



## wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 12:09 PM UTC

PDB ID : 7TGH / pdb\_00007tgh  
EMDB ID : EMD-25882  
Title : Cryo-EM structure of respiratory super-complex CI+III2 from Tetrahymena thermophila  
Authors : Zhou, L.; Maldonado, M.; Padavannil, A.; Guo, F.; Letts, J.A.  
Deposited on : 2022-01-07  
Resolution : 2.60 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 : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

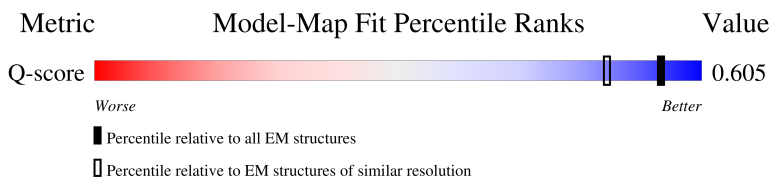
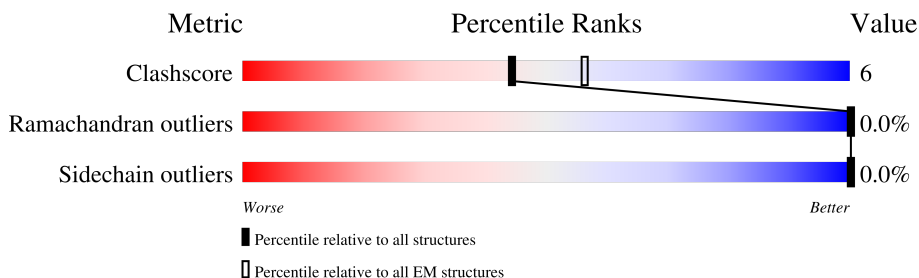
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

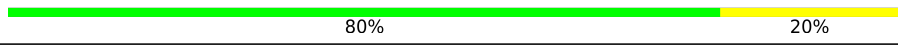
The reported resolution of this entry is 2.60 Å.

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



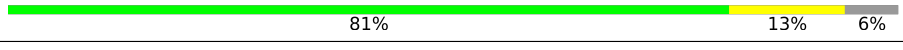
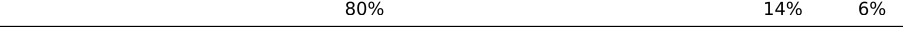
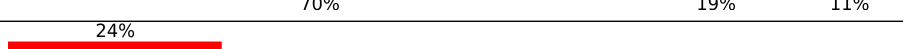
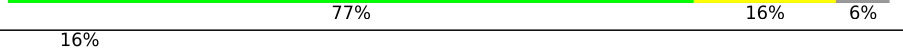
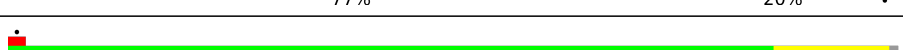
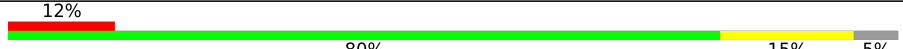
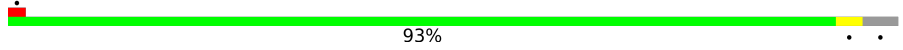
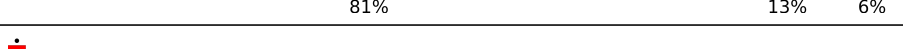
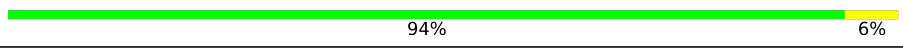
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 8728 ( 2.10 - 3.10 )                                     |

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

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | 1     | 284    |  |
| 2   | 1B    | 59     |  |
| 3   | 2     | 360    |  |
| 4   | 2B    | 178    |  |

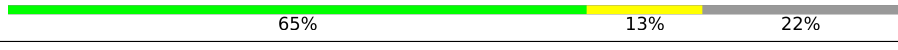
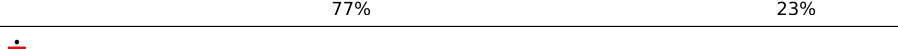
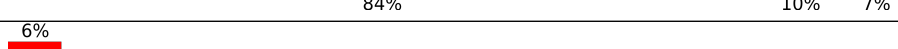
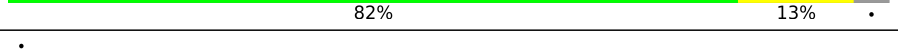
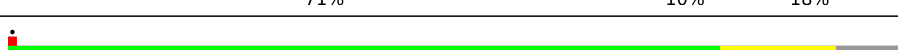
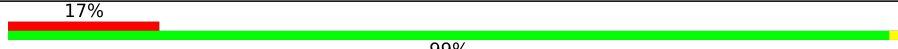
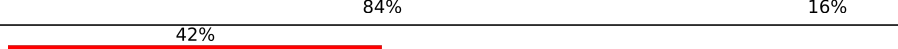
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 5   | 3     | 121    |    |
| 6   | 3A    | 482    |    |
| 6   | 3a    | 482    |    |
| 7   | 3B    | 513    |    |
| 7   | 3b    | 513    |    |
| 8   | 3C    | 426    |    |
| 8   | 3c    | 426    |    |
| 9   | 3D    | 319    |    |
| 9   | 3d    | 319    |    |
| 10  | 3E    | 269    |   |
| 10  | 3e    | 269    |  |
| 11  | 3F    | 90     |  |
| 11  | 3f    | 90     |  |
| 12  | 3G    | 328    |  |
| 12  | 3g    | 328    |  |
| 13  | 3H    | 130    |  |
| 13  | 3h    | 130    |  |
| 14  | 3I    | 119    |  |
| 14  | 3i    | 119    |  |
| 15  | 3J    | 62     |  |
| 15  | 3j    | 62     |  |
| 16  | 3M    | 19     |  |
| 17  | 3l    | 24     |  |
| 18  | 3m    | 17     |  |
| 19  | 4     | 505    |  |

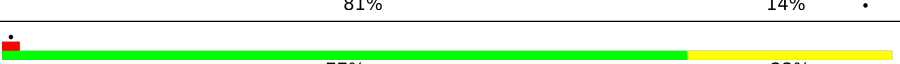
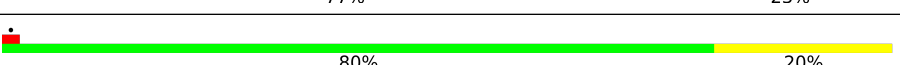
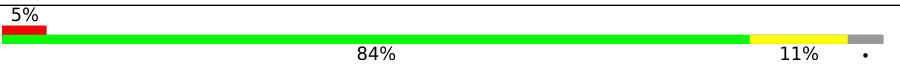
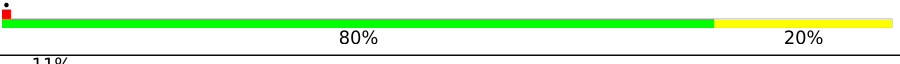
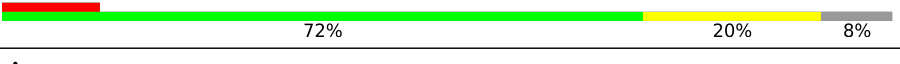
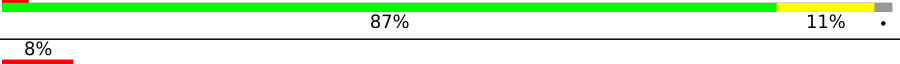
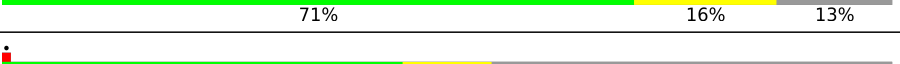
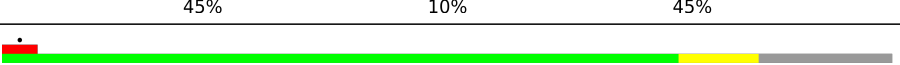
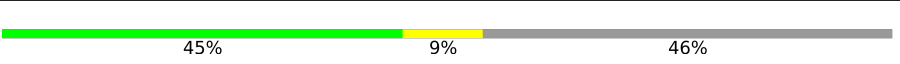
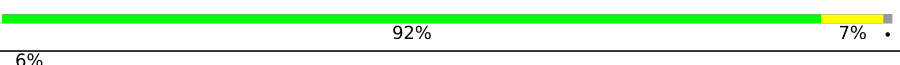
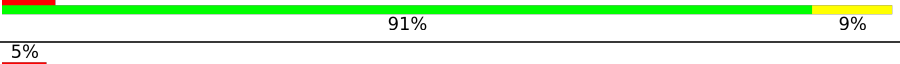
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 20  | 4L    | 116    |    |
| 21  | 5     | 750    |    |
| 22  | 5B    | 100    |    |
| 23  | 6     | 255    |    |
| 24  | A2    | 103    |    |
| 25  | A5    | 206    |    |
| 26  | A6    | 172    |    |
| 27  | A7    | 282    |    |
| 28  | A9    | 362    |    |
| 29  | AB    | 138    |   |
| 30  | AC    | 133    |  |
| 31  | AL    | 194    |  |
| 32  | AM    | 175    |  |
| 33  | B7    | 120    |  |
| 34  | B8    | 207    |  |
| 35  | BL    | 188    |  |
| 36  | C     | 209    |  |
| 37  | C1    | 257    |  |
| 38  | C2    | 233    |  |
| 39  | C3    | 346    |  |
| 40  | TD    | 73     |  |
| 41  | J1    | 317    |  |
| 42  | FX    | 172    |  |
| 43  | T2    | 333    |  |
| 44  | T1    | 516    |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 45  | A1    | 94     |    |
| 46  | X1    | 150    |    |
| 47  | T6    | 144    |    |
| 48  | T5    | 205    |    |
| 49  | R     | 124    |    |
| 50  | S1    | 718    |    |
| 51  | S2    | 442    |    |
| 52  | S3    | 198    |    |
| 53  | S4    | 185    |    |
| 54  | S6    | 132    |    |
| 55  | S7    | 162    |   |
| 56  | S8    | 236    |  |
| 57  | B9    | 189    |  |
| 58  | TX    | 166    |  |
| 59  | A8    | 238    |  |
| 60  | TB    | 113    |  |
| 61  | V1    | 474    |  |
| 62  | V2    | 274    |  |
| 63  | B6    | 129    |  |
| 64  | BM    | 214    |  |
| 65  | C4    | 102    |  |
| 66  | AN    | 231    |  |
| 67  | B4    | 108    |  |
| 68  | T4    | 212    |  |
| 69  | T8    | 135    |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 70  | B2    | 126    |                  |
| 71  | T3    | 311    |                  |
| 72  | P1    | 251    |                  |
| 73  | B3    | 83     |                  |
| 74  | TA    | 102    |                  |
| 75  | S5    | 94     |                  |
| 76  | TC    | 93     |                  |
| 77  | P2    | 189    |                  |
| 78  | A3    | 135    |                  |
| 79  | T9    | 135    |                  |
| 80  | TE    | 71     |                  |
| 81  | T7    | 143    |                  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 93  | SF4  | S1    | 802 | -         | -        | X       | -                |
| 93  | SF4  | S8    | 302 | -         | -        | X       | -                |

