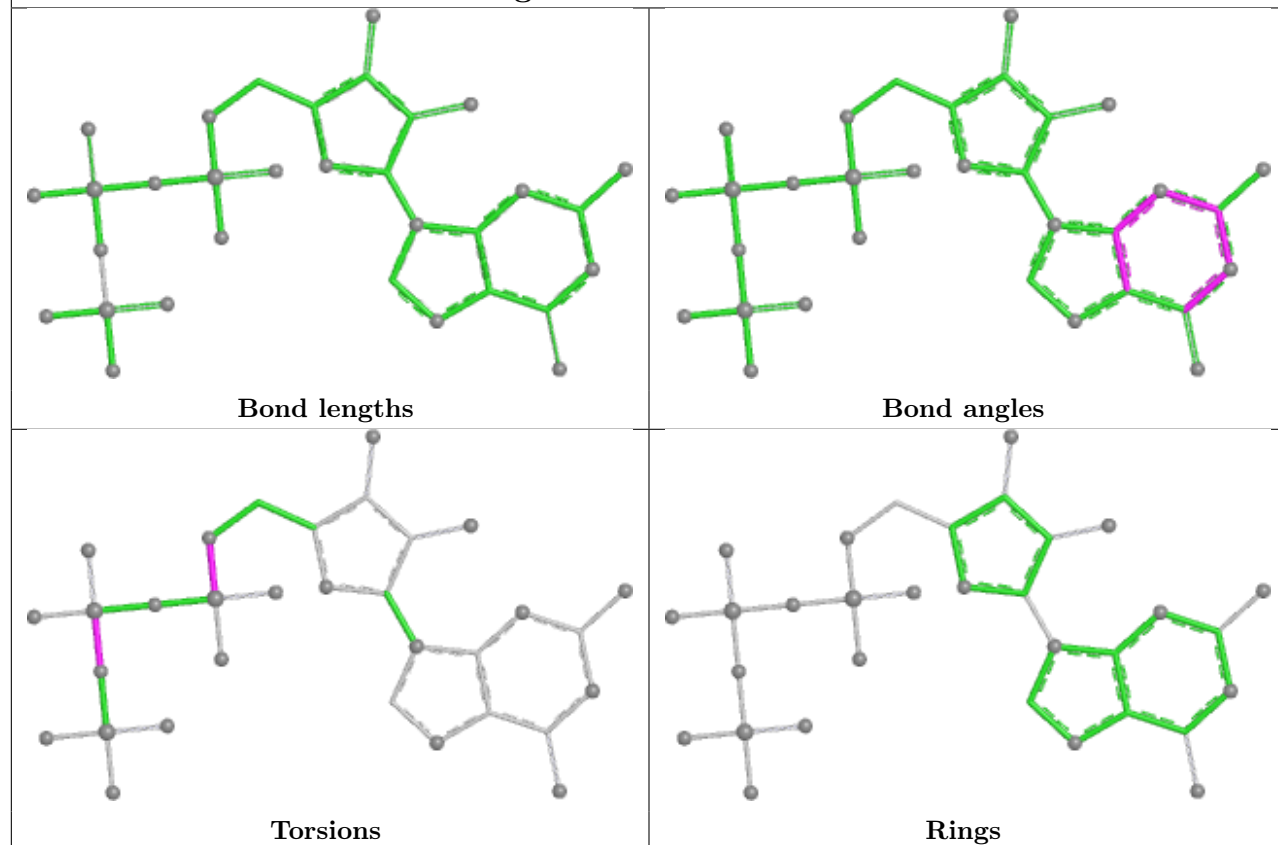
## Ligand GTP CX 602



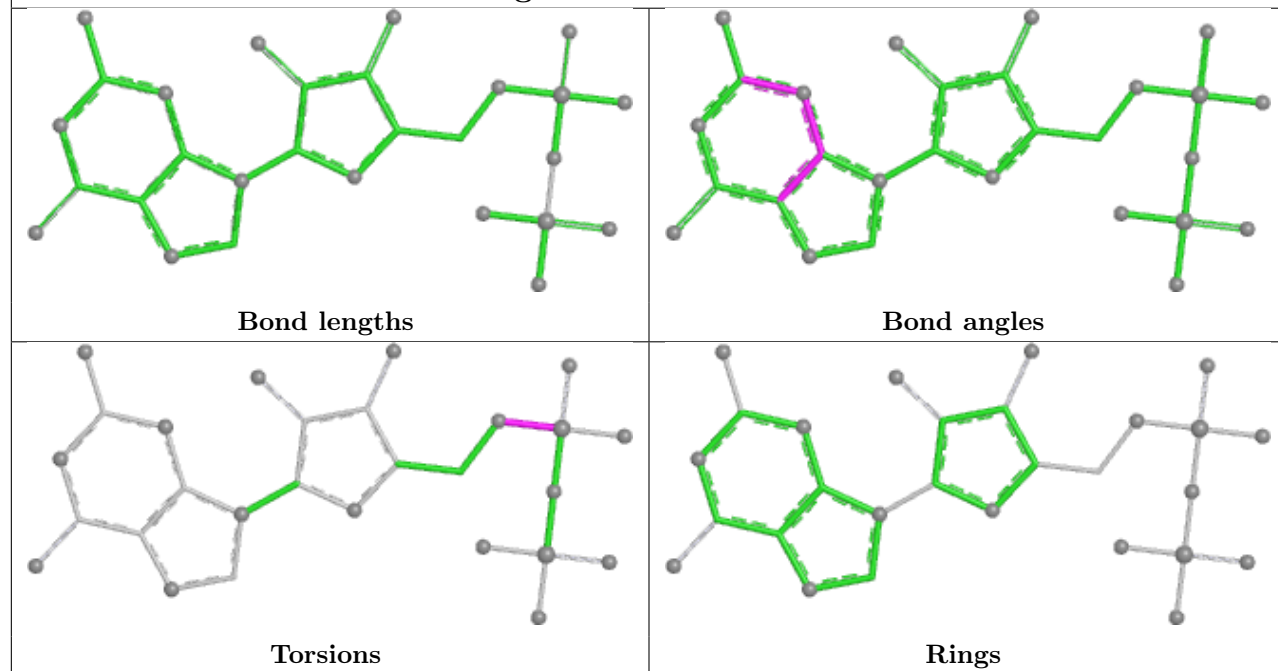
## Ligand GDP KI 501

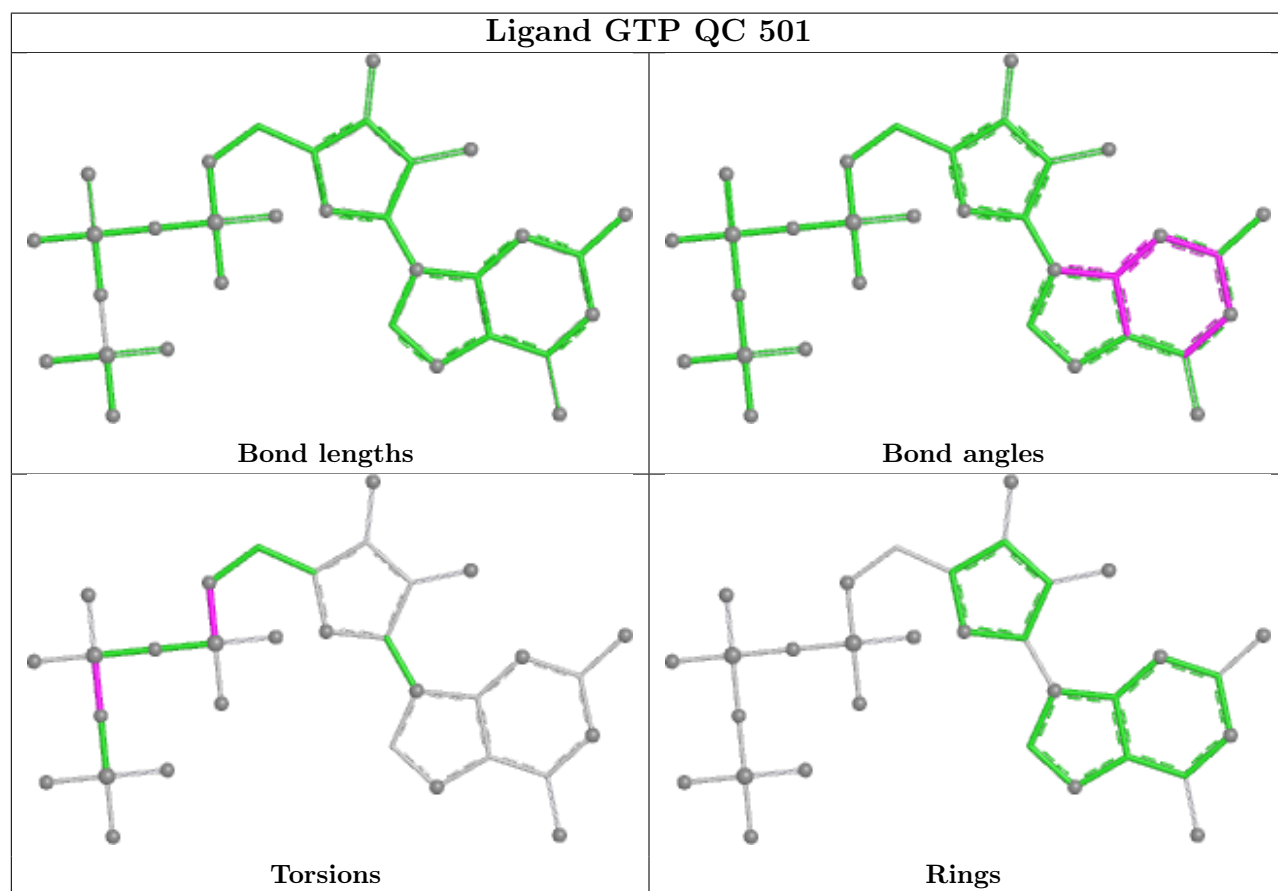
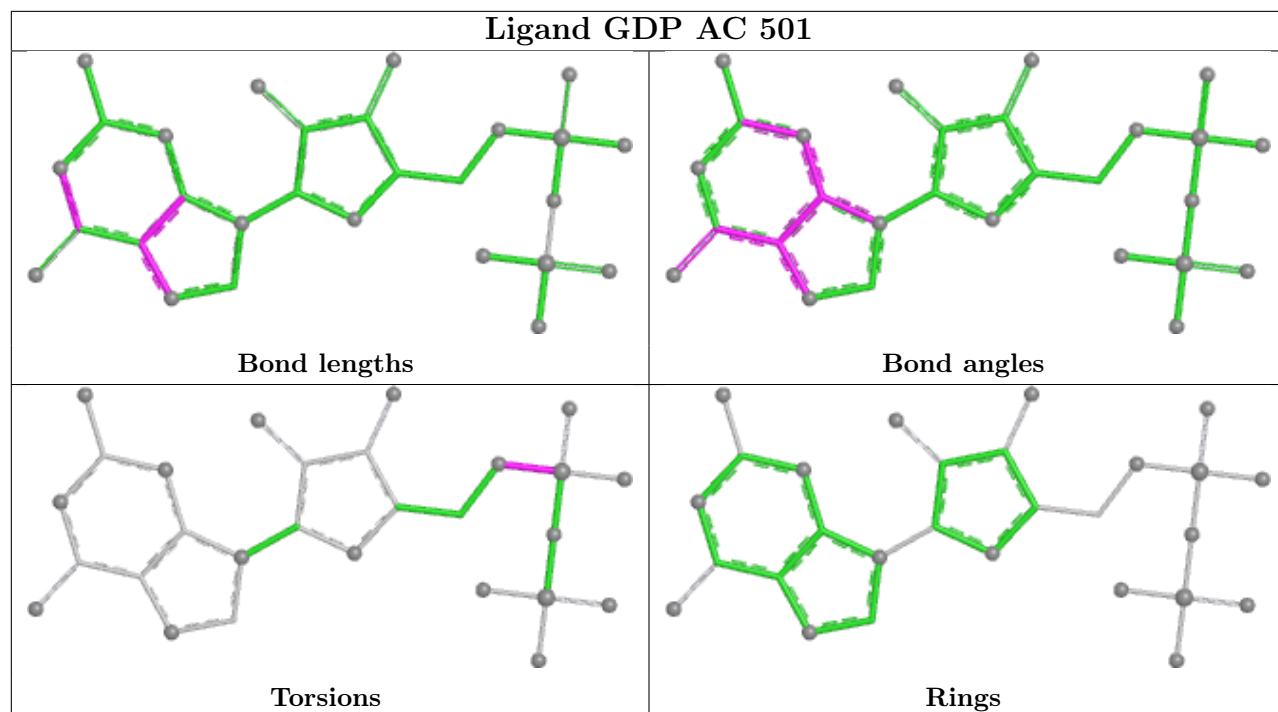


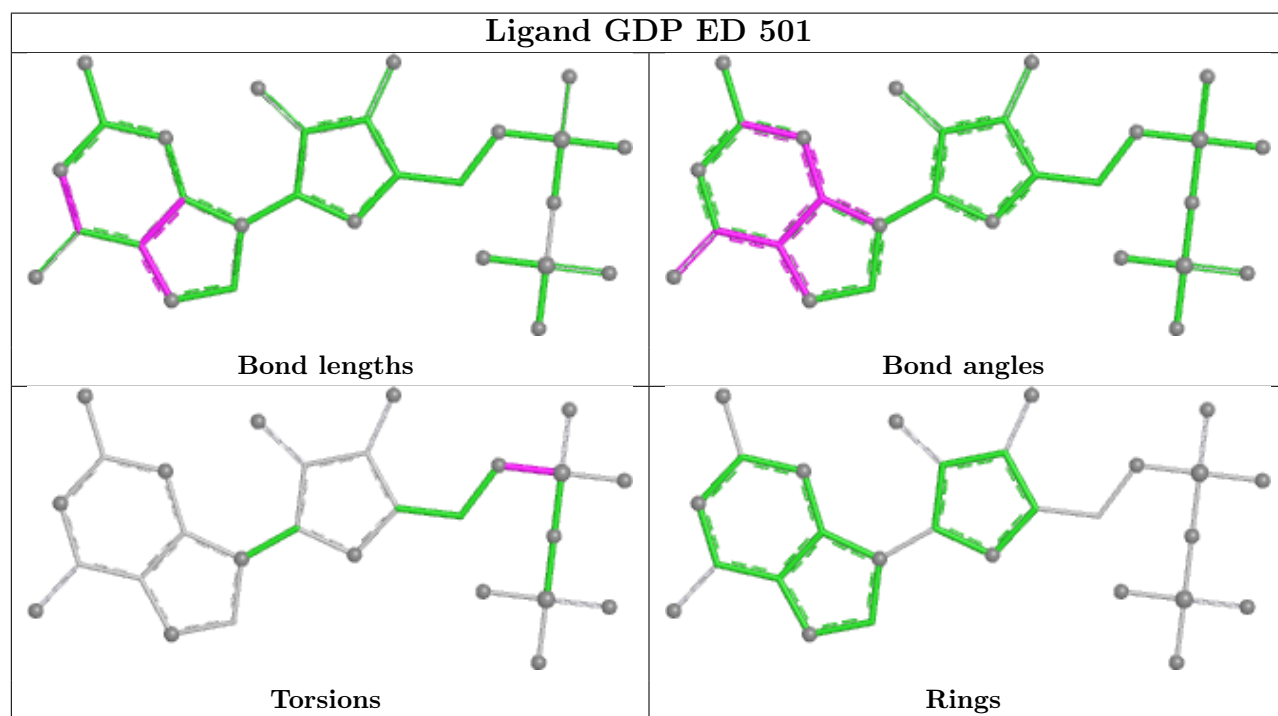
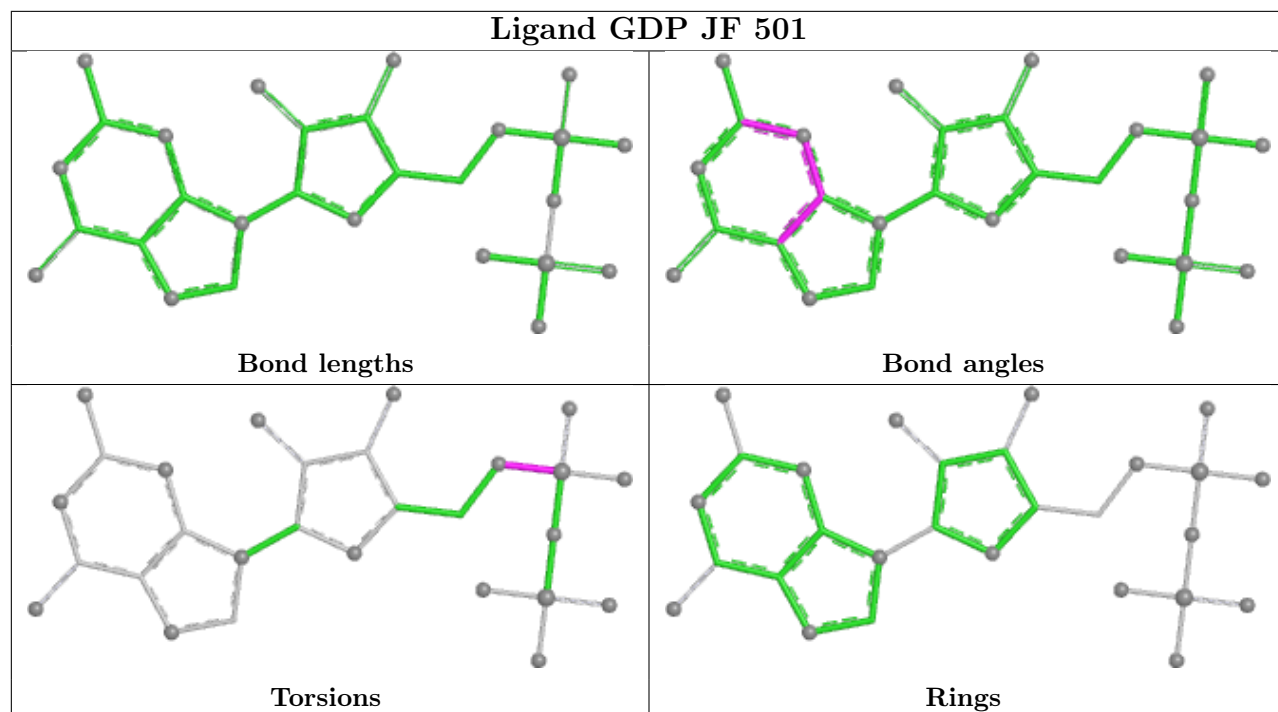
## Ligand GTP TM 501