## 2 Entry composition

There are 94 unique types of molecules in this entry. The entry contains 153366 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 NADH-ubiquinone oxidoreductase chain 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | 1     | 284      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2313  | 1586 | 335 | 379 | 13 |         |       |

- Molecule 2 is a protein called NADH dehydrogenase subunit 1.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 2   | 1B    | 59       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 516   | 362 | 78 | 73 | 3 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| 1B    | 49      | VAL      | LEU    | conflict | UNP Q09FB0 |
| 1B    | 56      | THR      | SER    | conflict | UNP Q09FB0 |

- Molecule 3 is a protein called Ymf65.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | 2     | 359      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3065  | 2129 | 435 | 494 | 7 |         |       |

- Molecule 4 is a protein called NADH dehydrogenase subunit 2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4   | 2B    | 178      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1483  | 1015 | 215 | 248 | 5 |         |       |

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase chain 3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | 3     | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1017  | 705 | 142 | 166 | 4 |         |       |

- Molecule 6 is a protein called M16 family peptidase, putative.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | 3A    | 453      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3511  | 2210 | 598 | 697 | 6 |         |       |
| 6   | 3a    | 451      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3495  | 2199 | 595 | 695 | 6 |         |       |

- Molecule 7 is a protein called Peptidase M16 inactive domain protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7   | 3B    | 479      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3826  | 2426 | 667 | 728 | 5 |         |       |
| 7   | 3b    | 478      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3815  | 2420 | 663 | 727 | 5 |         |       |

- Molecule 8 is a protein called Apocytochrome b.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 8   | 3C    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3590  | 2417 | 541 | 610 | 22 |         |       |
| 8   | 3c    | 426      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3589  | 2417 | 541 | 609 | 22 |         |       |

- Molecule 9 is a protein called Cytochrome protein c1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9   | 3D    | 295      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2488  | 1627 | 418 | 430 | 13 |         |       |
| 9   | 3d    | 285      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2403  | 1569 | 405 | 416 | 13 |         |       |

- Molecule 10 is a protein called Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10  | 3E    | 230      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1846  | 1178 | 325 | 334 | 9 |         |       |
| 10  | 3e    | 104      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 882   | 567  | 162 | 152 | 1 |         |       |

- Molecule 11 is a protein called Ubiquinol-cytochrome C reductase hinge protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | 3F    | 89       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 703   | 439 | 125 | 130 | 9 |         |       |
| 11  | 3f    | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 597   | 374 | 105 | 109 | 9 |         |       |

- Molecule 12 is a protein called UQCRB.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 12  | 3G    | 307      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2595  | 1676 | 450 | 463 | 6 |         |       |
| 12  | 3g    | 317      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2682  | 1738 | 464 | 474 | 6 |         |       |

- Molecule 13 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | 3H    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1098  | 708 | 195 | 187 | 8 |         |       |
| 13  | 3h    | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1046  | 669 | 190 | 179 | 8 |         |       |

- Molecule 14 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | 3I    | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 971   | 651 | 161 | 158 | 1 |         |       |
| 14  | 3i    | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 948   | 638 | 157 | 152 | 1 |         |       |

- Molecule 15 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 15  | 3J    | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 501   | 341 | 79 | 79 | 2 |         |       |
| 15  | 3j    | 51       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 443   | 306 | 65 | 70 | 2 |         |       |

- Molecule 16 is a protein called UNK1.

| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 16  | 3M    | 19       | Total | C  | N  | O  | S | 0       | 0     |
|     |       |          | 150   | 94 | 27 | 27 | 2 |         |       |

- Molecule 17 is a protein called UNK2.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 17  | 3l    | 24       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 124   | 74 | 24 | 26 |         |       |

- Molecule 18 is a protein called UNK3.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 18  | 3m    | 17       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 121   | 78 | 25 | 18 |         |       |

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 19  | 4     | 505      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4170  | 2859 | 601 | 692 | 18 |         |       |

- Molecule 20 is a protein called Ymf58.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | 4L    | 116      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 957   | 648 | 142 | 163 | 4 |         |       |

- Molecule 21 is a protein called NADH dehydrogenase subunit 5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 21  | 5     | 587      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4844  | 3313 | 696 | 819 | 16 |         |       |

- Molecule 22 is a protein called Ymf57.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | 5B    | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 888   | 620 | 128 | 137 | 3 |         |       |

- Molecule 23 is a protein called Ymf62.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 23  | 6     | 244      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2076  | 1419 | 295 | 358 | 4 |         |       |

- Molecule 24 is a protein called Ribosomal protein L51/S25/CI-B8 domain protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | A2    | 92       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 765   | 486 | 136 | 141 | 2 |         |       |

- Molecule 25 is a protein called ETC complex I subunit motif protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | A5    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1307  | 838 | 219 | 244 | 6 |         |       |

- Molecule 26 is a protein called NADH dehydrogenase, putative.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | A6    | 172      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1421  | 903 | 253 | 257 | 8 |         |       |

- Molecule 27 is a protein called NDUA7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 27  | A7    | 281      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2339  | 1473 | 412 | 452 | 2 |         |       |

- Molecule 28 is a protein called NAD-dependent epimerase/dehydratase family protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 28  | A9    | 338      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2718  | 1737 | 475 | 494 | 12 |         |       |

- Molecule 29 is a protein called Acyl carrier protein.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 29  | AB    | 112      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 926   | 586 | 158 | 182 |         |       |

- Molecule 30 is a protein called Acyl carrier protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | AC    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 806   | 513 | 134 | 158 | 1 |         |       |

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 31  | AL    | 193      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1612  | 1019 | 303 | 285 | 5 |         |       |

- Molecule 32 is a protein called NDUA13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | AM    | 160      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1349  | 858 | 256 | 227 | 8 |         |       |

- Molecule 33 is a protein called NDUB7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | B7    | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 937   | 593 | 162 | 176 | 6 |         |       |

- Molecule 34 is a protein called NDUB8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | B8    | 169      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1408  | 904 | 238 | 260 | 6 |         |       |

- Molecule 35 is a protein called NDUB10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | BL    | 175      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1461  | 925 | 264 | 268 | 4 |         |       |

- Molecule 36 is a protein called UNK4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | C     | 209      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1045  | 627 | 209 | 209 |   |         |       |

- Molecule 37 is a protein called Gamma-carbonic anhydrase.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 37  | C1    | 229      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1769  | 1110 | 304 | 350 | 5 |         |       |

- Molecule 38 is a protein called Gamma-carbonic anhydrase.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 38  | C2    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1624  | 1020 | 294 | 303 | 7 |         |       |

- Molecule 39 is a protein called Transcription factor apfi protein, putative.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 39  | C3    | 346      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2804  | 1766 | 481 | 549 | 8 |         |       |

- Molecule 40 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | TD    | 71       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 608   | 399 | 108 | 101 |   |         |       |

- Molecule 41 is a protein called DnaJ domain protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 41  | J1    | 262      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2146  | 1361 | 396 | 386 | 3 |         |       |

- Molecule 42 is a protein called 2 iron, 2 sulfur cluster-binding protein.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 42  | FX    | 146      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1162  | 722 | 207 | 223 | 10 |         |       |

- Molecule 43 is a protein called Acyl-CoA synthetase (AMP-forming)/AMP-acid ligase II.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 43  | T2    | 271      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2117  | 1347 | 362 | 407 | 1 |         |       |

- Molecule 44 is a protein called Lipid-A-disaccharide synthase.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 44  | T1    | 481      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3884  | 2492 | 662 | 717 | 13 |         |       |

- Molecule 45 is a protein called NDUA1.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 45  | A1    | 92       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 799   | 526 | 138 | 135 |         |       |

- Molecule 46 is a protein called NADH-ubiquinone oxidoreductase complex I, 21 kDa subunit.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 46  | X1    | 149      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1227  | 800 | 213 | 214 |         |       |

- Molecule 47 is a protein called NDUTT6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | T6    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 903   | 562 | 161 | 174 | 6 |         |       |

- Molecule 48 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | T5    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1088  | 699 | 193 | 194 | 2 |         |       |

- Molecule 49 is a protein called UNK5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | R     | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 943   | 613 | 160 | 167 | 3 |         |       |

- Molecule 50 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 50  | S1    | 687      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5394  | 3404 | 933 | 1029 | 28 |         |       |

- Molecule 51 is a protein called NADH dehydrogenase subunit 7.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 51  | S2    | 442      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3599  | 2291 | 624 | 660 | 24 |         |       |

- Molecule 52 is a protein called NADH dehydrogenase subunit 9.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 52  | S3    | 198      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1681  | 1096 | 267 | 312 | 6 |         |       |

- Molecule 53 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53  | S4    | 177      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1463  | 928 | 257 | 269 | 9 |         |       |

- Molecule 54 is a protein called Zinc-finger protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 54  | S6    | 90       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 722   | 456 | 128 | 134 | 4 |         |       |

- Molecule 55 is a protein called NADH dehydrogenase subunit 10.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 55  | S7    | 162      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1286  | 827 | 221 | 227 | 11 |         |       |

- Molecule 56 is a protein called NADH-ubiquinone oxidoreductase 1, chain, putative.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 56  | S8    | 218      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1812  | 1155 | 299 | 347 | 11 |         |       |

- Molecule 57 is a protein called NDUB9.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 57  | B9    | 186      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1579  | 1021 | 252 | 302 | 4 |         |       |

- Molecule 58 is a protein called Thioredoxin.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 58  | TX    | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1206  | 767 | 205 | 227 | 7 |         |       |

- Molecule 59 is a protein called NDUA8.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 59  | A8    | 132      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1075  | 676 | 180 | 208 | 11 |         |       |

- Molecule 60 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 60  | TB    | 96       | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 801   | 515 | 139 | 147 |  |         |       |

- Molecule 61 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 61  | V1    | 442      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3410  | 2146 | 600 | 640 | 24 |         |       |

- Molecule 62 is a protein called NADH-ubiquinone oxidoreductase 24 kDa subunit.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 62  | V2    | 231      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1858  | 1173 | 318 | 357 | 10 |         |       |

- Molecule 63 is a protein called NDUB6.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 63  | B6    | 70       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 596   | 400 | 98 | 94 | 4 |         |       |

- Molecule 64 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 64  | BM    | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1163  | 737 | 195 | 226 | 5 |         |       |

- Molecule 65 is a protein called NDUC2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 65  | C4    | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 842   | 548 | 138 | 149 | 7 |         |       |

- Molecule 66 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 66  | AN    | 231      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1879  | 1219 | 317 | 336 | 7 |         |       |

- Molecule 67 is a protein called NDUB4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 67  | B4    | 108      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 898   | 601 | 138 | 157 | 2 |         |       |

- Molecule 68 is a protein called NDUTT4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 68  | T4    | 170      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1408  | 918 | 242 | 245 | 3 |         |       |

- Molecule 69 is a protein called NDUTT8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 69  | T8    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1064  | 691 | 189 | 184 |   |         |       |

- Molecule 70 is a protein called NDUB2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 70  | B2    | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 955   | 615 | 165 | 172 | 3 |         |       |

- Molecule 71 is a protein called NDUTT3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 71  | T3    | 305      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2442  | 1555 | 426 | 455 | 6 |         |       |

- Molecule 72 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 72  | P1    | 228      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1896  | 1235 | 320 | 336 | 5 |         |       |

- Molecule 73 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 73  | B3    | 68       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 594   | 392 | 104 | 97 | 1 |         |       |

- Molecule 74 is a protein called NDUTT10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 74  | TA    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 854   | 553 | 141 | 155 | 5 |         |       |

- Molecule 75 is a protein called GRAM domain protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 75  | S5    | 85       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 693   | 440 | 118 | 129 | 6 |         |       |

- Molecule 76 is a protein called NDUTT12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 76  | TC    | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 781   | 491 | 145 | 144 | 1 |         |       |

- Molecule 77 is a protein called NDUPH2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 77  | P2    | 167      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1414  | 926 | 225 | 258 | 5 |         |       |

- Molecule 78 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 78  | A3    | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1065  | 691 | 193 | 178 | 3 |         |       |

- Molecule 79 is a protein called NDUTT9.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 79  | T9    | 132      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1066  | 670 | 185 | 201 | 10 |         |       |

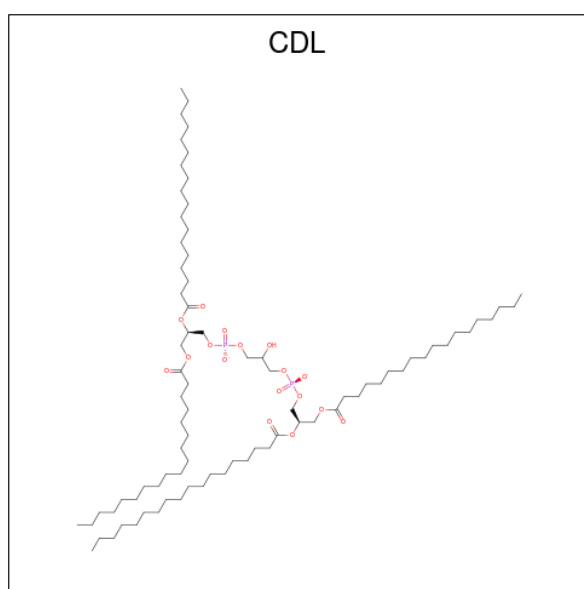
- Molecule 80 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 80  | TE    | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 413   | 277 | 63 | 71 | 2 |         |       |

- Molecule 81 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 81  | T7    | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1187  | 770 | 202 | 209 | 6 |         |       |

- Molecule 82 is CARDIOLIPIN (CCD ID: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 82  | 1     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 50    | 31 | 17 | 2 |         |
| 82  | 2B    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 53    | 34 | 17 | 2 |         |
| 82  | 3     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 44    | 25 | 17 | 2 |         |
| 82  | 3B    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 78    | 59 | 17 | 2 |         |
| 82  | 3C    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 65    | 46 | 17 | 2 |         |
| 82  | 3G    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 66    | 47 | 17 | 2 |         |
| 82  | 3H    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 62    | 43 | 17 | 2 |         |

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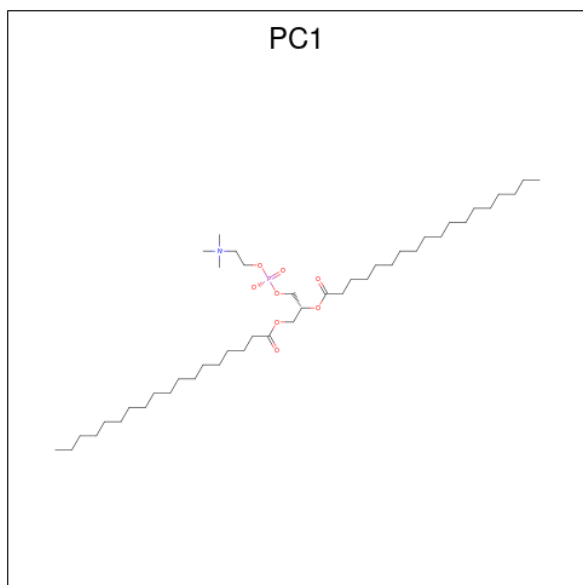
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 82  | 3H    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 66    | 47 | 17 | 2 |         |
| 82  | 3I    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 71    | 52 | 17 | 2 |         |
| 82  | 3I    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 37    | 18 | 17 | 2 |         |
| 82  | 3b    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 68    | 49 | 17 | 2 |         |
| 82  | 3c    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 64    | 45 | 17 | 2 |         |
| 82  | 3c    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 56    | 37 | 17 | 2 |         |
| 82  | 3i    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 71    | 52 | 17 | 2 |         |
| 82  | 5     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 90    | 71 | 17 | 2 |         |
| 82  | 5     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 96    | 77 | 17 | 2 |         |
| 82  | AL    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 53    | 34 | 17 | 2 |         |
| 82  | AM    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 62    | 43 | 17 | 2 |         |
| 82  | B8    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 45    | 26 | 17 | 2 |         |
| 82  | TD    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 66    | 47 | 17 | 2 |         |
| 82  | T1    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 55    | 36 | 17 | 2 |         |
| 82  | A1    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 53    | 34 | 17 | 2 |         |
| 82  | R     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 84    | 65 | 17 | 2 |         |
| 82  | BM    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 86    | 67 | 17 | 2 |         |
| 82  | C4    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 98    | 79 | 17 | 2 |         |
| 82  | AN    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 53    | 34 | 17 | 2 |         |
| 82  | B4    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 40    | 21 | 17 | 2 |         |
| 82  | P2    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 82    | 63 | 17 | 2 |         |