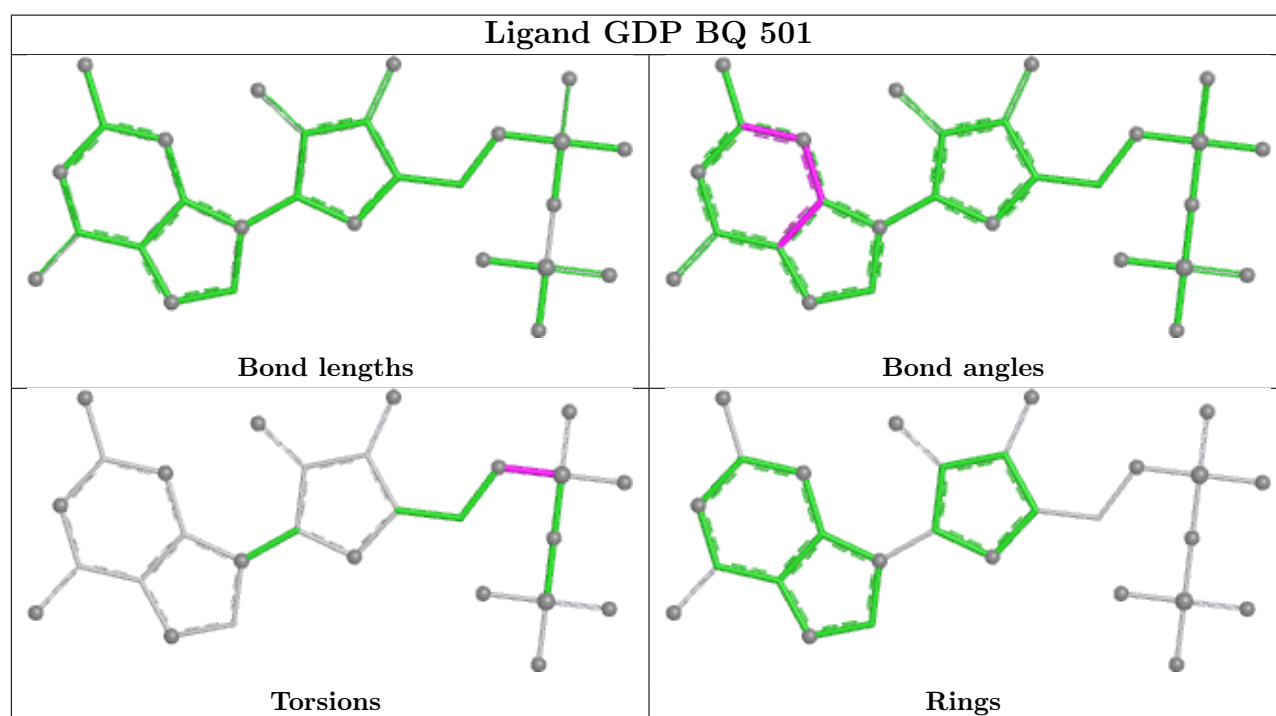
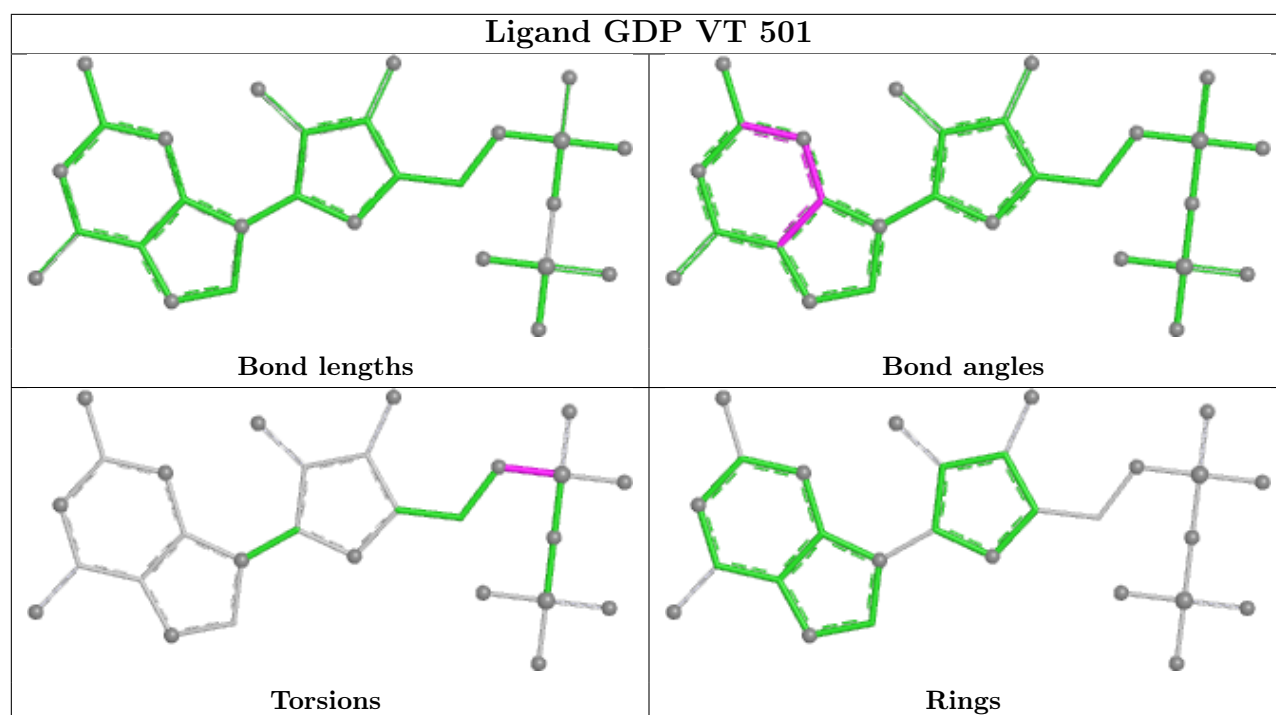
## Ligand GDP OG 501

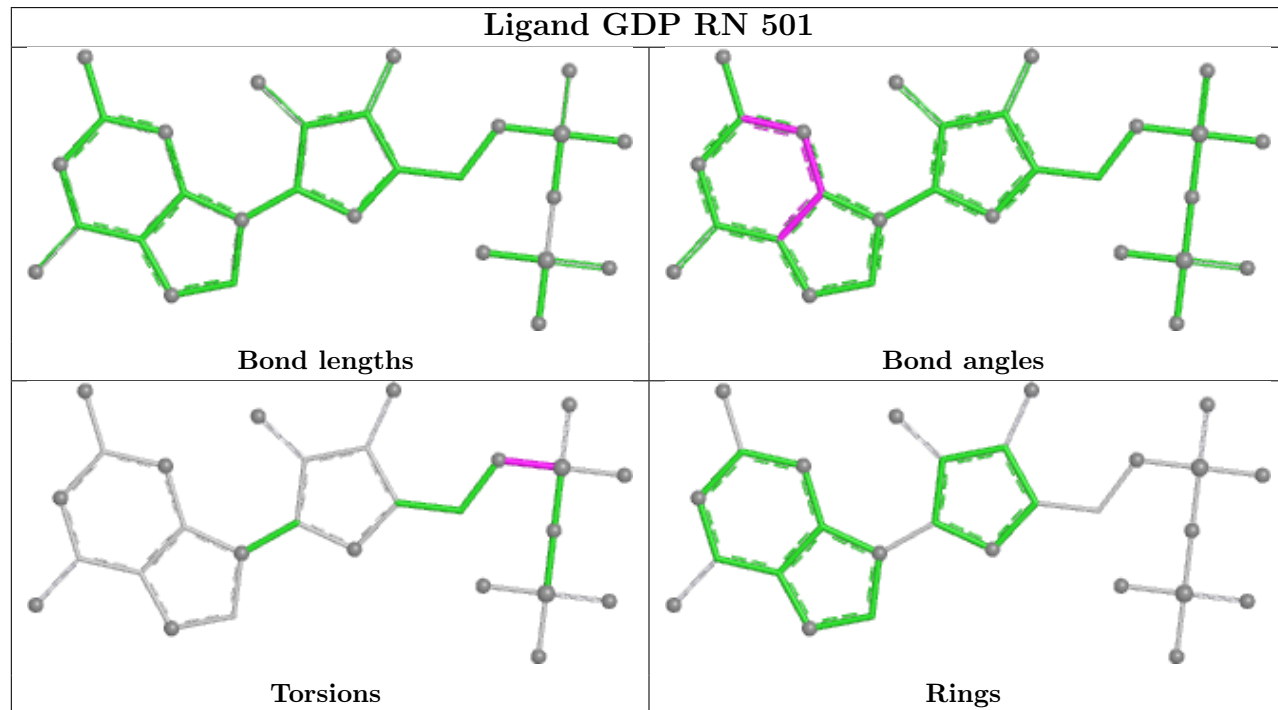
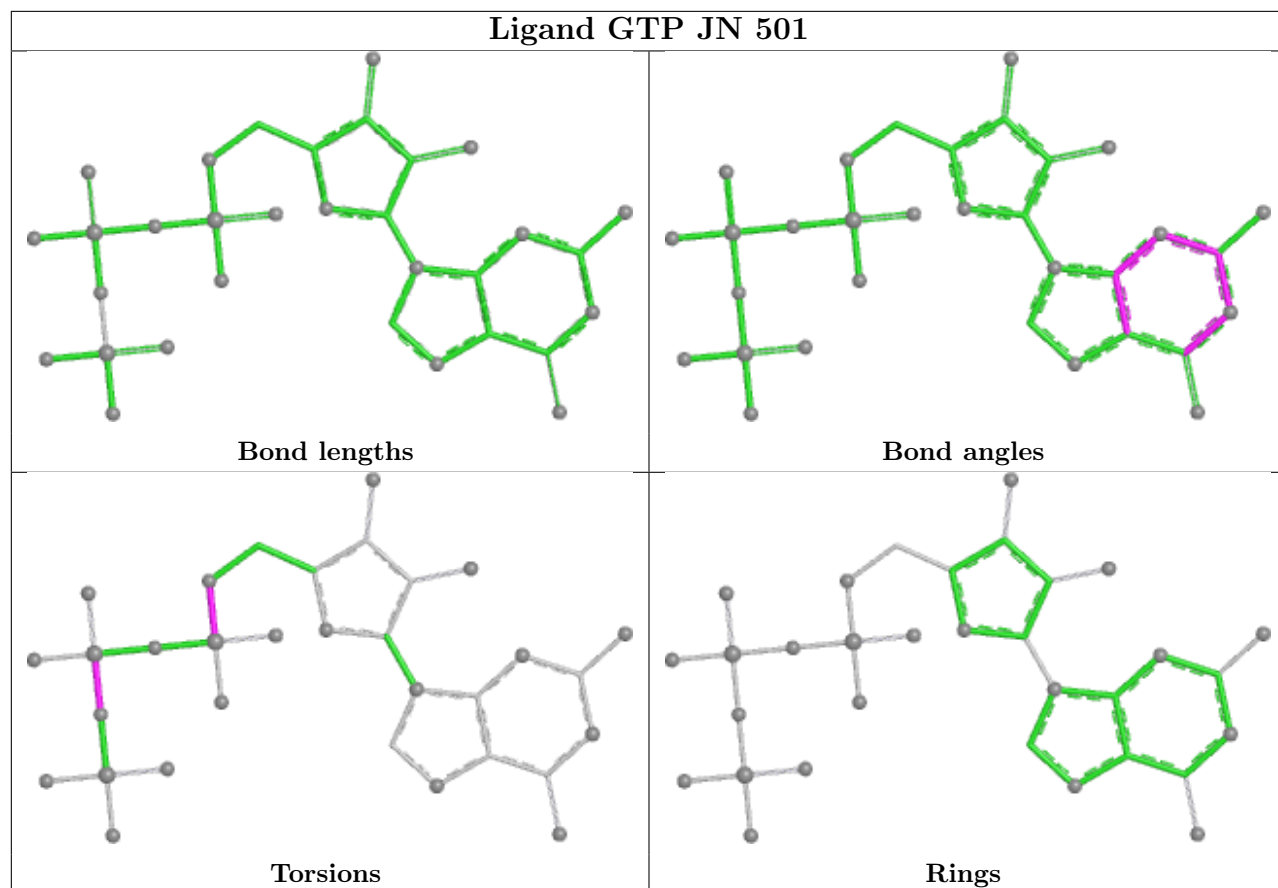


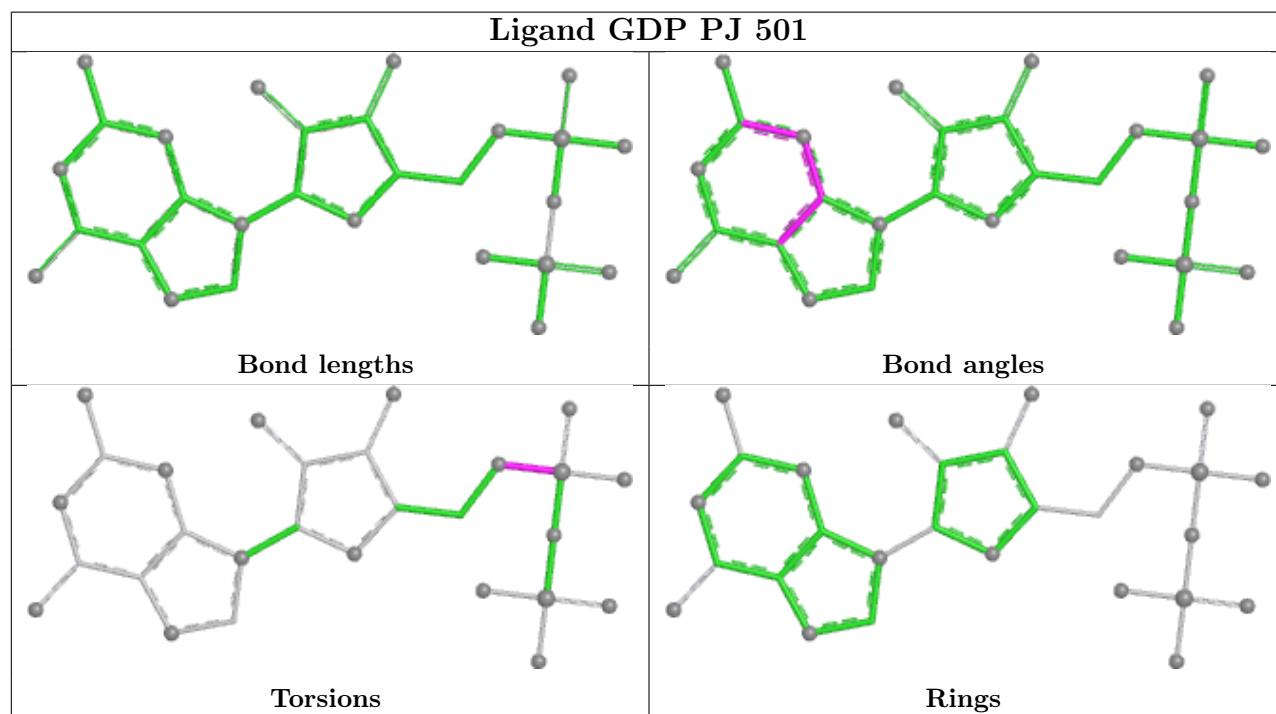
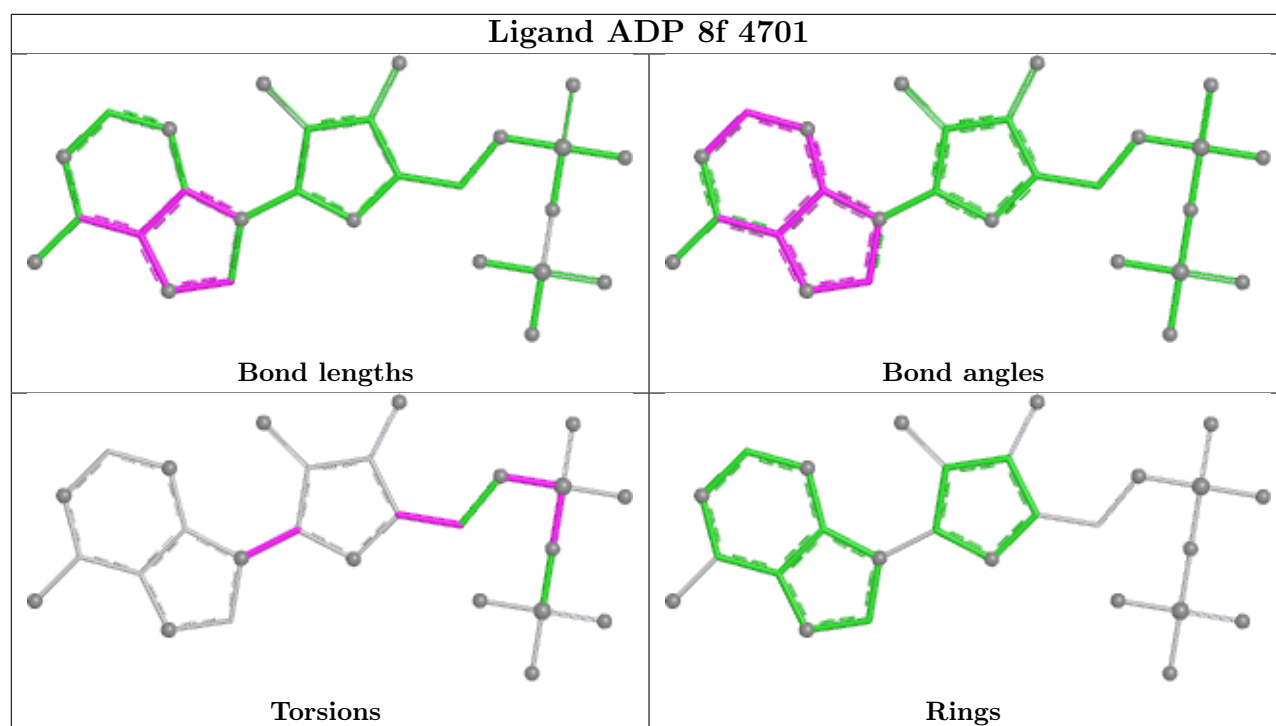