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| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 82  | T7    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 48    | 29 | 17 | 2 |         |

- Molecule 83 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula:  $C_{44}H_{88}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 83  | 1     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 36    | 26 | 1 | 8 | 1 |         |
| 83  | 3     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 31    | 21 | 1 | 8 | 1 |         |
| 83  | 3C    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 46    | 36 | 1 | 8 | 1 |         |
| 83  | 3C    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 44    | 34 | 1 | 8 | 1 |         |
| 83  | 3C    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 29    | 19 | 1 | 8 | 1 |         |
| 83  | 3E    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 54    | 44 | 1 | 8 | 1 |         |
| 83  | 3E    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 24    | 14 | 1 | 8 | 1 |         |
| 83  | 3F    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 22    | 12 | 1 | 8 | 1 |         |
| 83  | 3I    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 32    | 22 | 1 | 8 | 1 |         |
| 83  | 3I    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 46    | 36 | 1 | 8 | 1 |         |

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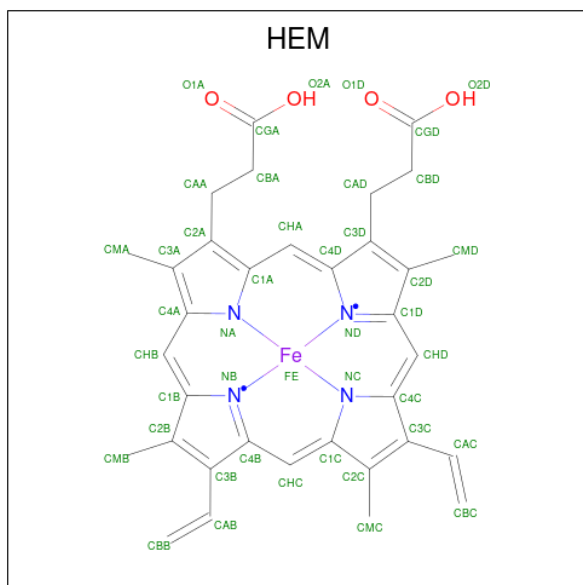
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 83  | 3J    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 37    | 27 | 1 | 8 | 1 |         |
| 83  | 3b    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 30    | 20 | 1 | 8 | 1 |         |
| 83  | 3c    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 31    | 21 | 1 | 8 | 1 |         |
| 83  | 3c    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 38    | 28 | 1 | 8 | 1 |         |
| 83  | 3e    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 50    | 40 | 1 | 8 | 1 |         |
| 83  | 3g    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 33    | 23 | 1 | 8 | 1 |         |
| 83  | 3j    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 36    | 26 | 1 | 8 | 1 |         |
| 83  | 5     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 54    | 44 | 1 | 8 | 1 |         |
| 83  | 5     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 39    | 29 | 1 | 8 | 1 |         |
| 83  | 5     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 54    | 44 | 1 | 8 | 1 |         |
| 83  | 6     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 39    | 29 | 1 | 8 | 1 |         |
| 83  | 6     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 54    | 44 | 1 | 8 | 1 |         |
| 83  | AM    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 30    | 20 | 1 | 8 | 1 |         |
| 83  | J1    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 40    | 30 | 1 | 8 | 1 |         |
| 83  | T1    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 26    | 16 | 1 | 8 | 1 |         |
| 83  | X1    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 49    | 39 | 1 | 8 | 1 |         |
| 83  | B6    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 83  | C4    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 32    | 22 | 1 | 8 | 1 |         |
| 83  | AN    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 36    | 26 | 1 | 8 | 1 |         |
| 83  | B2    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 48    | 38 | 1 | 8 | 1 |         |
| 83  | P1    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 40    | 30 | 1 | 8 | 1 |         |

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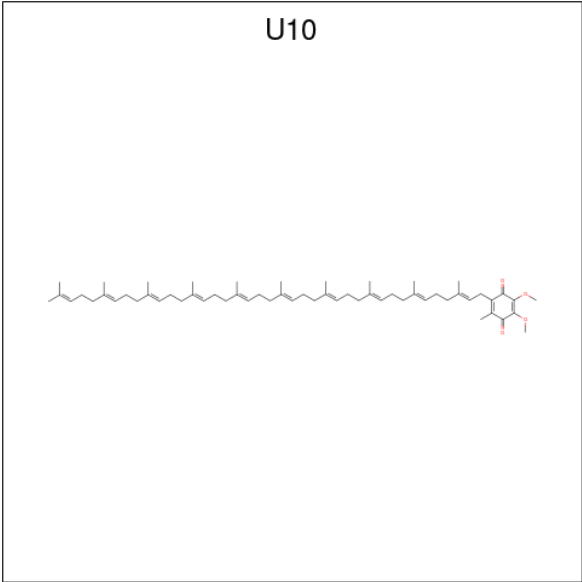
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 83  | TC    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 42    | 32 | 1 | 8 | 1 |         |

- Molecule 84 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).



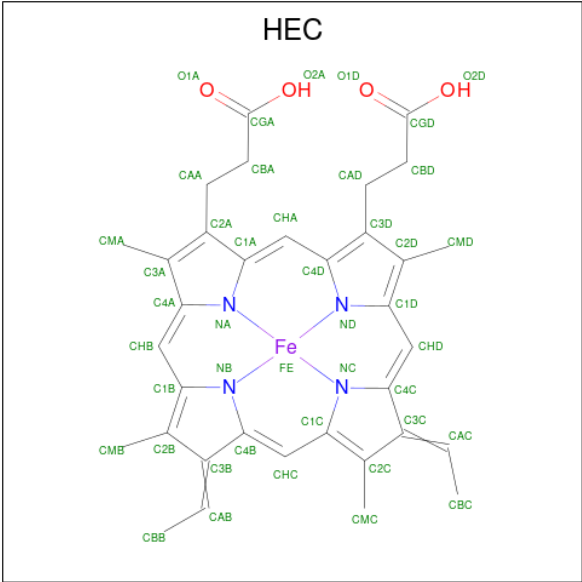
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 84  | 3C    | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 84  | 3C    | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 84  | 3c    | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 84  | 3c    | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |

- Molecule 85 is UBIQUINONE-10 (CCD ID: U10) (formula:  $C_{59}H_{90}O_4$ ) (labeled as "Ligand of Interest" by depositor).



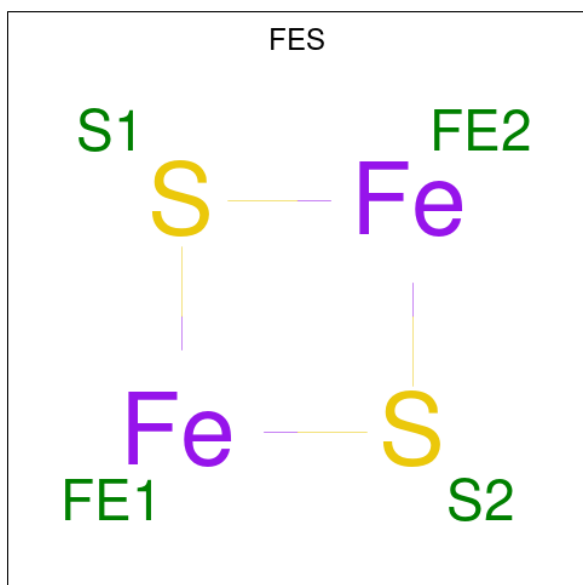
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 85  | 3C    | 1        | Total | C  |   | 0       |
|     |       |          | 26    | 26 |   |         |
| 85  | 3H    | 1        | Total | C  | O | 0       |
|     |       |          | 29    | 25 | 4 |         |
| 85  | 5B    | 1        | Total | C  | O | 0       |
|     |       |          | 63    | 59 | 4 |         |

- Molecule 86 is HEME C (CCD ID: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).



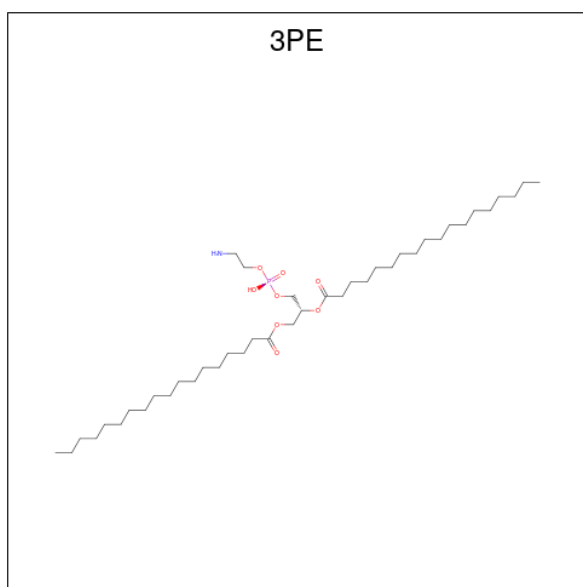
| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 86  | 3D    | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |
| 86  | 3d    | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |

- Molecule 87 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 87  | 3E    | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |
| 87  | FX    | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |
| 87  | S1    | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |
| 87  | V2    | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |

- Molecule 88 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula:  $\text{C}_{41}\text{H}_{82}\text{NO}_8\text{P}$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 88  | 3E    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 34    | 24 | 1 | 8 | 1 |         |
| 88  | 3d    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 47    | 37 | 1 | 8 | 1 |         |
| 88  | 4     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 47    | 37 | 1 | 8 | 1 |         |
| 88  | 4     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 36    | 26 | 1 | 8 | 1 |         |
| 88  | 5     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 37    | 27 | 1 | 8 | 1 |         |
| 88  | 5     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 35    | 25 | 1 | 8 | 1 |         |
| 88  | 5B    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 24    | 14 | 1 | 8 | 1 |         |
| 88  | B8    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 36    | 26 | 1 | 8 | 1 |         |
| 88  | S8    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 41    | 31 | 1 | 8 | 1 |         |
| 88  | C4    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 88  | AN    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 88  | AN    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 35    | 25 | 1 | 8 | 1 |         |
| 88  | T4    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 25    | 15 | 1 | 8 | 1 |         |
| 88  | T8    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 39    | 29 | 1 | 8 | 1 |         |

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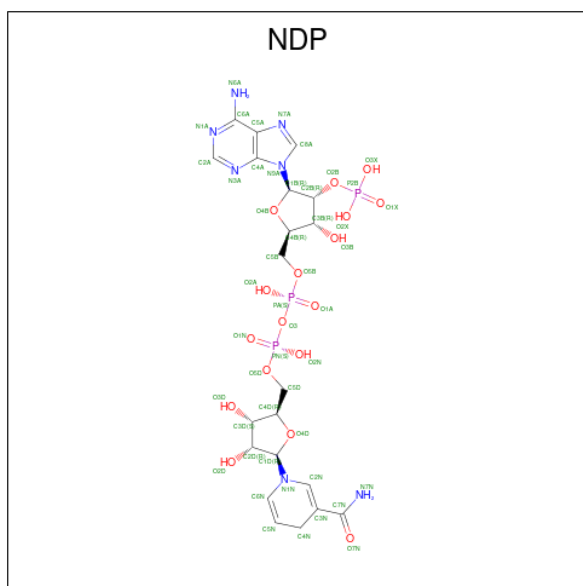
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| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 88  | P1    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 47    | 37 | 1 | 8 | 1 |         |
| 88  | TA    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 26    | 16 | 1 | 8 | 1 |         |
| 88  | A3    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |

- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 89  | 3F    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 89  | A9    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 89  | S6    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

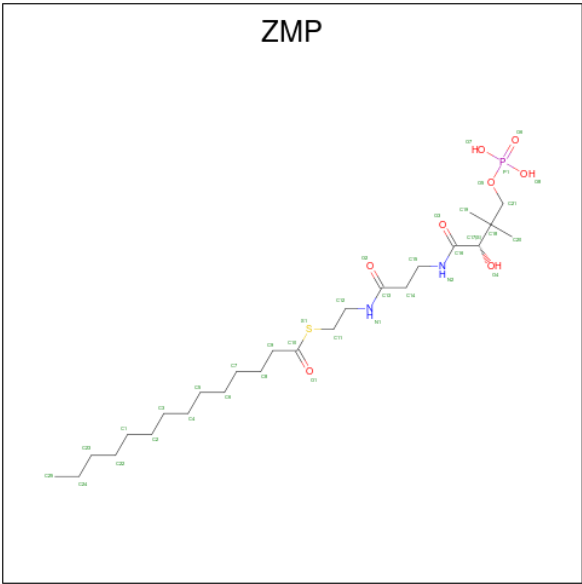
- Molecule 90 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 90  | A9    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 48    | 21 | 7 | 17 | 3 |         |

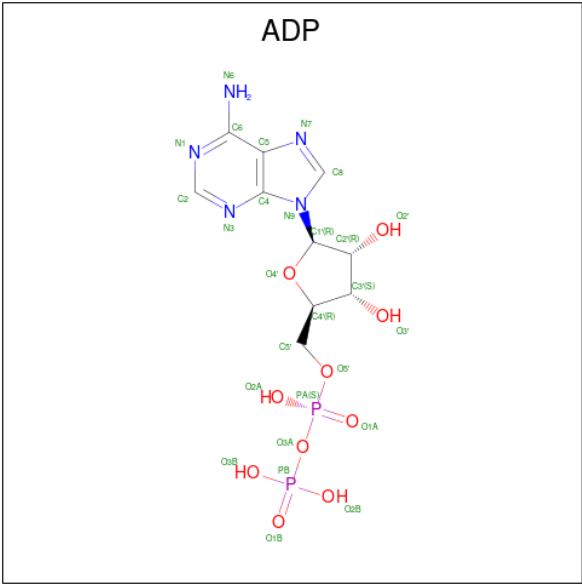
- Molecule 91 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alan

yl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C<sub>25</sub>H<sub>49</sub>N<sub>2</sub>O<sub>8</sub>PS) (labeled as "Ligand of Interest" by depositor).



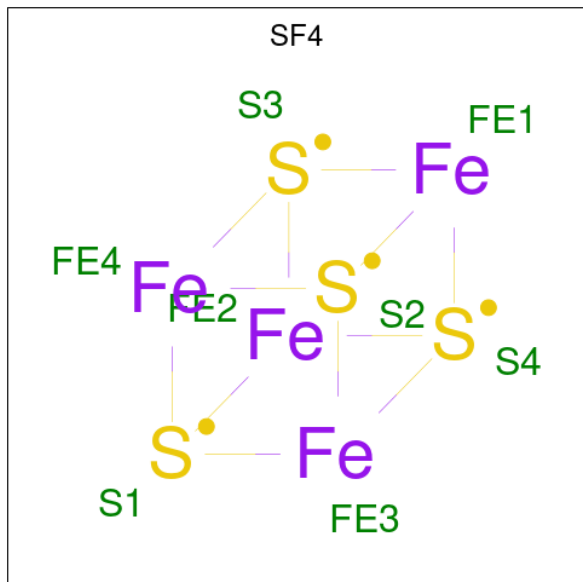
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |   |
|-----|-------|----------|-------|----|---|---|---|---------|---|
| 91  | AB    | 1        | Total | C  | N | O | P | S       | 0 |
|     |       |          | 34    | 23 | 2 | 7 | 1 | 1       |   |

- Molecule 92 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



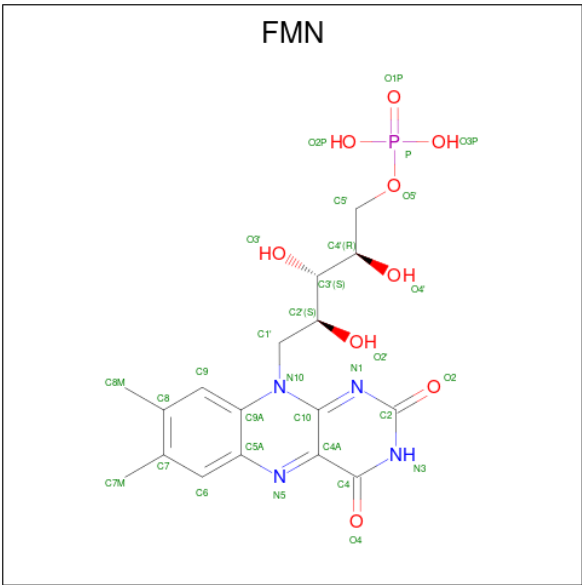
| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
|     |       |          | Total | C  | N | O  | P |         |
| 92  | B8    | 1        | 27    | 10 | 5 | 10 | 2 | 0       |

- Molecule 93 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 93  | S1    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 93  | S1    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 93  | S7    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 93  | S8    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 93  | S8    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 93  | V1    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

- Molecule 94 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula:  $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$ ) (labeled as "Ligand of Interest" by depositor).