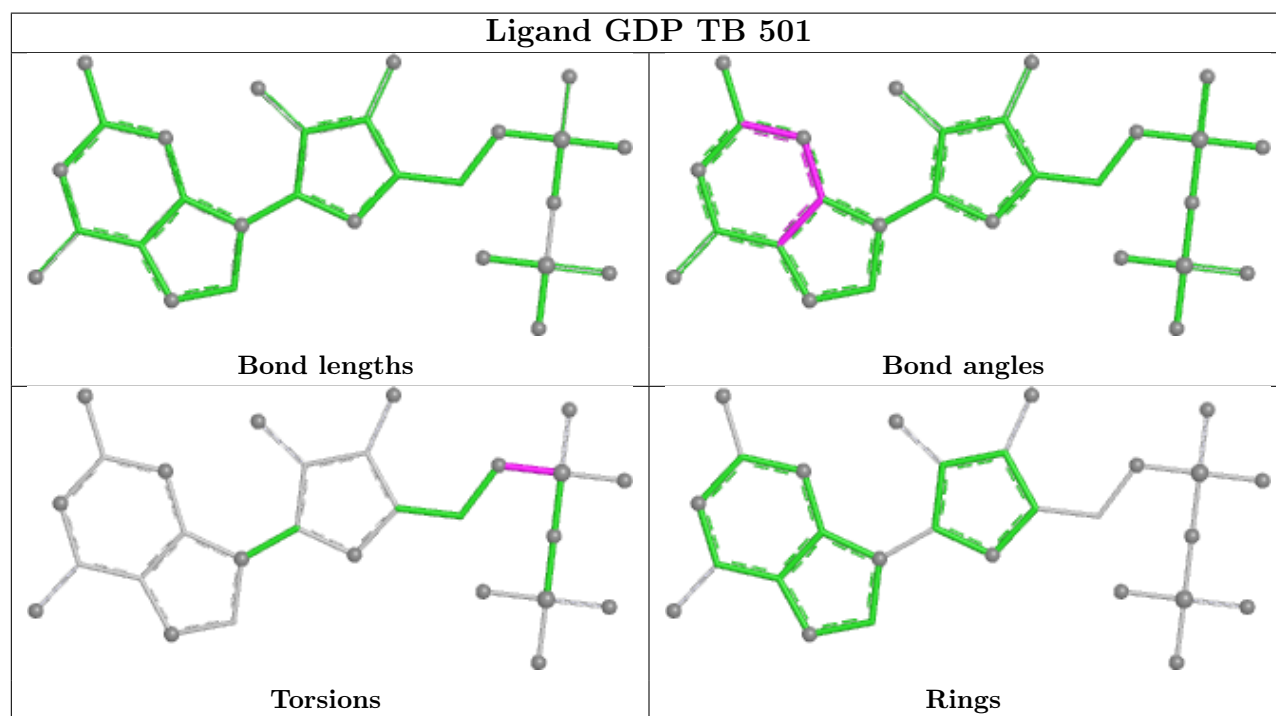
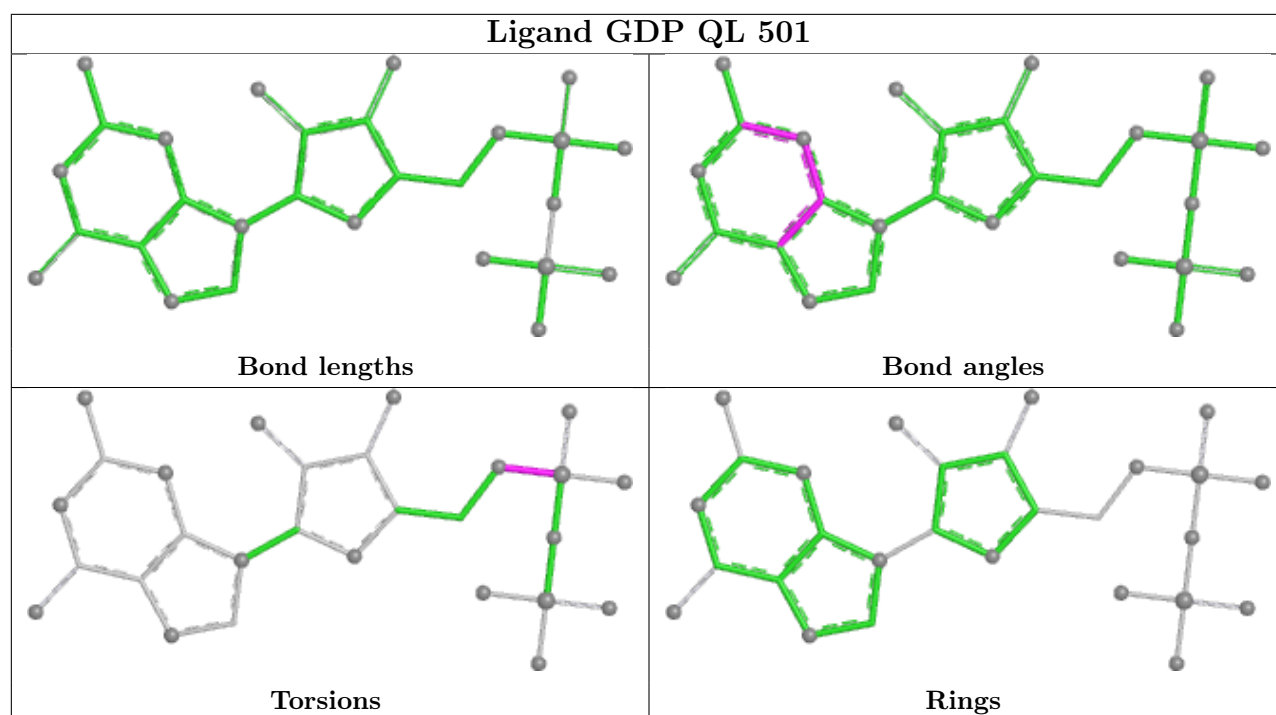




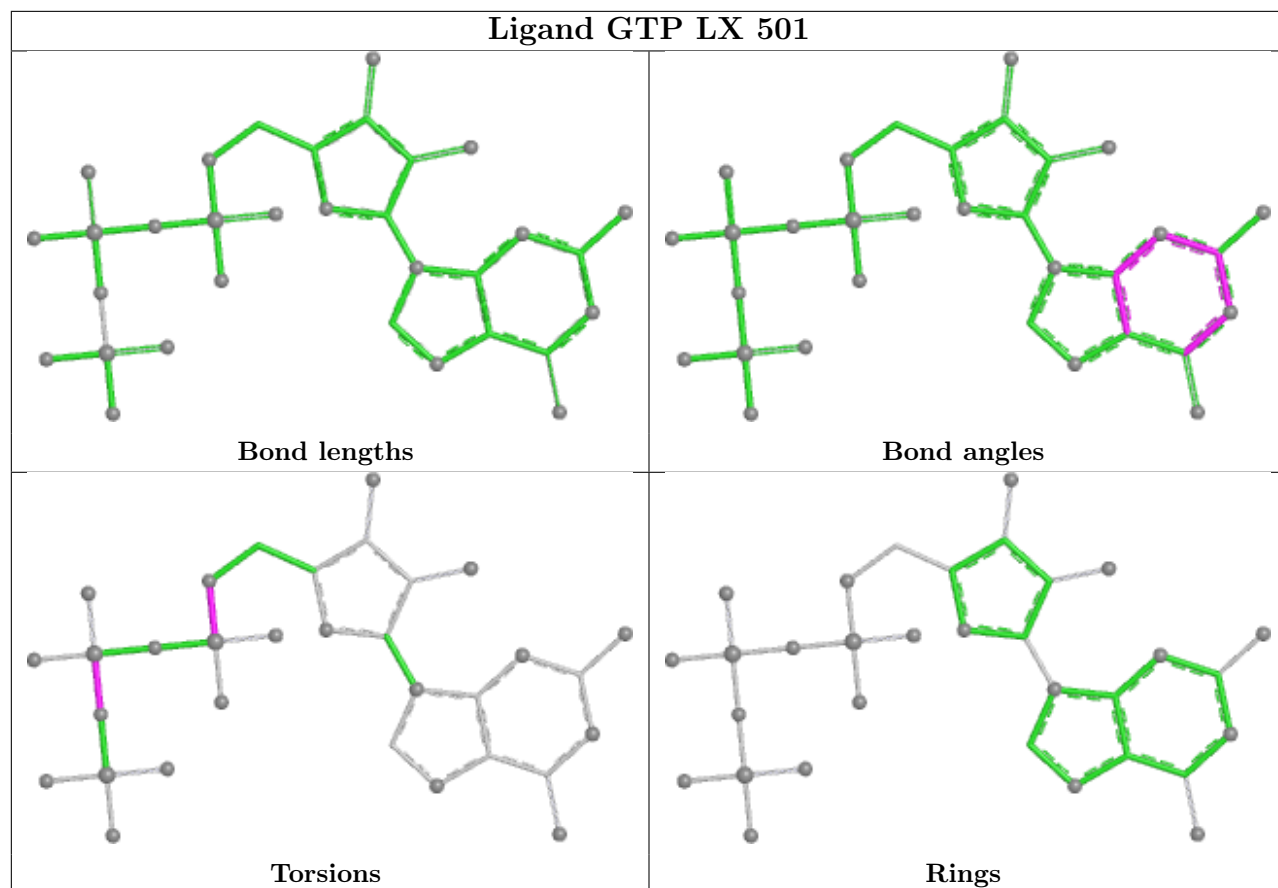




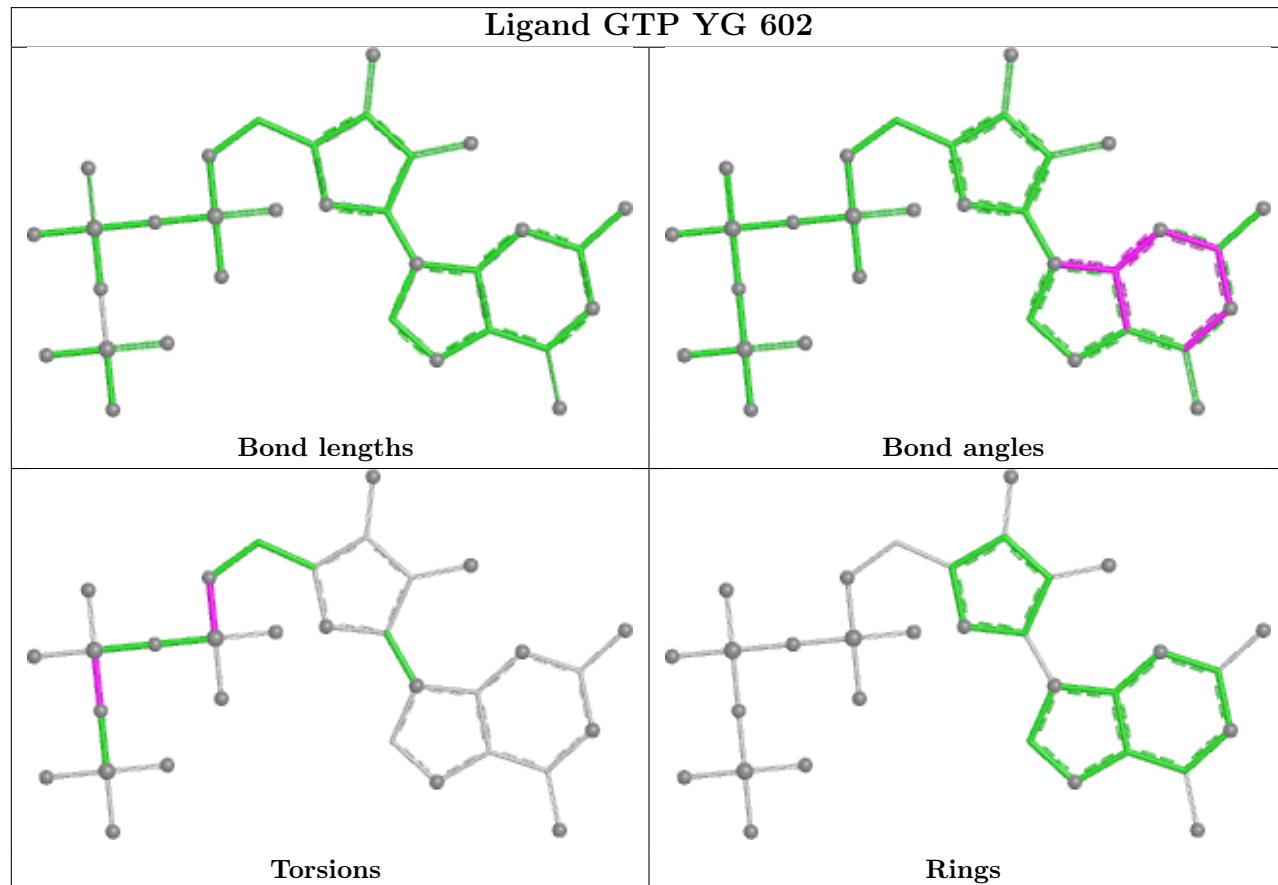


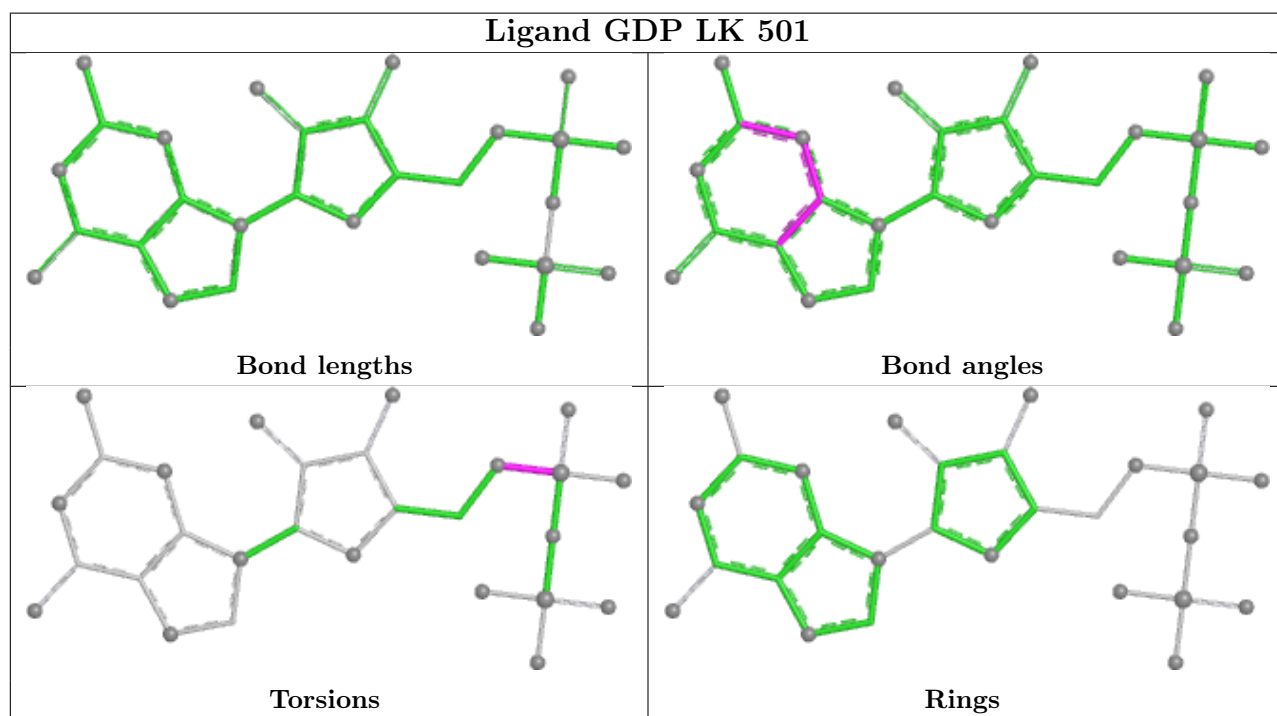
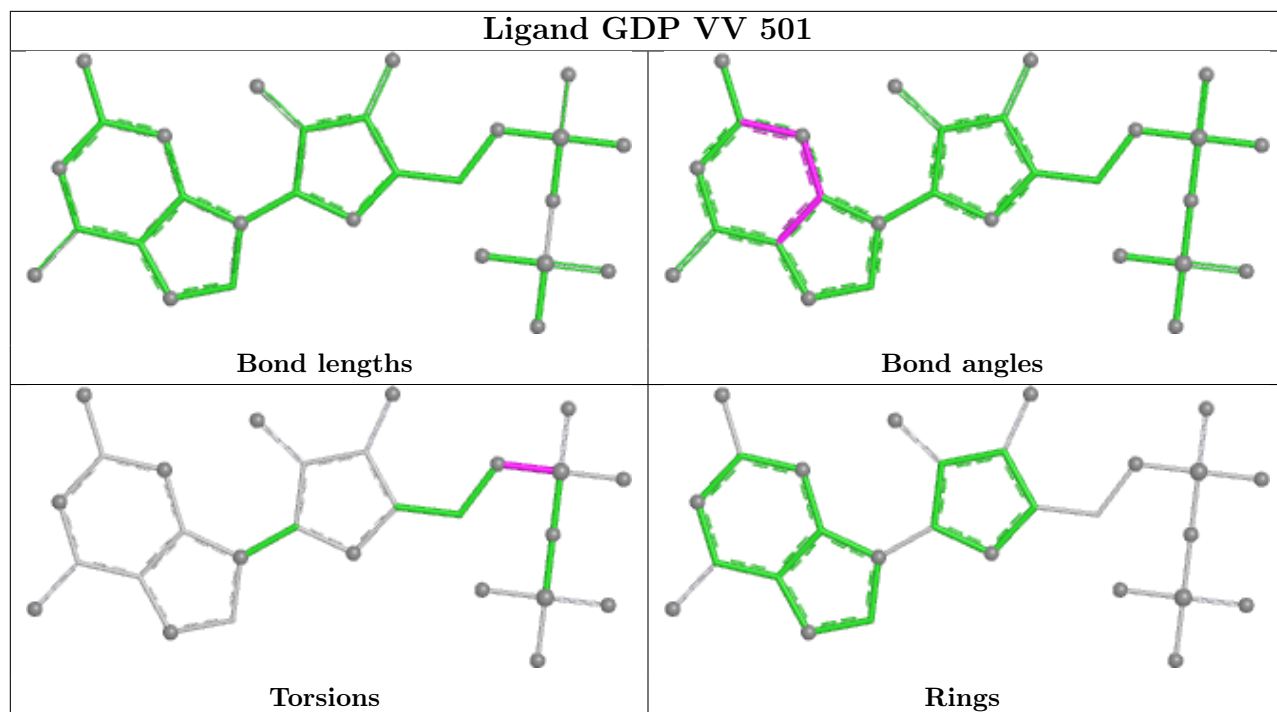


## Ligand GTP LX 501

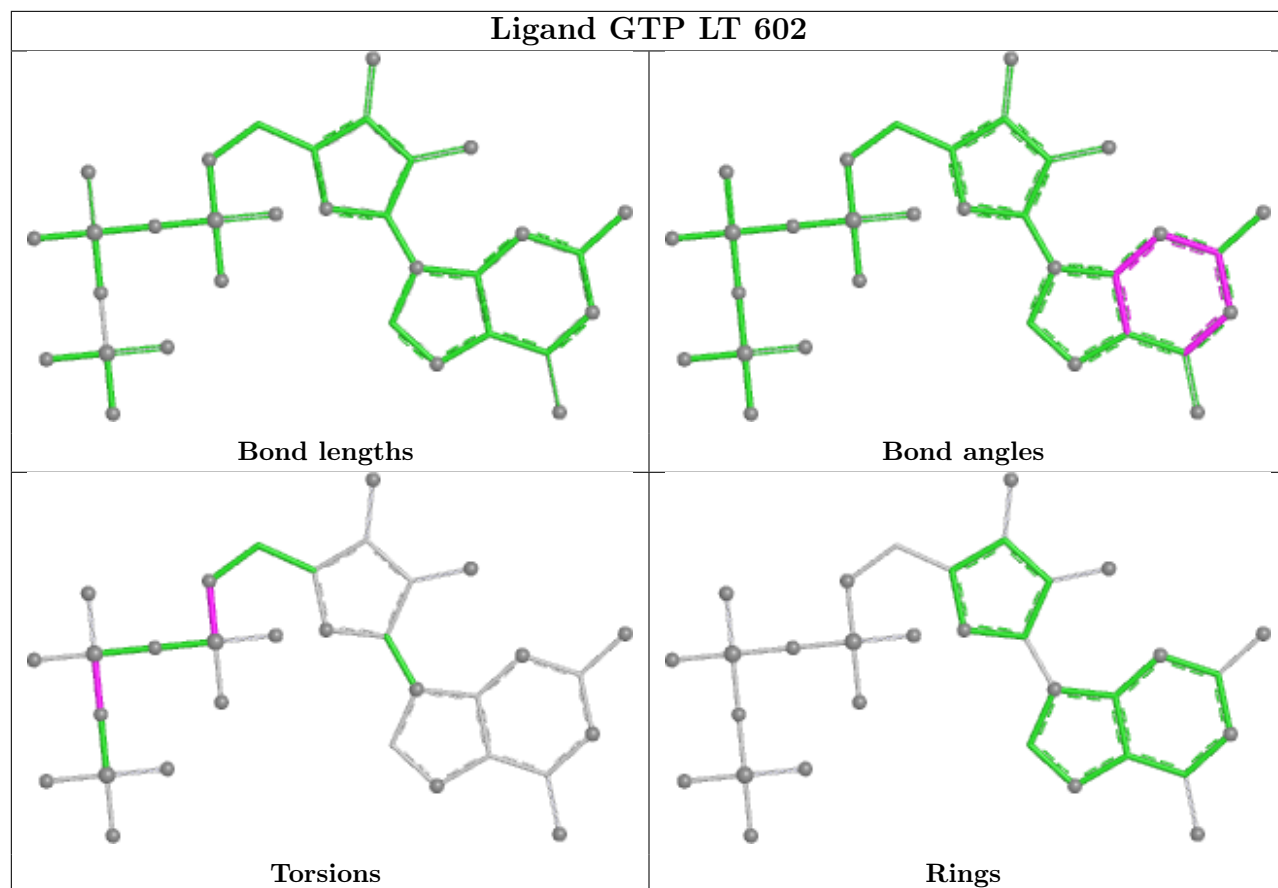


## Ligand GTP YG 602

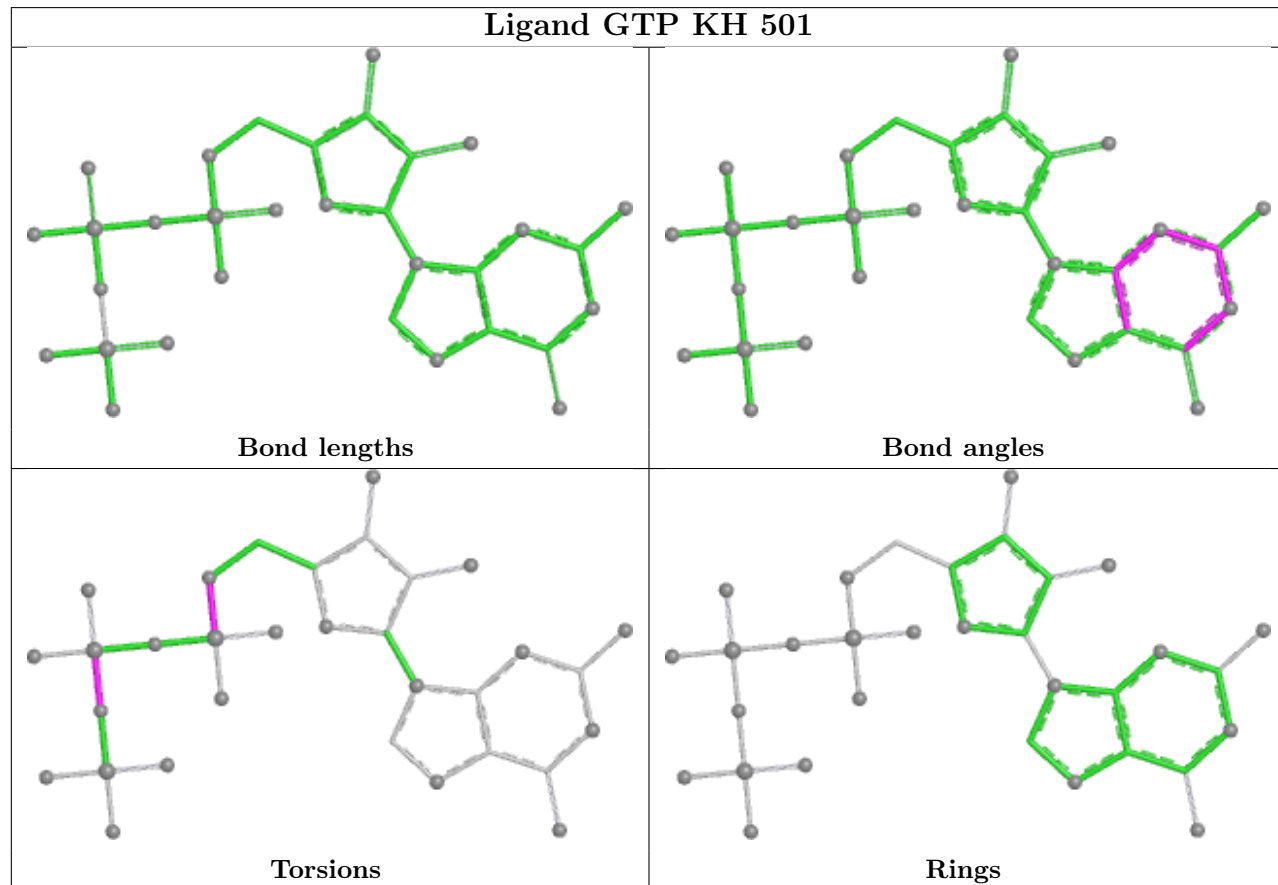


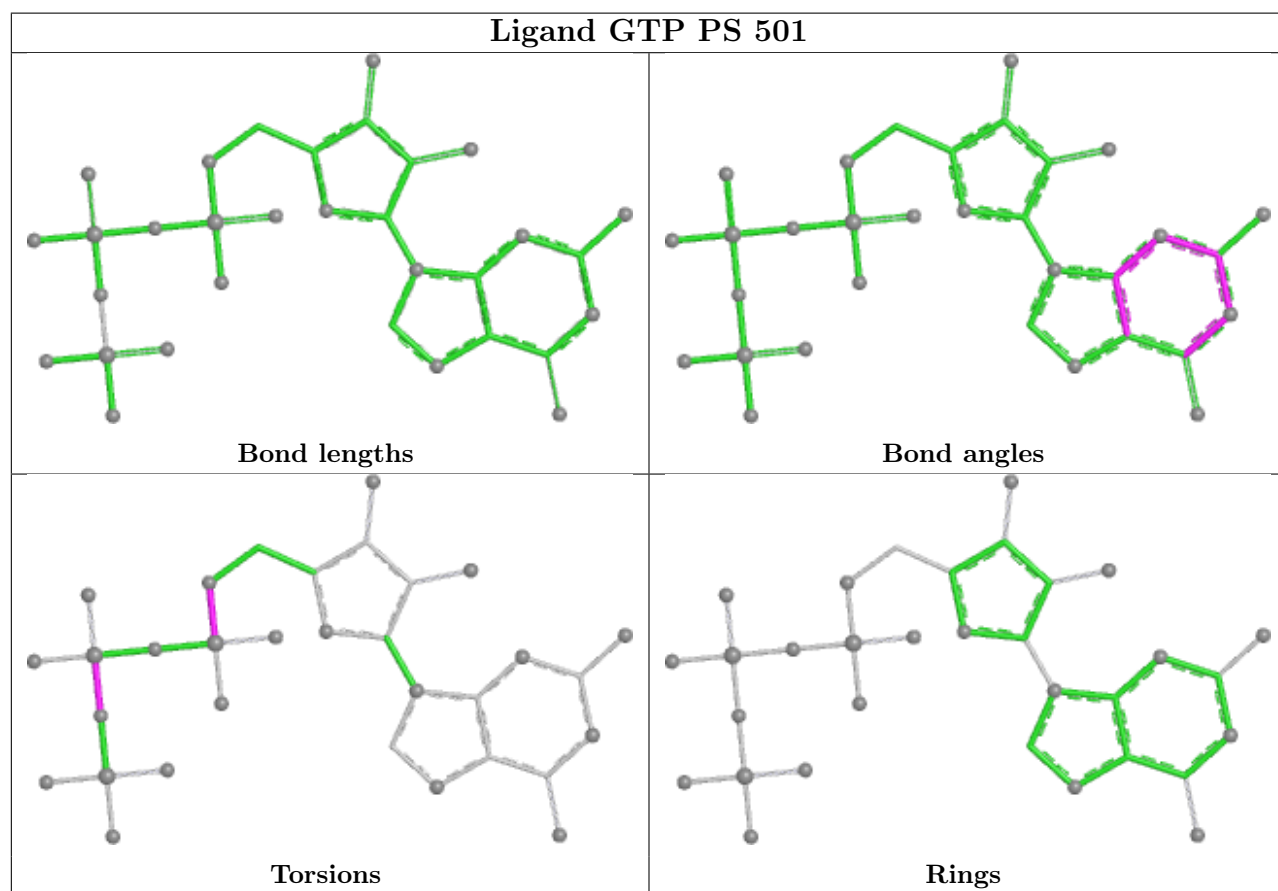
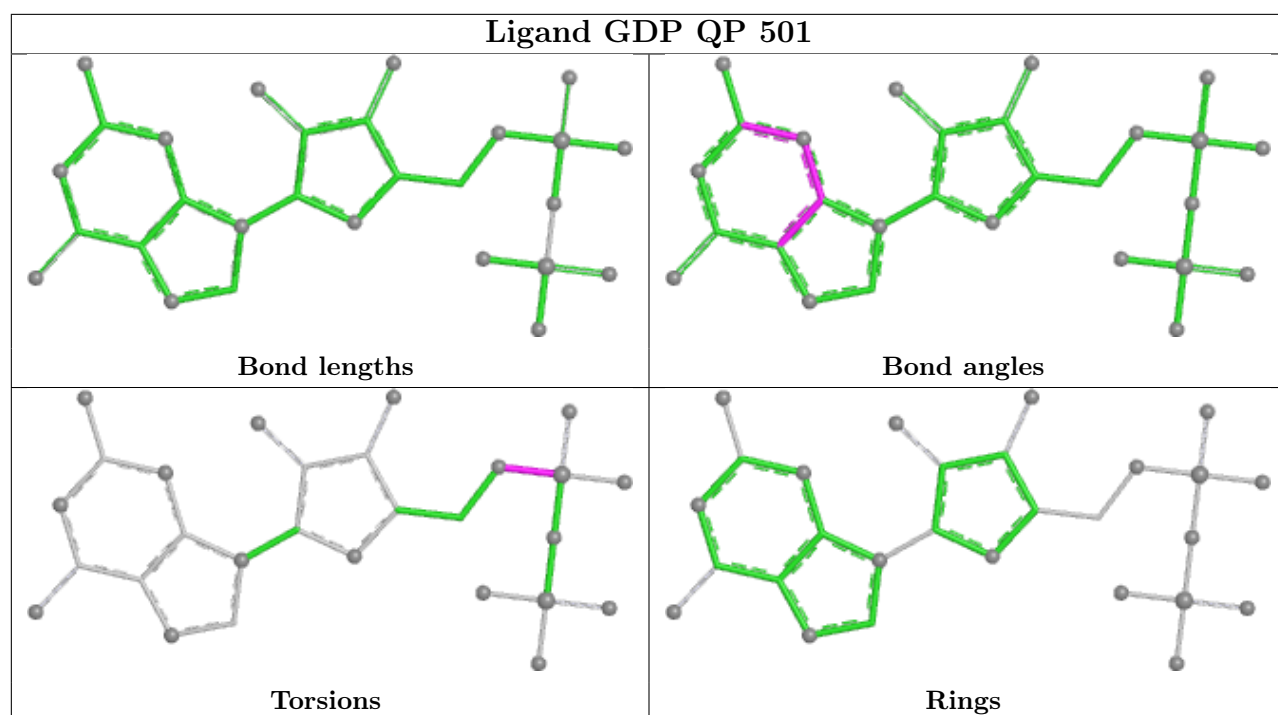