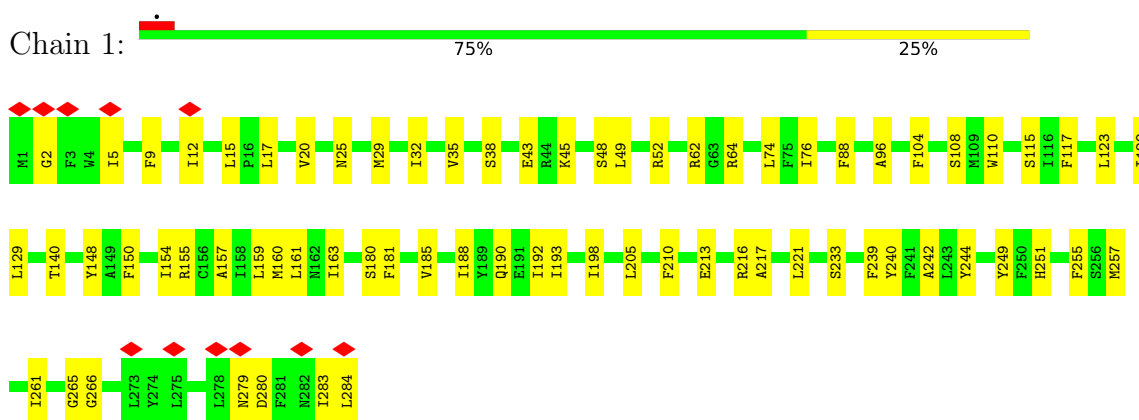


| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 94  | V1    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 31    | 17 | 4 | 9 | 1 |         |

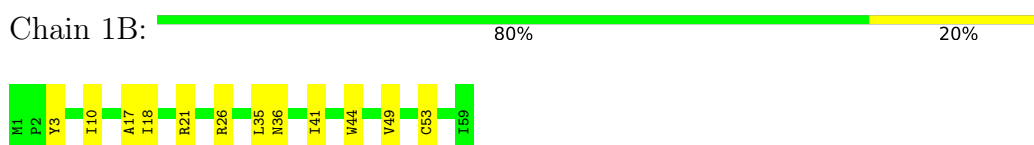
### 3 Residue-property plots

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

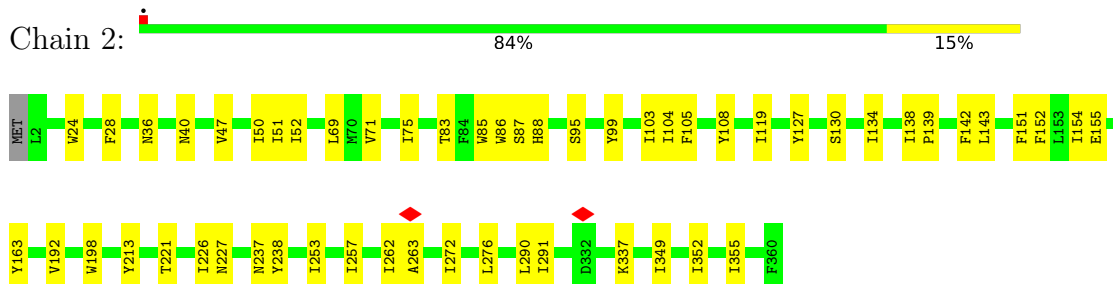
- Molecule 1: NADH-ubiquinone oxidoreductase chain 1



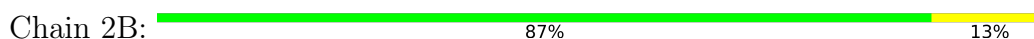
- Molecule 2: NADH dehydrogenase subunit 1

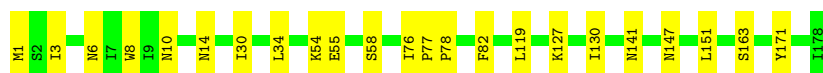


- Molecule 3: Ymf65

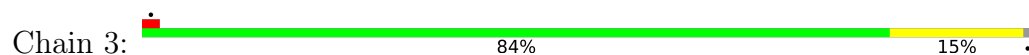


- Molecule 4: NADH dehydrogenase subunit 2

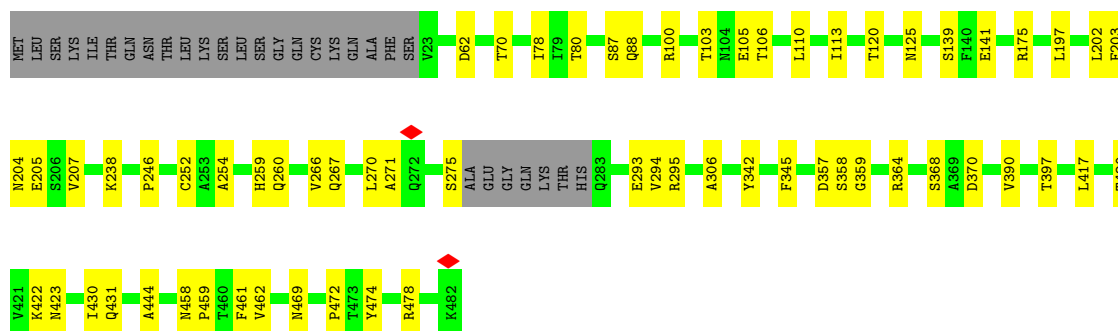
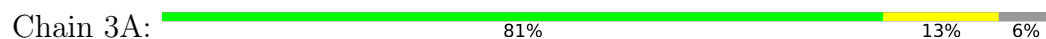




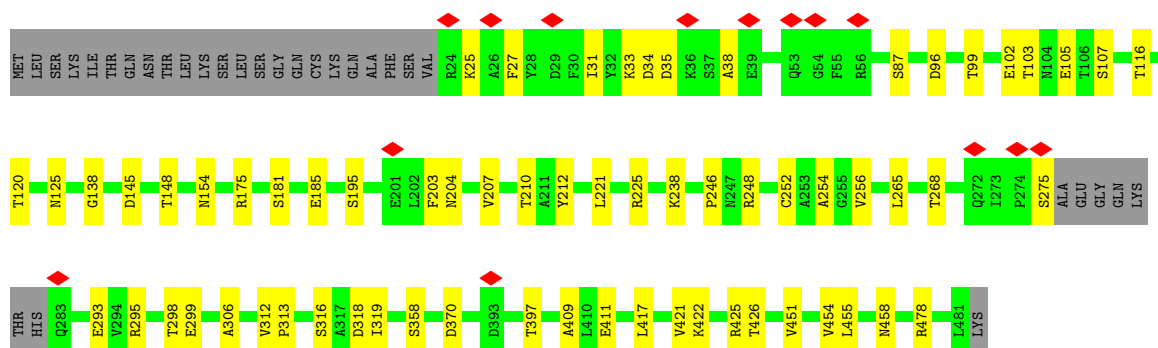
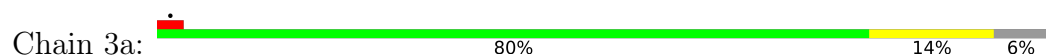
- Molecule 5: NADH-ubiquinone oxidoreductase chain 3



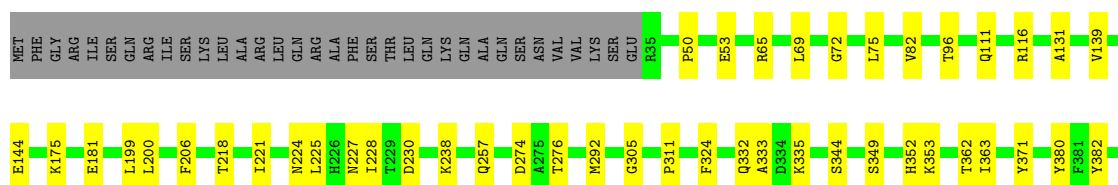
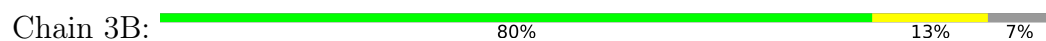
- Molecule 6: M16 family peptidase, putative



- Molecule 6: M16 family peptidase, putative



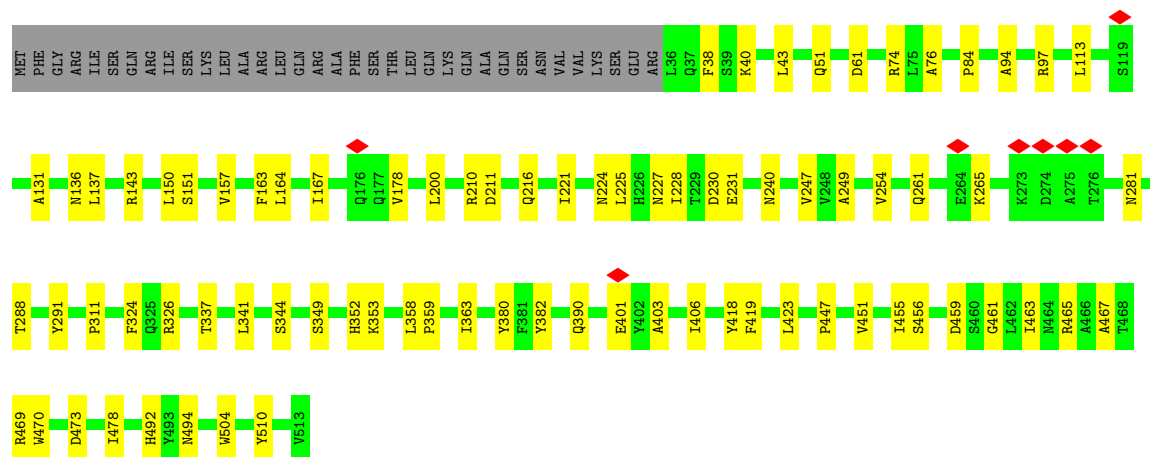
- Molecule 7: Peptidase M16 inactive domain protein