## Ligand GTP LT 602



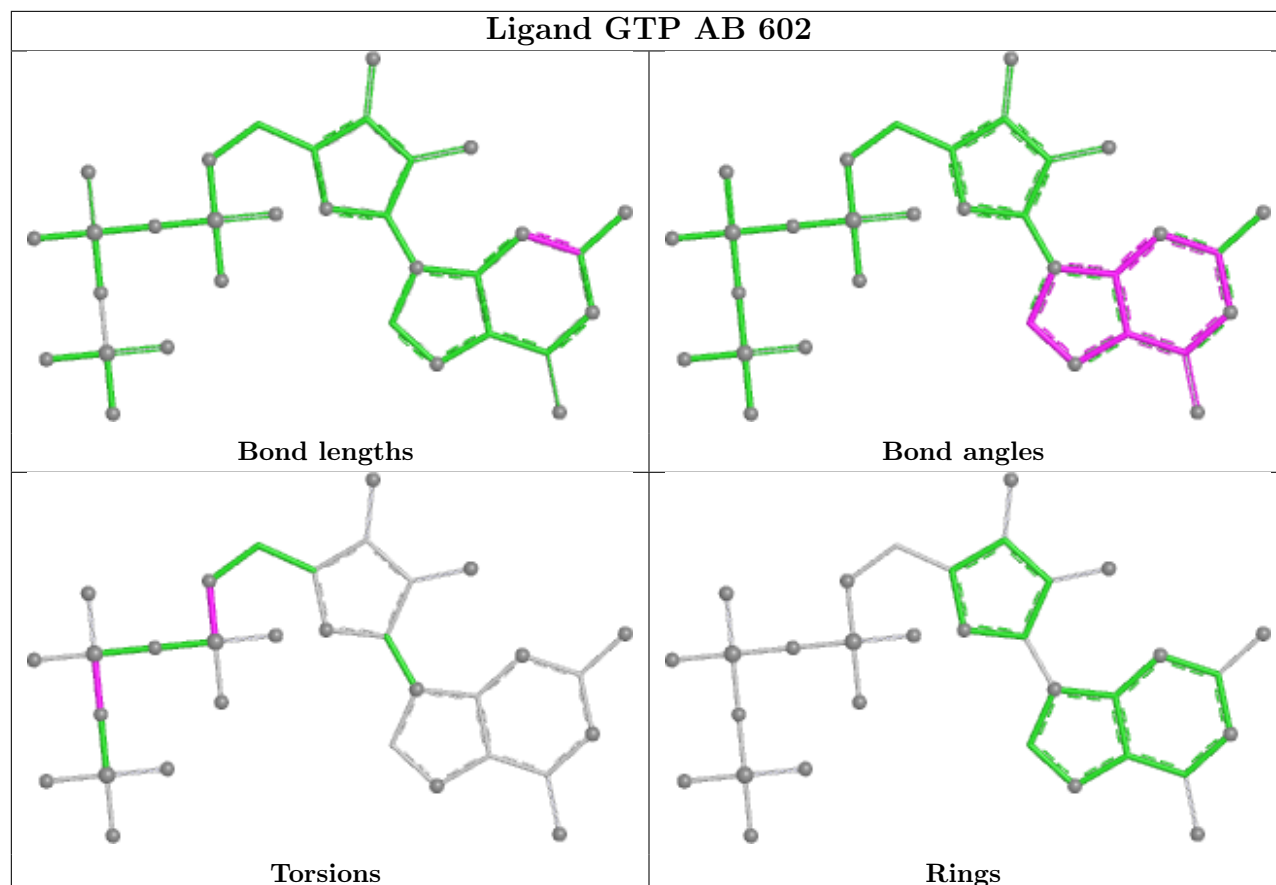
## Ligand GTP KH 501



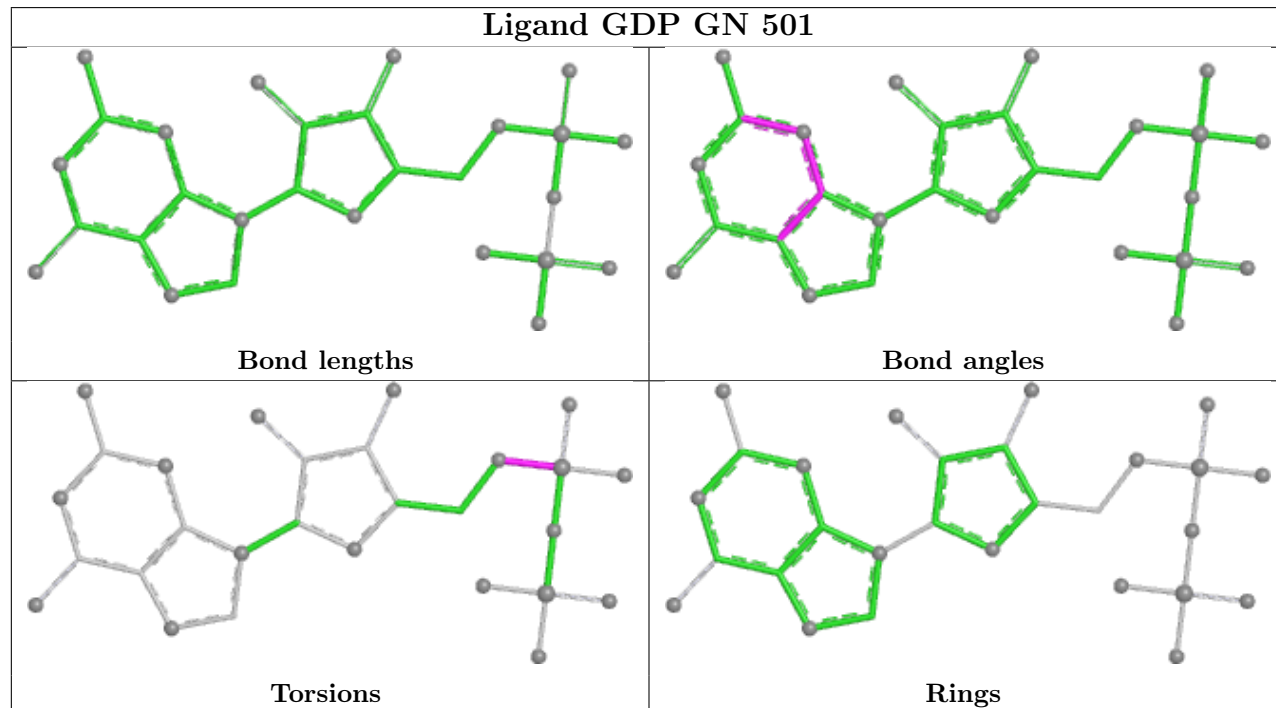


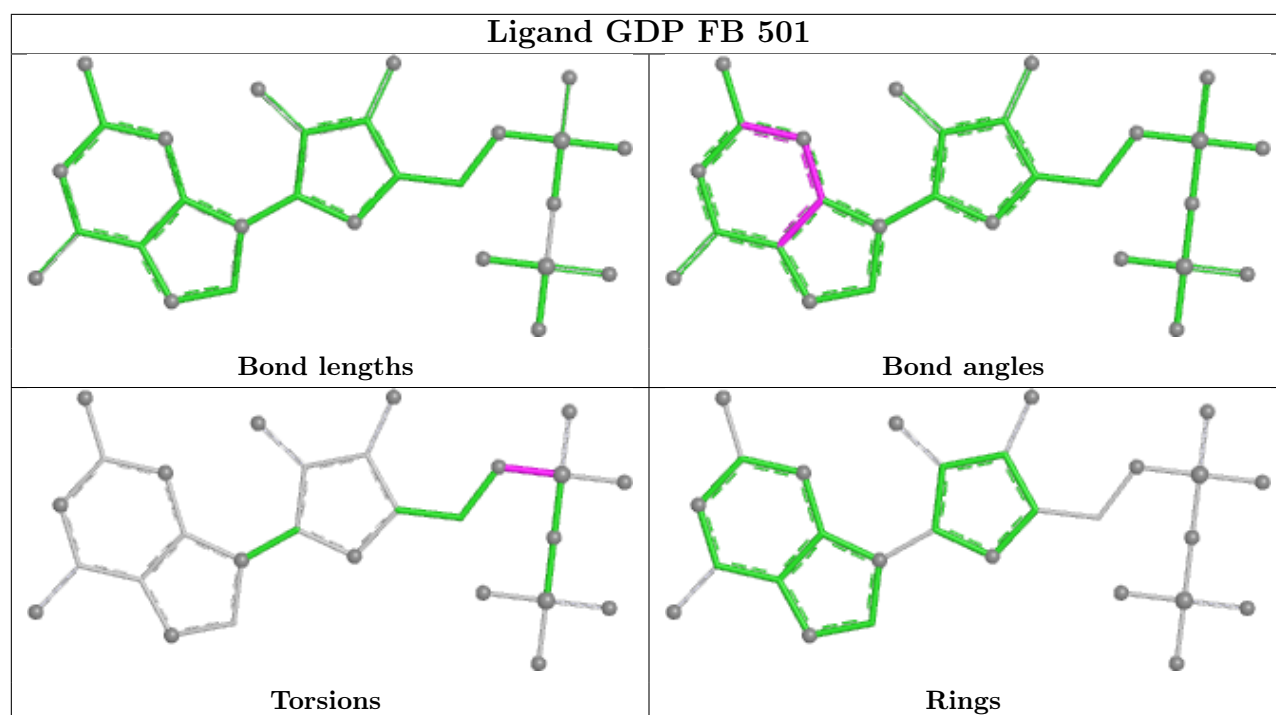


## Ligand GTP AB 602



## Ligand GDP GN 501





#### 4.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

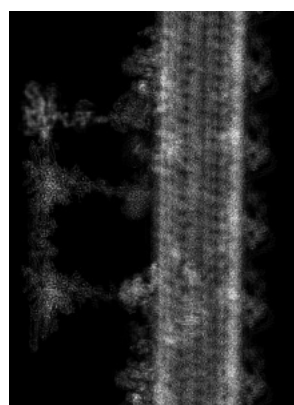
## 5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47524. These allow visual inspection of the internal detail of the map and identification of artifacts.

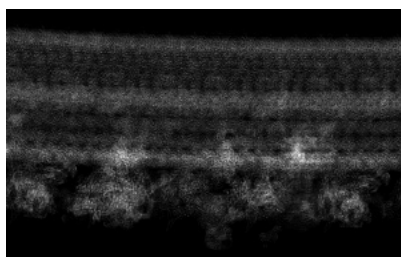
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

#### 5.1.1 Primary map



X



Y



Z

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

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

#### 5.2.1 Primary map



X Index: 380



Y Index: 430



Z Index: 600

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

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

### 5.3.1 Primary map



X Index: 314



Y Index: 676

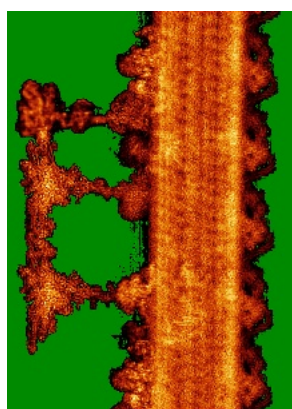


Z Index: 362

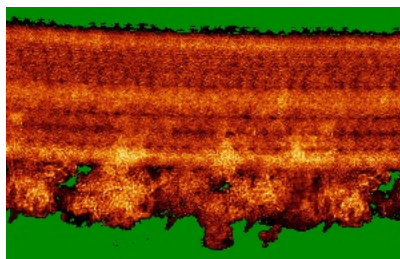
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 5.4.1 Primary map



X



Y

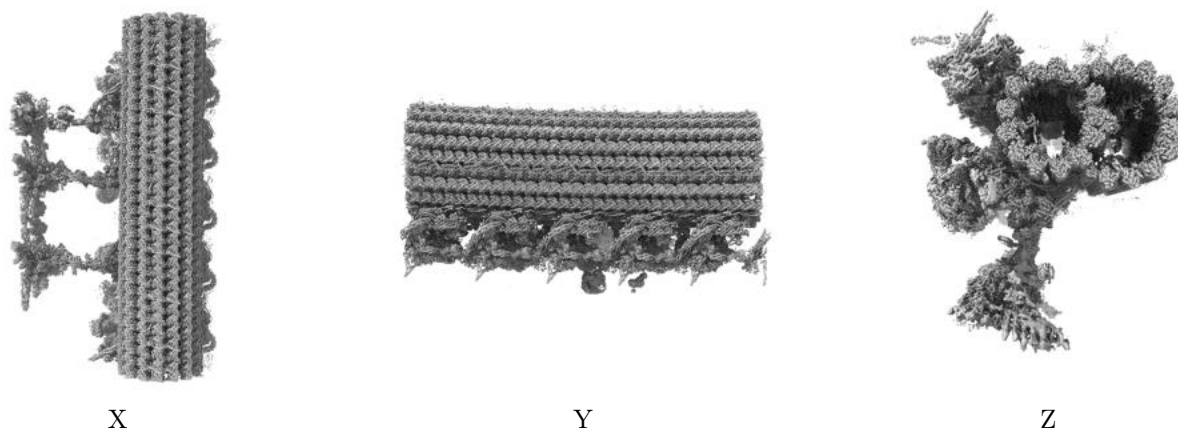


Z

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

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

### 5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

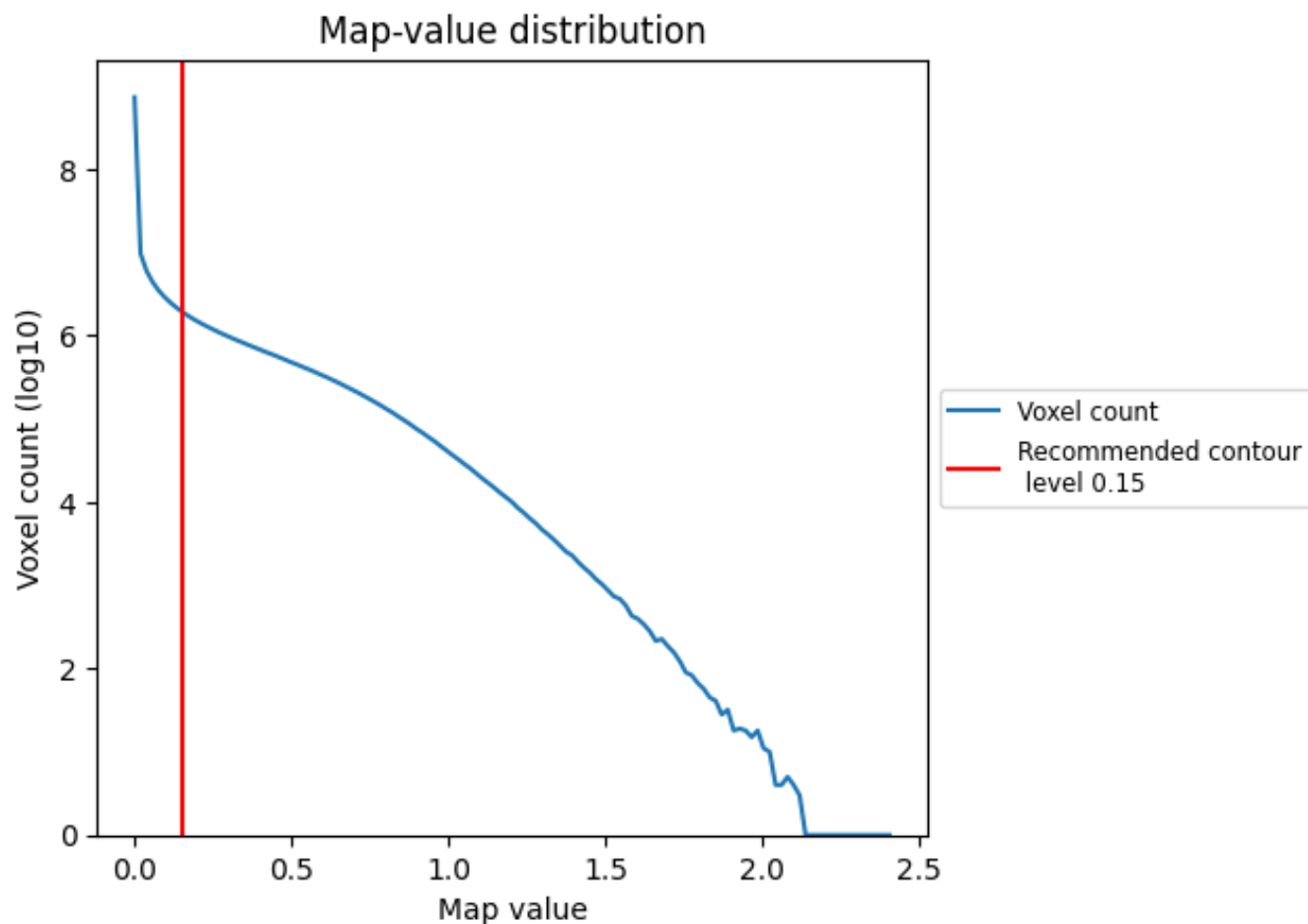
## 5.6 Mask visualisation [i](#)

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

## 6 Map analysis [i](#)

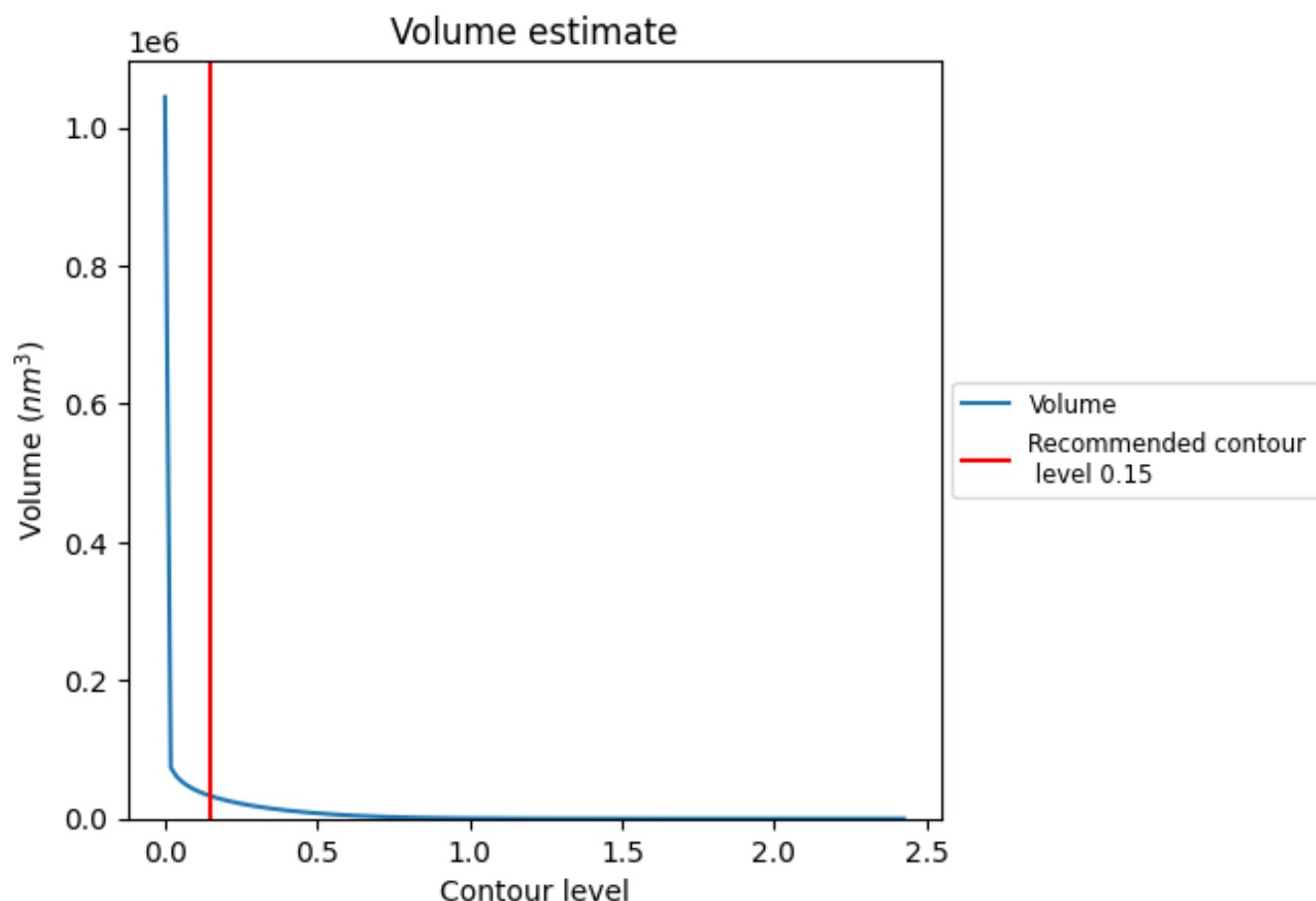
This section contains the results of statistical analysis of the map.

### 6.1 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.

## 6.2 Volume estimate [i](#)



The volume at the recommended contour level is 32681 nm<sup>3</sup>; this corresponds to an approximate mass of 29522 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.

## 6.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

## 7 Fourier-Shell correlation

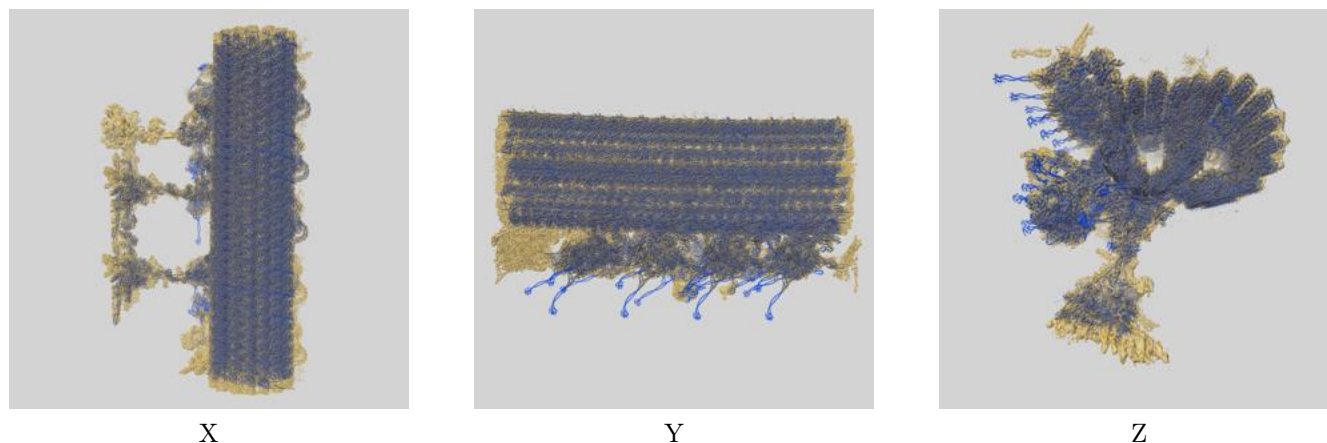
This section was not generated. No FSC curve or half-maps provided.



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

This section contains information regarding the fit between EMDB map EMD-47524 and PDB model 9E5C. Per-residue inclusion information can be found in section ?? on page ??.

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

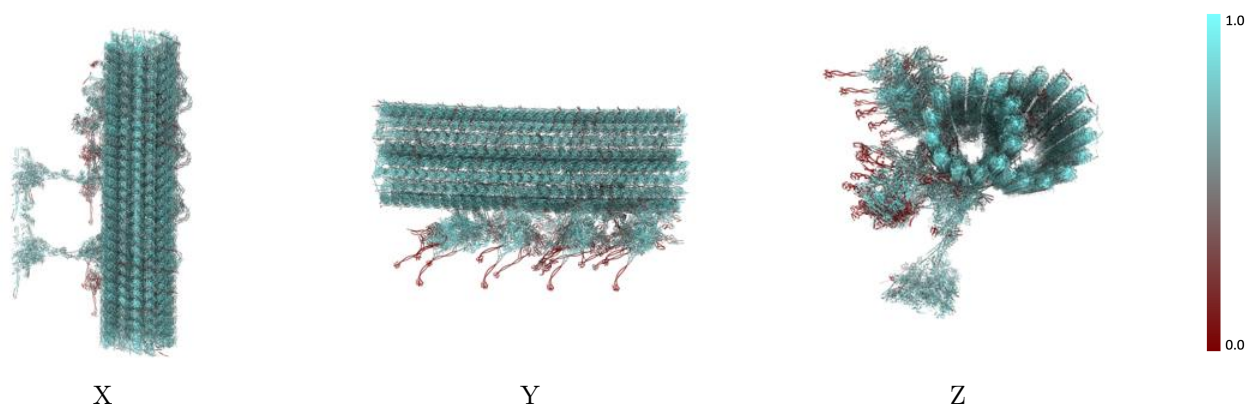


The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

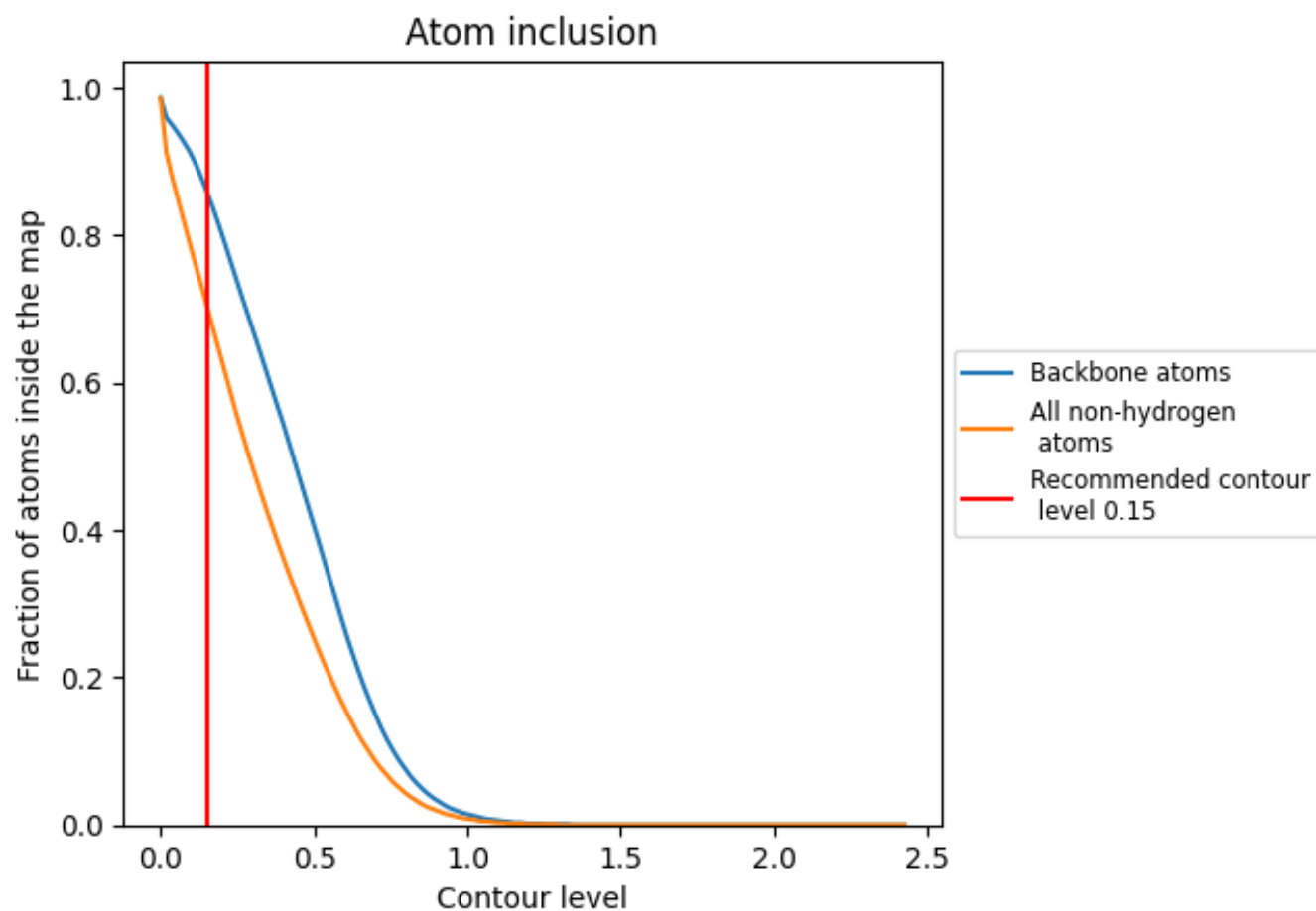
This section was not generated.

## 8.3 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 (0.15).

## 8.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

## 8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             |
|-------|--------------------------------------------------------------------------------------------|
| All   |  0.7050   |
| 0A    |  0.6470   |
| 0B    |  0.6610   |
| 0C    |  0.6720   |
| 0D    |  0.6540   |
| 0E    |  0.6770   |
| 0F    |  0.6060   |
| 0G    |  0.6650   |
| 0H    |  0.6830   |
| 0I    |  0.6690   |
| 0J    |  0.7060   |
| 0K    |  0.7160   |
| 0L    |  0.7090   |
| 0M    |  0.5530   |
| 0N    |  0.6670  |
| 0O    |  0.8180 |
| 0P    |  0.8210 |
| 0Q    |  0.8200 |
| 0R    |  0.7930 |
| 0S    |  0.7890 |
| 0T    |  0.7960 |
| 0U    |  0.6580 |
| 0V    |  0.6470 |
| 0W    |  0.6740 |
| 0X    |  0.6540 |
| 0Y    |  0.6300 |
| 0Z    |  0.6190 |
| 0a    |  0.6390 |
| 0b    |  0.6470 |
| 0c    |  0.6700 |
| 0d    |  0.6740 |
| 0e    |  0.6450 |
| 0f    |  0.6540 |
| 0g    |  0.3530 |
| 0h    |  0.4940 |



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| Chain | Atom inclusion                                                                             |
|-------|--------------------------------------------------------------------------------------------|
| 0i    |  0.3000   |
| 0j    |  0.5490   |
| 0k    |  0.3870   |
| 0l    |  0.5390   |
| 0m    |  0.4100   |
| 0n    |  0.5720   |
| 0o    |  0.3300   |
| 0p    |  0.5140   |
| 0q    |  0.8510   |
| 0r    |  0.7550   |
| 0s    |  0.7210   |
| 0t    |  0.4600   |
| 0u    |  0.4960   |
| 0v    |  0.6890   |
| 0w    |  0.6480   |
| 0x    |  0.6380   |
| 0y    |  0.6450   |
| 0z    |  0.5820   |
| 1A    |  0.6190   |
| 1B    |  0.6550  |
| 1C    |  0.7760 |
| 1D    |  0.7870 |
| 1E    |  0.7020 |
| 1F    |  0.7330 |
| 1G    |  0.7650 |
| 1H    |  0.7260 |
| 1I    |  0.7440 |
| 1J    |  0.6640 |
| 1K    |  0.6970 |
| 1L    |  0.6040 |
| 1M    |  0.6110 |
| 1N    |  0.3830 |
| 1O    |  0.3940 |
| 1P    |  0.6070 |
| 1Q    |  0.6530 |
| 1R    |  0.6590 |
| 1S    |  0.6940 |
| 1T    |  0.8010 |
| 1U    |  0.8070 |
| 1V    |  0.8080 |
| 1W    |  0.7300 |
| 1X    |  0.7500 |

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| Chain | Atom inclusion                                                                             |
|-------|--------------------------------------------------------------------------------------------|
| 1Y    |  0.8280   |
| 1Z    |  0.8230   |
| 1a    |  0.4880   |
| 1b    |  0.4490   |
| 1c    |  0.4610   |
| 1d    |  0.3930   |
| 1e    |  0.5410   |
| 1f    |  0.5360   |
| 1g    |  0.6060   |
| 1h    |  0.5710   |
| 1i    |  0.7950   |
| 1j    |  0.5320   |
| 1k    |  0.5210   |
| 1l    |  0.4410   |
| 1m    |  0.6020   |
| 1n    |  0.5350   |
| 1o    |  0.5650   |
| 1p    |  0.1330   |
| 1r    |  0.4290   |
| 1t    |  0.5310  |
| 2A    |  0.7170 |
| 2B    |  0.7490 |
| 2C    |  0.7100 |
| 2D    |  0.7890 |
| 2E    |  0.7680 |
| 2F    |  0.7900 |
| 2G    |  0.7100 |
| 2H    |  0.7510 |
| 2I    |  0.7220 |
| 2J    |  0.7610 |
| 2K    |  0.7670 |
| 2L    |  0.7560 |
| 2M    |  0.7510 |
| 2N    |  0.7530 |
| 2O    |  0.7130 |
| 2P    |  0.6940 |
| 2Q    |  0.7210 |
| 2R    |  0.7070 |
| 2S    |  0.7410 |
| 2T    |  0.6890 |
| 2U    |  0.7970 |
| 2V    |  0.8030 |

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| Chain | Atom inclusion                                                                             |
|-------|--------------------------------------------------------------------------------------------|
| 2W    |  0.8040   |
| 2X    |  0.6800   |
| 2Y    |  0.6790   |
| 2Z    |  0.6500   |
| 2a    |  0.7010   |
| 2b    |  0.6680   |
| 2c    |  0.6990   |
| 2d    |  0.6550   |
| 2e    |  0.6560   |
| 2f    |  0.6240   |
| 2g    |  0.6520   |
| 2h    |  0.6340   |
| 2i    |  0.6470   |
| 2j    |  0.6770   |
| 2k    |  0.6600   |
| 2l    |  0.7110   |
| 2m    |  0.7030   |
| 2n    |  0.6780   |
| 2o    |  0.7040  |
| 2p    |  0.6790 |
| 2q    |  0.7340 |
| 2r    |  0.6410 |
| 2s    |  0.7200 |
| 2t    |  0.6350 |
| 2u    |  0.6720 |
| 2v    |  0.7130 |
| 2w    |  0.6060 |
| 2x    |  0.7020 |
| 2y    |  0.5950 |
| 2z    |  0.7310 |
| 3A    |  0.7040 |
| 3B    |  0.6950 |
| 3C    |  0.7210 |
| 3D    |  0.7040 |
| 3E    |  0.8290 |
| 3F    |  0.8090 |
| 3G    |  0.8350 |
| 3H    |  0.8160 |
| 3I    |  0.8320 |
| 3J    |  0.3940 |
| 3K    |  0.5400 |
| 3L    |  0.7300 |