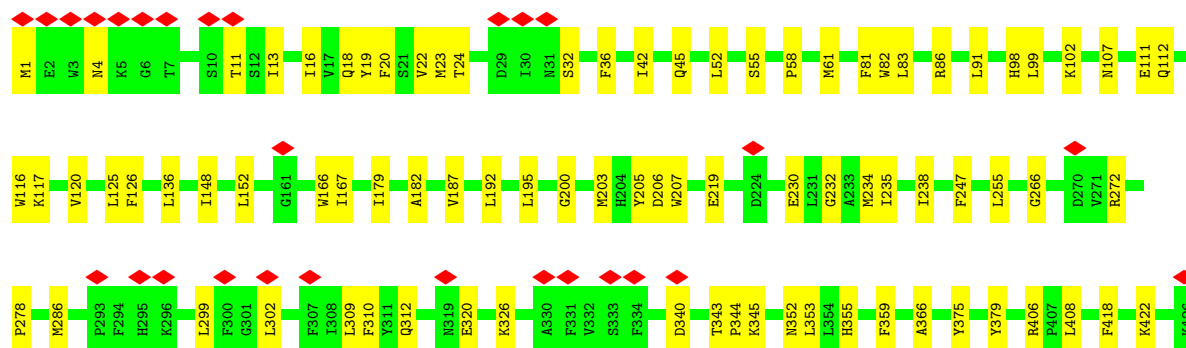
• Molecule 7: Peptidase M16 inactive domain protein

Chain 3b: 78% 16% 7%



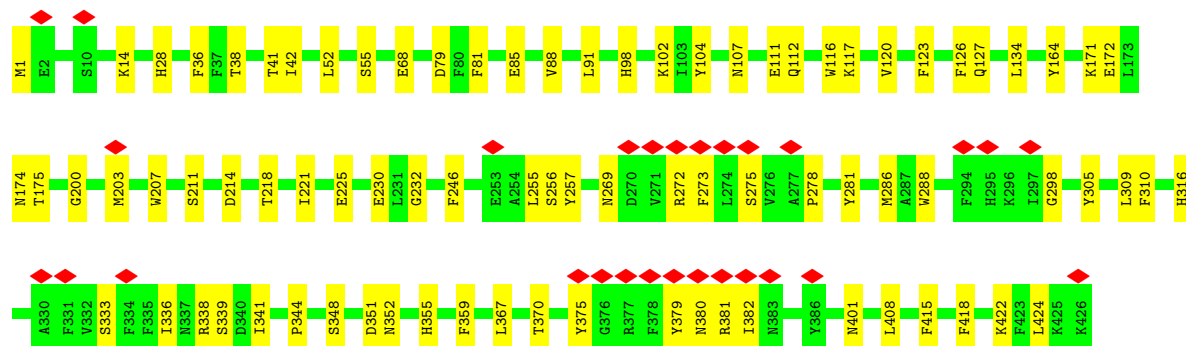
• Molecule 8: Apocytochrome b

Chain 3C: 7% 80% 20%



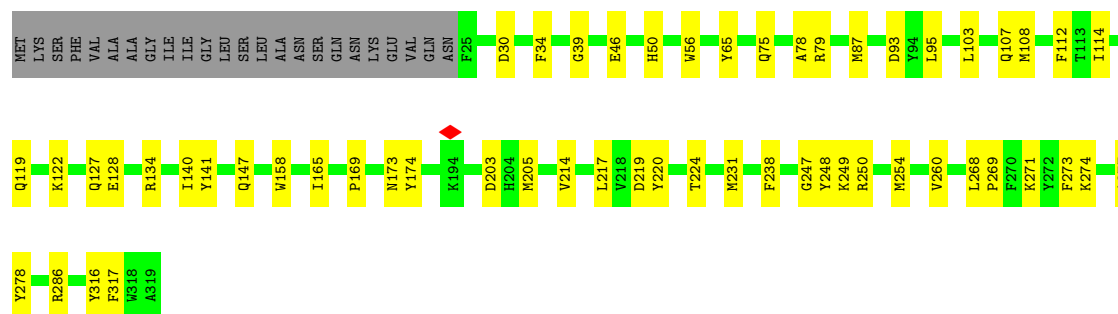
• Molecule 8: Apocytochrome b

Chain 3c: 7% 80% 20%



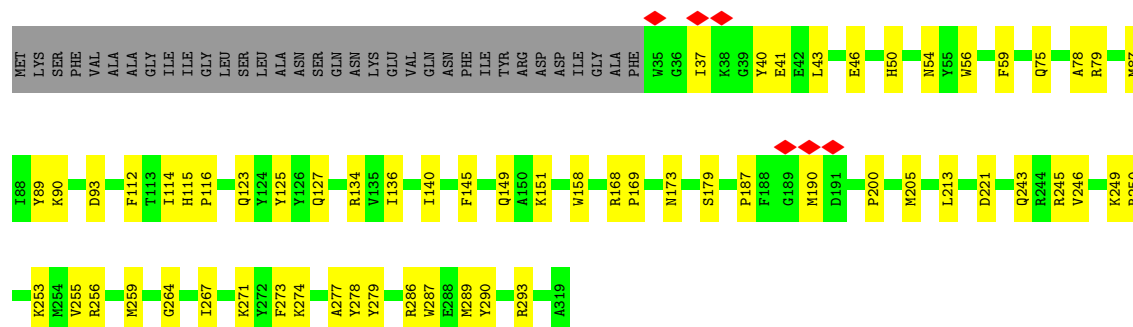
- Molecule 9: Cytochrome protein c1

Chain 3D: 



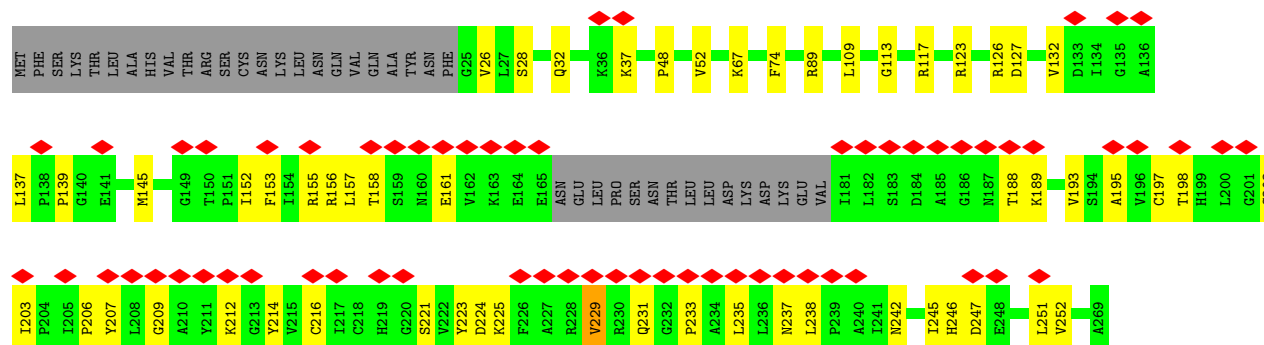
- Molecule 9: Cytochrome protein c1

Chain 3d: 



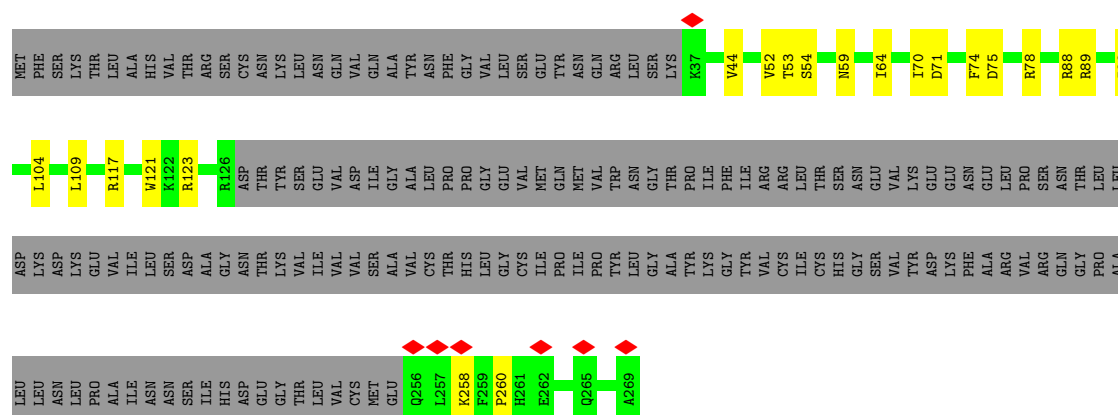
- Molecule 10: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit

Chain 3E: 

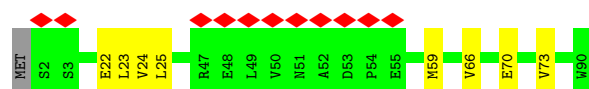
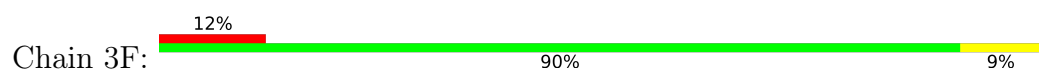


- Molecule 10: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit

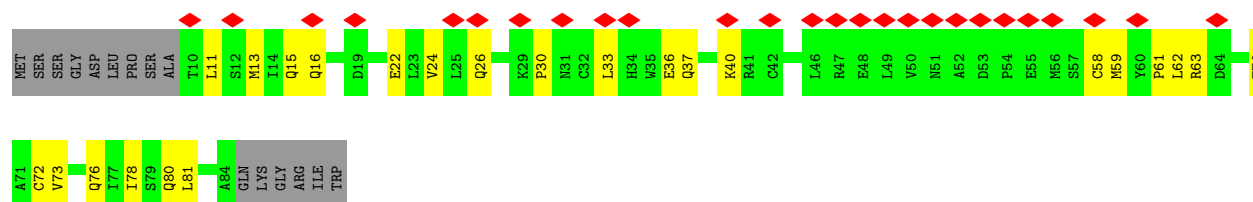
Chain 3e: 