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| Chain | Atom inclusion                                                                             |
|-------|--------------------------------------------------------------------------------------------|
| 3M    |  0.7960   |
| 3N    |  0.7180   |
| 3O    |  0.7720   |
| 3P    |  0.7620   |
| 3Q    |  0.7730   |
| 3R    |  0.7550   |
| 3S    |  0.8050   |
| 3T    |  0.7200   |
| 3U    |  0.7270   |
| 3V    |  0.7670   |
| 3W    |  0.7540   |
| 3X    |  0.7350   |
| 3Y    |  0.7300   |
| 3Z    |  0.7970   |
| 3a    |  0.6540   |
| 3b    |  0.7070   |
| 3c    |  0.6690   |
| 3d    |  0.7110   |
| 3e    |  0.5170   |
| 3f    |  0.7150  |
| 3g    |  0.4540 |
| 3h    |  0.7350 |
| 3i    |  0.7180 |
| 3j    |  0.5890 |
| 3k    |  0.7640 |
| 3l    |  0.6770 |
| 3m    |  0.6480 |
| 3o    |  0.6840 |
| 3p    |  0.6160 |
| 3q    |  0.6720 |
| 3r    |  0.6410 |
| 3s    |  0.6690 |
| 3t    |  0.6480 |
| 3u    |  0.6840 |
| 3v    |  0.6570 |
| 3w    |  0.6740 |
| 3x    |  0.6610 |
| 3y    |  0.7420 |
| 3z    |  0.7060 |
| 4A    |  0.7410 |
| 4B    |  0.7630 |
| 4C    |  0.7770 |

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| Chain | Atom inclusion                                                                             |
|-------|--------------------------------------------------------------------------------------------|
| 4D    |  0.8150   |
| 4E    |  0.7860   |
| 4F    |  0.8090   |
| 4G    |  0.7980   |
| 4H    |  0.7960   |
| 4I    |  0.7530   |
| 4J    |  0.7980   |
| 4K    |  0.8100   |
| 4L    |  0.8100   |
| 4M    |  0.7370   |
| 4N    |  0.7680   |
| 4O    |  0.7280   |
| 4P    |  0.7100   |
| 4Q    |  0.7680   |
| 4R    |  0.7450   |
| 4S    |  0.7460   |
| 4T    |  0.8130   |
| 4U    |  0.7300   |
| 4V    |  0.7180   |
| 4W    |  0.7350  |
| 4X    |  0.7170 |
| 4Y    |  0.7350 |
| 4Z    |  0.7130 |
| 4a    |  0.6670 |
| 4b    |  0.6580 |
| 4c    |  0.7210 |
| 4d    |  0.7370 |
| 4e    |  0.7800 |
| 4f    |  0.7760 |
| 4g    |  0.7880 |
| 4h    |  0.8020 |
| 4i    |  0.7890 |
| 4j    |  0.7930 |
| 4k    |  0.6070 |
| 4l    |  0.5990 |
| 4m    |  0.6470 |
| 4n    |  0.5290 |
| 4o    |  0.6530 |
| 4p    |  0.6990 |
| 4q    |  0.6550 |
| 4r    |  0.7070 |
| 4s    |  0.7130 |

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| Chain | Atom inclusion                                                                             |
|-------|--------------------------------------------------------------------------------------------|
| 4t    |  0.7100   |
| 4u    |  0.6680   |
| 4v    |  0.6900   |
| 4w    |  0.6280   |
| 4x    |  0.8260   |
| 4y    |  0.6250   |
| 4z    |  0.6170   |
| 5A    |  0.6530   |
| 5B    |  0.5890   |
| 5C    |  0.7440   |
| 5D    |  0.7450   |
| 5E    |  0.7390   |
| 5F    |  0.7590   |
| 5G    |  0.7480   |
| 5H    |  0.7590   |
| 5I    |  0.7370   |
| 5J    |  0.8010   |
| 5K    |  0.6760   |
| 5L    |  0.7920  |
| 5M    |  0.7560 |
| 5N    |  0.7520 |
| 5O    |  0.7190 |
| 5P    |  0.7340 |
| 5Q    |  0.7480 |
| 5R    |  0.7410 |
| 5S    |  0.5740 |
| 5T    |  0.6260 |
| 5U    |  0.6150 |
| 5V    |  0.5800 |
| 5W    |  0.5650 |
| 5X    |  0.5560 |
| 5Y    |  0.6370 |
| 5Z    |  0.6330 |
| 5a    |  0.7430 |
| 5b    |  0.6460 |
| 5c    |  0.6780 |
| 5d    |  0.5580 |
| 5e    |  0.8220 |
| 5f    |  0.7390 |
| 5g    |  0.6660 |
| 5h    |  0.7360 |
| 5i    |  0.5760 |

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| Chain | Atom inclusion                                                                             |
|-------|--------------------------------------------------------------------------------------------|
| 5j    |  0.6360   |
| 5k    |  0.4240   |
| 5l    |  0.7160   |
| 5m    |  0.7910   |
| 5n    |  0.6840   |
| 5o    |  0.6790   |
| 5p    |  0.8410   |
| 5q    |  0.6570   |
| 5r    |  0.6080   |
| 5s    |  0.7080   |
| 5t    |  0.6740   |
| 5u    |  0.7880   |
| 5v    |  0.8110   |
| 5w    |  0.8320   |
| 5x    |  0.9130   |
| 5y    |  0.9420   |
| 6A    |  0.6450   |
| 6B    |  0.6020   |
| 6C    |  0.6540   |
| 6D    |  0.6240  |
| 6E    |  0.5880 |
| 6F    |  0.6010 |
| 6G    |  0.5990 |
| 6H    |  0.5930 |
| 6I    |  0.5660 |
| 6J    |  0.5640 |
| 6K    |  0.5810 |
| 6L    |  0.4670 |
| 6M    |  0.5480 |
| 6N    |  0.5440 |
| 6O    |  0.4750 |
| 6P    |  0.5320 |
| 6Q    |  0.4560 |
| 6R    |  0.7150 |
| 6S    |  0.6780 |
| 6T    |  0.6830 |
| 6U    |  0.5870 |
| 6V    |  0.6030 |
| 6W    |  0.5990 |
| 6X    |  0.4740 |
| 6Y    |  0.6210 |
| 6Z    |  0.6140 |

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| Chain | Atom inclusion                                                                             |
|-------|--------------------------------------------------------------------------------------------|
| 6a    |  0.3090   |
| 6b    |  0.7140   |
| 6c    |  0.3820   |
| 6d    |  0.2500   |
| 6e    |  0.3700   |
| 6f    |  0.6910   |
| 6g    |  0.6640   |
| 6h    |  0.7320   |
| 6i    |  0.5610   |
| 6j    |  0.7250   |
| 6k    |  0.7020   |
| 6l    |  0.6990   |
| 6m    |  0.7180   |
| 6n    |  0.5880   |
| 6o    |  0.6870   |
| 6p    |  0.7180   |
| 6q    |  0.6320   |
| 6r    |  0.7080   |
| 6s    |  0.6320  |
| 6t    |  0.5920 |
| 6u    |  0.6870 |
| 7A    |  0.5960 |
| 7B    |  0.6500 |
| 7C    |  0.6360 |
| 7D    |  0.6250 |
| 7E    |  0.5680 |
| 7F    |  0.6130 |
| 7G    |  0.6140 |
| 7H    |  0.3780 |
| 7I    |  0.5370 |
| 7J    |  0.4930 |
| 7K    |  0.3630 |
| 7L    |  0.5920 |
| 7M    |  0.5340 |
| 7N    |  0.6570 |
| 7O    |  0.7010 |
| 7P    |  0.6490 |
| 7Q    |  0.7470 |
| 7R    |  0.7520 |
| 7S    |  0.7420 |
| 7T    |  0.8200 |
| 7U    |  0.8450 |

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| Chain | Atom inclusion                                                                             |
|-------|--------------------------------------------------------------------------------------------|
| 7V    |  0.4570   |
| 7W    |  0.6160   |
| 7X    |  0.4950   |
| 7Y    |  0.4800   |
| 7Z    |  0.6040   |
| 7a    |  0.6460   |
| 7b    |  0.6370   |
| 7c    |  0.7090   |
| 7d    |  0.8130   |
| 7e    |  0.6260   |
| 7f    |  0.6100   |
| 7g    |  0.6710   |
| 7h    |  0.6720   |
| 7i    |  0.3410   |
| 7j    |  0.6910   |
| 7k    |  0.6110   |
| 7l    |  0.6760   |
| 7m    |  0.6560   |
| 7n    |  0.6730   |
| 7o    |  0.5830  |
| 7p    |  0.6100 |
| 7q    |  0.4240 |
| 7r    |  0.5890 |
| 7s    |  0.4680 |
| 7t    |  0.3880 |
| 8A    |  0.5110 |
| 8B    |  0.4240 |
| 8C    |  0.5990 |
| 8D    |  0.3040 |
| 8E    |  0.4270 |
| 8F    |  0.3560 |
| 8G    |  0.3510 |
| 8H    |  0.4120 |
| 8I    |  0.3500 |
| 8J    |  0.3100 |
| 8K    |  0.4040 |
| 8L    |  0.8400 |
| 8M    |  0.3990 |
| 8N    |  0.5990 |
| 8O    |  0.5570 |
| 8P    |  0.4020 |
| 8Q    |  0.6090 |

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| Chain | Atom inclusion                                                                             |
|-------|--------------------------------------------------------------------------------------------|
| 8R    |  0.5520   |
| 8S    |  0.3750   |
| 8T    |  0.5910   |
| 8U    |  0.3290   |
| 8V    |  0.6060   |
| 8W    |  0.2350   |
| 8X    |  0.3350   |
| 8Y    |  0.5790   |
| 8Z    |  0.3010   |
| 8c    |  0.7030   |
| 8d    |  0.8140   |
| 8e    |  0.6220   |
| 8f    |  0.6020   |
| 8g    |  0.6620   |
| 8h    |  0.6640   |
| 8i    |  0.3170   |
| 8j    |  0.6730   |
| 8k    |  0.6170   |
| 8l    |  0.6640  |
| 8m    |  0.6580 |
| 8n    |  0.6320 |
| 8o    |  0.5580 |
| 8p    |  0.5370 |
| 8q    |  0.4390 |
| 8r    |  0.5720 |
| 8s    |  0.5410 |
| 8t    |  0.4910 |
| 9A    |  0.3390 |
| 9B    |  0.5750 |
| 9C    |  0.5160 |
| 9D    |  0.5290 |
| 9E    |  0.6280 |
| 9F    |  0.6500 |
| 9G    |  0.6690 |
| 9H    |  0.6670 |
| 9I    |  0.6580 |
| 9J    |  0.6800 |
| 9K    |  0.6960 |
| 9L    |  0.6570 |
| 9M    |  0.3730 |
| 9N    |  0.2980 |
| 9O    |  0.0990 |

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| Chain | Atom inclusion                                                                             |
|-------|--------------------------------------------------------------------------------------------|
| 9P    |  0.3790   |
| 9Q    |  0.3200   |
| 9R    |  0.1120   |
| 9S    |  0.3710   |
| 9T    |  0.4150   |
| 9U    |  0.5130   |
| 9V    |  0.4440   |
| 9W    |  0.5880   |
| 9X    |  0.6200   |
| 9Y    |  0.5780   |
| 9Z    |  0.5180   |
| 9a    |  0.6360   |
| 9b    |  0.6010   |
| 9c    |  0.7090   |
| 9d    |  0.8050   |
| 9e    |  0.6260   |
| 9f    |  0.6080   |
| 9g    |  0.6660   |
| 9h    |  0.6760   |
| 9i    |  0.3430  |
| 9j    |  0.6940 |
| 9k    |  0.6170 |
| 9l    |  0.6710 |
| 9m    |  0.6630 |
| 9n    |  0.6770 |
| 9o    |  0.5810 |
| 9p    |  0.6080 |
| 9q    |  0.4300 |
| 9r    |  0.5900 |
| 9s    |  0.5380 |
| 9t    |  0.4880 |
| AA    |  0.7700 |
| AB    |  0.7700 |
| AC    |  0.7800 |
| AD    |  0.7740 |
| AE    |  0.7750 |
| AF    |  0.7480 |
| AG    |  0.7690 |
| AH    |  0.7890 |
| AI    |  0.8020 |
| AJ    |  0.7980 |
| AK    |  0.8120 |

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| Chain | Atom inclusion                                                                             |
|-------|--------------------------------------------------------------------------------------------|
| AL    |  0.8120   |
| AM    |  0.8000   |
| AN    |  0.8050   |
| AO    |  0.8000   |
| AP    |  0.8060   |
| AQ    |  0.8050   |
| AR    |  0.7890   |
| AS    |  0.7920   |
| AT    |  0.7410   |
| AU    |  0.7450   |
| AV    |  0.7080   |
| AW    |  0.7120   |
| AX    |  0.7570   |
| AY    |  0.7710   |
| AZ    |  0.7770   |
| Aa    |  0.7790   |
| Ab    |  0.7890   |
| Ac    |  0.8020   |
| Ad    |  0.8000  |
| Ae    |  0.7960 |
| Af    |  0.7680 |
| Ag    |  0.7720 |
| Ah    |  0.7840 |
| Ai    |  0.7680 |
| Aj    |  0.7810 |
| Ak    |  0.7840 |
| Al    |  0.7850 |
| Am    |  0.7700 |
| An    |  0.7310 |
| Ao    |  0.7280 |
| Ap    |  0.7510 |
| BA    |  0.7840 |
| BB    |  0.7770 |
| BC    |  0.7500 |
| BD    |  0.7550 |
| BF    |  0.7240 |
| BG    |  0.7430 |
| BH    |  0.7310 |
| BI    |  0.7170 |
| BJ    |  0.7160 |
| BK    |  0.7430 |
| BL    |  0.7700 |

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| Chain | Atom inclusion                                                                             |
|-------|--------------------------------------------------------------------------------------------|
| BM    |  0.7960   |
| BN    |  0.7700   |
| BO    |  0.7920   |
| BP    |  0.7750   |
| BQ    |  0.7690   |
| BR    |  0.7580   |
| BS    |  0.7790   |
| BT    |  0.7850   |
| BU    |  0.7820   |
| BV    |  0.7680   |
| BW    |  0.7770   |
| BX    |  0.7250   |
| BY    |  0.6990   |
| BZ    |  0.6860   |
| CA    |  0.6810   |
| CB    |  0.7140   |
| CC    |  0.7380   |
| CD    |  0.7350   |
| CE    |  0.7400   |
| CF    |  0.7330  |
| CH    |  0.7160 |
| CI    |  0.7290 |
| CJ    |  0.7130 |
| CK    |  0.7300 |
| CL    |  0.7250 |
| CM    |  0.7170 |
| CN    |  0.7270 |
| CO    |  0.7470 |
| CP    |  0.7570 |
| CQ    |  0.7910 |
| CR    |  0.7750 |
| CS    |  0.8000 |
| CT    |  0.7350 |
| CU    |  0.7700 |
| CV    |  0.7760 |
| CW    |  0.7870 |
| CX    |  0.7950 |
| CY    |  0.8100 |
| CZ    |  0.7510 |
| DA    |  0.7690 |
| DB    |  0.7240 |
| DC    |  0.7310 |

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| Chain | Atom inclusion                                                                             |
|-------|--------------------------------------------------------------------------------------------|
| DD    |  0.7400   |
| DE    |  0.7010   |
| DF    |  0.6650   |
| DG    |  0.6950   |
| DH    |  0.7070   |
| DI    |  0.7360   |
| DJ    |  0.7230   |
| DK    |  0.7840   |
| DL    |  0.7590   |
| DM    |  0.6900   |
| DN    |  0.7010   |
| DO    |  0.7210   |
| DP    |  0.7790   |
| DQ    |  0.7780   |
| DR    |  0.7960   |
| DS    |  0.7410   |
| DT    |  0.7800   |
| DU    |  0.7800   |
| DV    |  0.7910  |
| DW    |  0.7530 |
| DX    |  0.8010 |
| DY    |  0.7900 |
| DZ    |  0.7900 |
| EA    |  0.7920 |
| EB    |  0.7820 |
| EC    |  0.7690 |
| ED    |  0.7760 |
| EE    |  0.7430 |
| EF    |  0.7810 |
| EG    |  0.7860 |
| EH    |  0.7080 |
| EI    |  0.6850 |
| EJ    |  0.6870 |
| EK    |  0.6900 |
| EL    |  0.7050 |
| EM    |  0.7190 |
| EN    |  0.7910 |
| EO    |  0.7930 |
| EQ    |  0.7660 |
| ER    |  0.7370 |
| ES    |  0.7100 |
| ET    |  0.7680 |

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| Chain | Atom inclusion                                                                             |
|-------|--------------------------------------------------------------------------------------------|
| EU    |  0.7900   |
| EV    |  0.8060   |
| EW    |  0.7540   |
| EX    |  0.7850   |
| EY    |  0.7810   |
| EZ    |  0.7970   |
| FA    |  0.7640   |
| FB    |  0.8000   |
| FC    |  0.7960   |
| FD    |  0.8120   |
| FE    |  0.7740   |
| FF    |  0.7850   |
| FG    |  0.7740   |
| FH    |  0.7730   |
| FI    |  0.7430   |
| FJ    |  0.7750   |
| FK    |  0.8300   |
| FL    |  0.8040   |
| FM    |  0.7730  |
| FN    |  0.7970 |
| FO    |  0.7780 |
| FP    |  0.7340 |
| FQ    |  0.7360 |
| FR    |  0.7850 |
| FS    |  0.8400 |
| FT    |  0.8300 |
| FV    |  0.7950 |
| FW    |  0.7450 |
| FX    |  0.7400 |
| FY    |  0.7480 |
| FZ    |  0.7840 |
| GA    |  0.7910 |
| GB    |  0.8090 |
| GC    |  0.7800 |
| GD    |  0.8030 |
| GE    |  0.7690 |
| GF    |  0.7940 |
| GG    |  0.7380 |
| GH    |  0.7800 |
| GI    |  0.7750 |
| GJ    |  0.8030 |
| GK    |  0.7850 |

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| Chain | Atom inclusion                                                                             |
|-------|--------------------------------------------------------------------------------------------|
| GL    |  0.8210   |
| GM    |  0.8100   |
| GN    |  0.8230   |
| GO    |  0.8090   |
| GP    |  0.8270   |
| GQ    |  0.7940   |
| GR    |  0.8180   |
| GS    |  0.7950   |
| GT    |  0.8000   |
| GU    |  0.7540   |
| GV    |  0.7830   |
| GW    |  0.8320   |
| GX    |  0.8320   |
| GZ    |  0.8150   |
| HA    |  0.8240   |
| HB    |  0.7670   |
| HC    |  0.7490   |
| HD    |  0.7610   |
| HE    |  0.8080  |
| HF    |  0.8540 |
| HG    |  0.8540 |
| HH    |  0.8530 |
| HI    |  0.8550 |
| HJ    |  0.8470 |
| HK    |  0.7930 |
| HL    |  0.7670 |
| HM    |  0.8250 |
| HN    |  0.8200 |
| HO    |  0.8460 |
| HP    |  0.8510 |
| HQ    |  0.8580 |
| HR    |  0.8530 |
| HS    |  0.8460 |
| HT    |  0.8560 |
| HU    |  0.8380 |
| HV    |  0.8360 |
| HW    |  0.8130 |
| HX    |  0.8280 |
| HY    |  0.8310 |
| HZ    |  0.7710 |
| IA    |  0.7610 |
| IB    |  0.7860 |

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| Chain | Atom inclusion                                                                             |
|-------|--------------------------------------------------------------------------------------------|
| ID    |  0.8190   |
| IE    |  0.8020   |
| IF    |  0.7720   |
| IG    |  0.7180   |
| IH    |  0.7320   |
| II    |  0.7510   |
| IJ    |  0.8030   |
| IK    |  0.7850   |
| IL    |  0.8210   |
| IM    |  0.8330   |
| IN    |  0.7910   |
| IO    |  0.7830   |
| IP    |  0.7730   |
| IQ    |  0.7930   |
| IR    |  0.8240   |
| IS    |  0.8220   |
| IT    |  0.8330   |
| IU    |  0.8110   |
| IV    |  0.8340   |
| IW    |  0.8200  |
| IX    |  0.8570 |
| IY    |  0.8150 |
| IZ    |  0.8270 |
| JA    |  0.8070 |
| JB    |  0.8300 |
| JC    |  0.8150 |
| JD    |  0.7980 |
| JE    |  0.7320 |
| JF    |  0.7580 |
| JG    |  0.8140 |
| JH    |  0.8180 |
| JI    |  0.8060 |
| JJ    |  0.8050 |
| JK    |  0.8110 |
| JL    |  0.7980 |
| JM    |  0.8230 |
| JN    |  0.8260 |
| JO    |  0.8350 |
| JP    |  0.8100 |
| JQ    |  0.8100 |
| JR    |  0.8090 |
| JS    |  0.8230 |

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| Chain | Atom inclusion                                                                             |
|-------|--------------------------------------------------------------------------------------------|
| JT    |  0.8400   |
| JU    |  0.8250   |
| JV    |  0.8260   |
| JW    |  0.8350   |
| JX    |  0.8280   |
| JY    |  0.8270   |
| JZ    |  0.8150   |
| KA    |  0.8450   |
| KB    |  0.8390   |
| KC    |  0.8210   |
| KD    |  0.8260   |
| KE    |  0.8300   |
| KF    |  0.8360   |
| KG    |  0.8080   |
| KH    |  0.8070   |
| KI    |  0.8230   |
| KJ    |  0.8130   |
| KK    |  0.8070   |
| KL    |  0.7910   |
| KM    |  0.7960  |
| KN    |  0.7810 |
| KO    |  0.8090 |
| KP    |  0.8010 |
| KQ    |  0.8140 |
| KR    |  0.8140 |
| KS    |  0.8330 |
| KT    |  0.8220 |
| KU    |  0.8270 |
| KV    |  0.8120 |
| KW    |  0.8090 |
| KX    |  0.7860 |
| KY    |  0.8040 |
| KZ    |  0.7970 |
| LA    |  0.8040 |
| LB    |  0.8060 |
| LC    |  0.8040 |
| LD    |  0.7870 |
| LE    |  0.8110 |
| LF    |  0.8170 |
| LG    |  0.8130 |
| LH    |  0.8090 |
| LI    |  0.8050 |

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| Chain | Atom inclusion                                                                             |
|-------|--------------------------------------------------------------------------------------------|
| LJ    |  0.7920   |
| LK    |  0.7930   |
| LL    |  0.7830   |
| LM    |  0.7990   |
| LN    |  0.8090   |
| LO    |  0.8730   |
| LP    |  0.8760   |
| LQ    |  0.8670   |
| LR    |  0.8510   |
| LS    |  0.8760   |
| LT    |  0.8560   |
| LU    |  0.8510   |
| LV    |  0.8520   |
| LW    |  0.8720   |
| LX    |  0.8540   |
| LY    |  0.8620   |
| LZ    |  0.8590   |
| MA    |  0.8700   |
| MB    |  0.8740  |
| MC    |  0.8620 |
| MD    |  0.8480 |
| ME    |  0.8690 |
| MF    |  0.8600 |
| MG    |  0.8510 |
| MH    |  0.8530 |
| MI    |  0.8710 |
| MJ    |  0.8750 |
| MK    |  0.8620 |
| ML    |  0.8590 |
| MM    |  0.8750 |
| MN    |  0.8740 |
| MO    |  0.8640 |
| MP    |  0.8490 |
| MQ    |  0.8630 |
| MR    |  0.8640 |
| MT    |  0.8380 |
| MU    |  0.8390 |
| MV    |  0.8360 |
| MW    |  0.8360 |
| MX    |  0.8280 |
| MY    |  0.8070 |
| MZ    |  0.8270 |

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| Chain | Atom inclusion                                                                             |
|-------|--------------------------------------------------------------------------------------------|
| NA    |  0.8430   |
| NB    |  0.8400   |
| NC    |  0.8280   |
| ND    |  0.8290   |
| NE    |  0.8370   |
| NF    |  0.8300   |
| NG    |  0.8450   |
| NH    |  0.8320   |
| NI    |  0.8360   |
| NJ    |  0.8280   |
| NK    |  0.8180   |
| NL    |  0.8260   |
| NM    |  0.8350   |
| NN    |  0.8540   |
| NO    |  0.8030   |
| NP    |  0.8100   |
| NQ    |  0.8370   |
| NR    |  0.8330   |
| NS    |  0.8360  |
| NT    |  0.8350 |
| NU    |  0.8360 |
| NV    |  0.8340 |
| NX    |  0.8200 |
| NY    |  0.8260 |
| NZ    |  0.8150 |
| OA    |  0.8250 |
| OB    |  0.8140 |
| OC    |  0.7970 |
| OD    |  0.8190 |
| OE    |  0.8330 |
| OF    |  0.8370 |
| OG    |  0.8360 |
| OH    |  0.8220 |
| OI    |  0.8440 |
| OJ    |  0.8160 |
| OK    |  0.8330 |
| OL    |  0.8350 |
| OM    |  0.8480 |
| ON    |  0.8350 |
| OO    |  0.8320 |
| OP    |  0.8060 |
| OQ    |  0.8070 |

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| Chain | Atom inclusion                                                                             |
|-------|--------------------------------------------------------------------------------------------|
| OR    |  0.8170   |
| OS    |  0.7760   |
| OT    |  0.7890   |
| OU    |  0.8300   |
| OV    |  0.8240   |
| OW    |  0.8250   |
| OX    |  0.8160   |
| OY    |  0.8260   |
| OZ    |  0.8200   |
| PA    |  0.8000   |
| PC    |  0.6350   |
| PD    |  0.6530   |
| PE    |  0.6310   |
| PF    |  0.6340   |
| PG    |  0.6820   |
| PH    |  0.6700   |
| PI    |  0.7000   |
| PJ    |  0.7400   |
| PK    |  0.7430   |
| PL    |  0.7160  |
| PM    |  0.6630 |
| PN    |  0.6560 |
| PO    |  0.6740 |
| PP    |  0.6900 |
| PQ    |  0.6850 |
| PR    |  0.6960 |
| PS    |  0.6780 |
| PT    |  0.6730 |
| PU    |  0.6780 |
| PV    |  0.6920 |
| PW    |  0.7030 |
| PX    |  0.6290 |
| PY    |  0.6180 |
| PZ    |  0.6240 |
| QA    |  0.6300 |
| QB    |  0.6520 |
| QC    |  0.6270 |
| QD    |  0.6250 |
| QE    |  0.7020 |
| QF    |  0.7090 |
| QG    |  0.6980 |
| QH    |  0.7020 |

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| Chain | Atom inclusion                                                                             |
|-------|--------------------------------------------------------------------------------------------|
| QI    |  0.6700   |
| QJ    |  0.6940   |
| QK    |  0.7020   |
| QL    |  0.7150   |
| QM    |  0.7420   |
| QN    |  0.7480   |
| QO    |  0.7330   |
| QP    |  0.7440   |
| QQ    |  0.6970   |
| QR    |  0.6970   |
| QS    |  0.7320   |
| QT    |  0.7440   |
| QU    |  0.7460   |
| QV    |  0.7440   |
| QW    |  0.7310   |
| QX    |  0.7190   |
| QY    |  0.6780   |
| QZ    |  0.6650   |
| RA    |  0.6900   |
| RB    |  0.6650  |
| RC    |  0.6800 |
| RD    |  0.7090 |
| RE    |  0.7000 |
| RF    |  0.7040 |
| RG    |  0.6720 |
| RH    |  0.6750 |
| RI    |  0.7190 |
| RJ    |  0.7270 |
| RK    |  0.7160 |
| RL    |  0.7210 |
| RM    |  0.6990 |
| RN    |  0.6920 |
| RO    |  0.6700 |
| RP    |  0.7000 |
| RQ    |  0.7290 |
| RR    |  0.7520 |
| RS    |  0.7480 |
| RT    |  0.7610 |
| RU    |  0.7130 |
| RV    |  0.6950 |
| RW    |  0.7400 |
| RX    |  0.7580 |

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| Chain | Atom inclusion                                                                             |
|-------|--------------------------------------------------------------------------------------------|
| RY    |  0.7510   |
| RZ    |  0.7610   |
| SA    |  0.7360   |
| SB    |  0.7370   |
| SC    |  0.6790   |
| SD    |  0.6360   |
| SE    |  0.6790   |
| SF    |  0.6980   |
| SG    |  0.7110   |
| SH    |  0.7260   |
| SI    |  0.7160   |
| SJ    |  0.7210   |
| SK    |  0.6970   |
| SL    |  0.6860   |
| SM    |  0.6840   |
| SN    |  0.7430   |
| SO    |  0.7210   |
| SP    |  0.7440   |
| SQ    |  0.6890  |
| SR    |  0.8180 |
| SS    |  0.7690 |
| ST    |  0.7540 |
| SU    |  0.7350 |
| SV    |  0.7610 |
| SW    |  0.7440 |
| SX    |  0.7610 |
| SY    |  0.7740 |
| SZ    |  0.7730 |
| TA    |  0.7200 |
| TB    |  0.7650 |
| TC    |  0.7420 |
| TD    |  0.7620 |
| TE    |  0.7490 |
| TF    |  0.7490 |
| TG    |  0.6620 |
| TH    |  0.6260 |
| TI    |  0.6900 |
| TJ    |  0.7250 |
| TK    |  0.7100 |
| TL    |  0.7450 |
| TM    |  0.7180 |
| TN    |  0.7390 |

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| Chain | Atom inclusion                                                                             |
|-------|--------------------------------------------------------------------------------------------|
| TO    |  0.6740   |
| TP    |  0.6560   |
| TQ    |  0.7480   |
| TR    |  0.6920   |
| TS    |  0.7240   |
| TT    |  0.7160   |
| TU    |  0.7220   |
| TV    |  0.7140   |
| TW    |  0.7830   |
| TX    |  0.7960   |
| TY    |  0.7530   |
| TZ    |  0.7410   |
| UA    |  0.7570   |
| UB    |  0.7300   |
| UC    |  0.7620   |
| UD    |  0.7680   |
| UE    |  0.7590   |
| UF    |  0.7270   |
| UG    |  0.7630  |
| UH    |  0.7480 |
| UI    |  0.7660 |
| UJ    |  0.7450 |
| UK    |  0.7690 |
| UL    |  0.7660 |
| UM    |  0.7800 |
| UN    |  0.6750 |
| UO    |  0.6990 |
| UP    |  0.6920 |
| UQ    |  0.7190 |
| UR    |  0.7120 |
| US    |  0.7270 |
| UT    |  0.6530 |
| UU    |  0.7450 |
| UW    |  0.7760 |
| UX    |  0.7950 |
| UY    |  0.7630 |
| UZ    |  0.7550 |
| VA    |  0.7990 |
| VB    |  0.8160 |
| VC    |  0.8020 |
| VD    |  0.7630 |
| VE    |  0.7720 |

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| Chain | Atom inclusion                                                                             |
|-------|--------------------------------------------------------------------------------------------|
| VF    |  0.7770   |
| VG    |  0.7660   |
| VH    |  0.7950   |
| VI    |  0.7890   |
| VJ    |  0.7960   |
| VK    |  0.7790   |
| VL    |  0.8110   |
| VM    |  0.7930   |
| VN    |  0.8130   |
| VO    |  0.7880   |
| VP    |  0.8130   |
| VQ    |  0.8250   |
| VR    |  0.8300   |
| VS    |  0.7480   |
| VT    |  0.7730   |
| VU    |  0.7740   |
| VV    |  0.7940   |
| VW    |  0.7630   |
| VX    |  0.7570  |
| VY    |  0.7960 |
| VZ    |  0.8170 |
| WA    |  0.6440 |
| WB    |  0.6550 |
| WC    |  0.6480 |
| WD    |  0.6550 |
| WE    |  0.7550 |
| WF    |  0.7450 |
| WG    |  0.7070 |
| WH    |  0.6790 |
| WI    |  0.6520 |
| WJ    |  0.6680 |
| WK    |  0.6510 |
| WL    |  0.6760 |
| WM    |  0.6940 |
| WN    |  0.7000 |
| WO    |  0.7250 |
| WP    |  0.7610 |
| WQ    |  0.7450 |
| WR    |  0.7390 |
| WS    |  0.7130 |
| WT    |  0.6950 |
| WU    |  0.7720 |

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| Chain | Atom inclusion                                                                             |
|-------|--------------------------------------------------------------------------------------------|
| WV    |  0.7800   |
| WW    |  0.6310   |
| WX    |  0.6410   |
| WY    |  0.6420   |
| WZ    |  0.6580   |
| XA    |  0.6470   |
| XB    |  0.6420   |
| XC    |  0.7280   |
| XD    |  0.7520   |
| XE    |  0.6910   |
| XF    |  0.6920   |
| XG    |  0.6690   |
| XH    |  0.6420   |
| XI    |  0.7100   |
| XJ    |  0.7490   |
| XK    |  0.6720   |
| XL    |  0.6640   |
| XM    |  0.6990   |
| XN    |  0.6960  |
| XO    |  0.7010 |
| XP    |  0.6800 |
| XQ    |  0.6700 |
| XR    |  0.7140 |
| XS    |  0.7400 |
| XT    |  0.7500 |
| XU    |  0.7410 |
| XV    |  0.7330 |
| XW    |  0.6610 |
| XX    |  0.6210 |
| XY    |  0.7620 |
| XZ    |  0.7420 |
| YA    |  0.7230 |
| YB    |  0.7090 |
| YC    |  0.7060 |
| YD    |  0.7030 |
| YE    |  0.6740 |
| YF    |  0.6350 |
| YG    |  0.7130 |
| YH    |  0.7480 |
| YJ    |  0.7670 |
| YK    |  0.7710 |
| YL    |  0.7270 |

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| Chain | Atom inclusion                                                                             |
|-------|--------------------------------------------------------------------------------------------|
| YM    |  0.7100   |
| YN    |  0.7650   |
| YO    |  0.7810   |
| YP    |  0.7520   |
| YQ    |  0.7590   |
| YR    |  0.7730   |
| YS    |  0.7740   |
| YT    |  0.7600   |
| YU    |  0.7510   |
| YV    |  0.7470   |
| YW    |  0.7910   |
| YX    |  0.7930   |
| YY    |  0.8000   |
| YZ    |  0.7880   |
| ZA    |  0.7870   |
| ZB    |  0.7660   |
| ZC    |  0.7460   |
| ZD    |  0.7710   |
| ZE    |  0.7590  |
| ZF    |  0.7750 |
| ZG    |  0.7830 |
| ZH    |  0.7750 |
| ZI    |  0.7720 |
| ZJ    |  0.7260 |
| ZK    |  0.7030 |
| ZL    |  0.7750 |
| ZM    |  0.7870 |
| ZN    |  0.7840 |
| ZO    |  0.7700 |
| ZP    |  0.7320 |
| ZQ    |  0.7420 |
| ZR    |  0.7330 |
| ZS    |  0.7490 |
| ZT    |  0.7620 |
| ZU    |  0.7790 |
| ZV    |  0.7970 |
| ZW    |  0.7970 |
| ZX    |  0.7780 |
| ZY    |  0.7750 |
| ZZ    |  0.7740 |