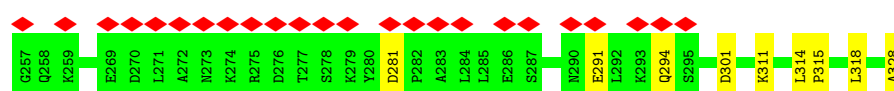
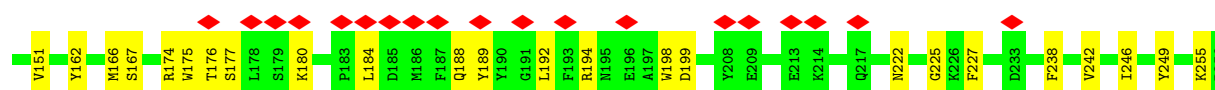
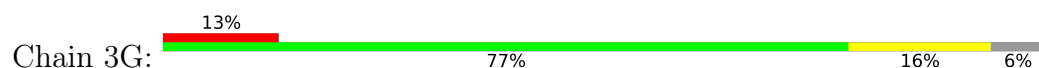
• Molecule 11: Ubiquinol-cytochrome C reductase hinge protein



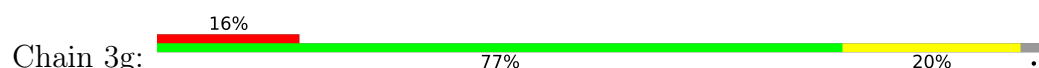
• Molecule 11: Ubiquinol-cytochrome C reductase hinge protein

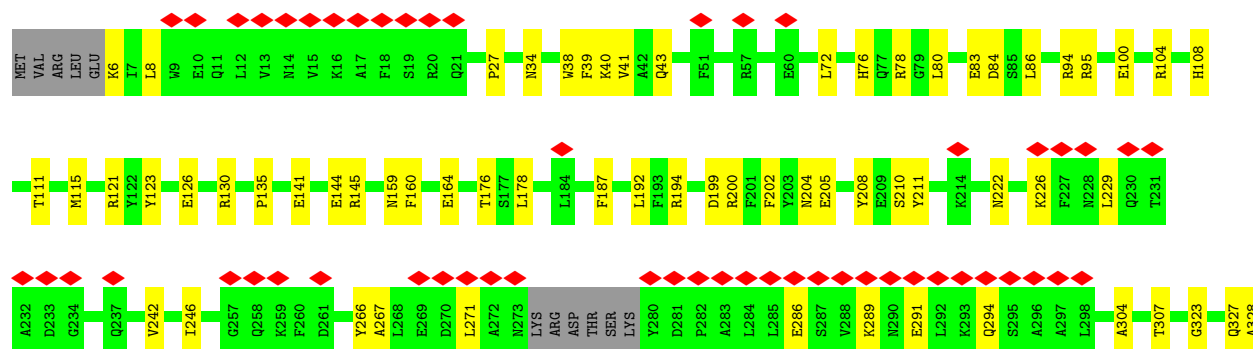


• Molecule 12: UQCRB

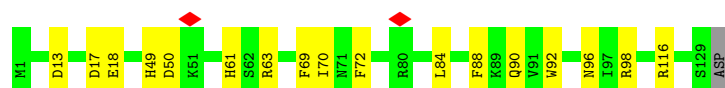


• Molecule 12: UQCRB

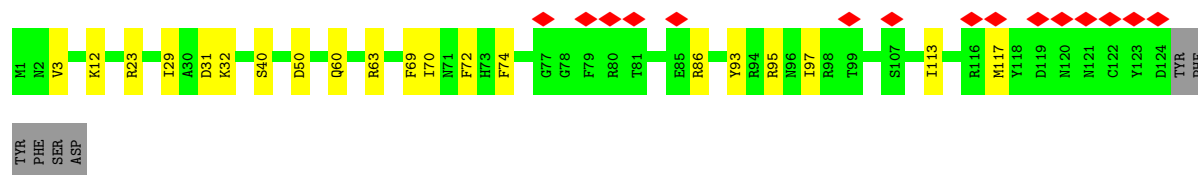
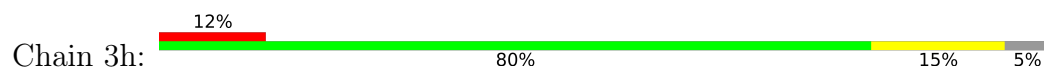




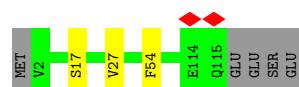
- Molecule 13: Transmembrane protein, putative



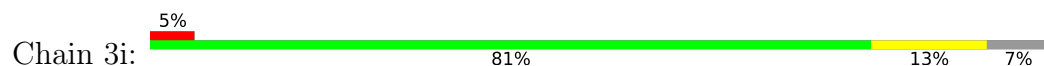
- Molecule 13: Transmembrane protein, putative



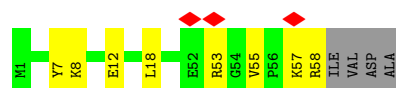
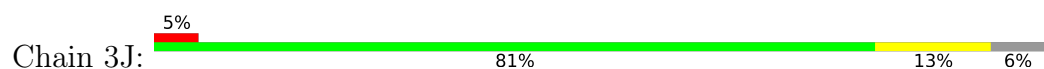
- Molecule 14: Transmembrane protein, putative



- Molecule 14: Transmembrane protein, putative

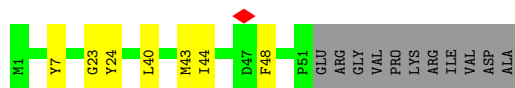


- Molecule 15: Transmembrane protein, putative



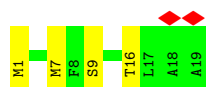
- Molecule 15: Transmembrane protein, putative

Chain 3j:  71% 11% 18%



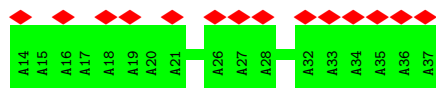
- Molecule 16: UNK1

Chain 3M:  11% 79% 21%

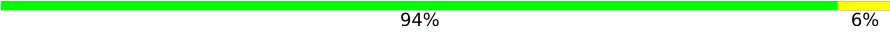


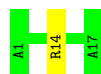
- Molecule 17: UNK2

Chain 3l:  58% 100%



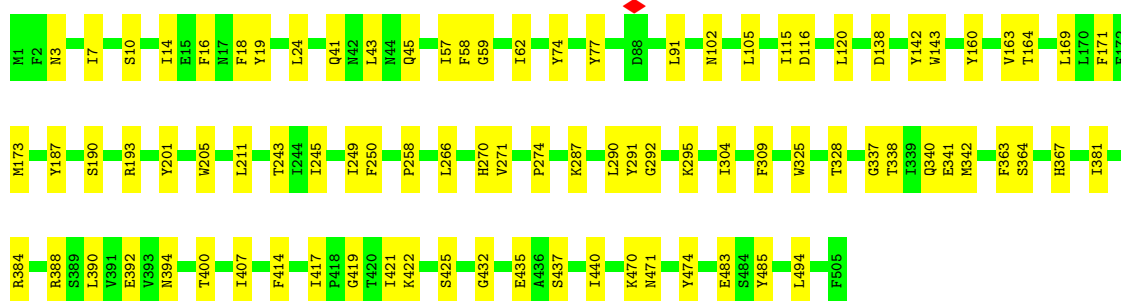
- Molecule 18: UNK3

Chain 3m:  94% 6%



- Molecule 19: NADH-ubiquinone oxidoreductase chain 4

Chain 4:  83% 17%

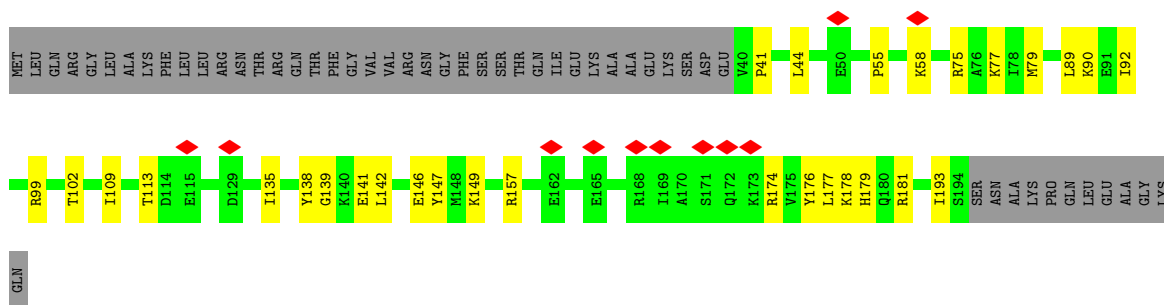


- Molecule 20: Ymf58

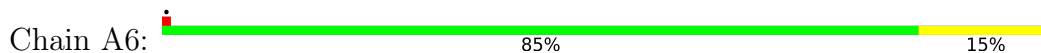
Chain 4L:  81% 19%



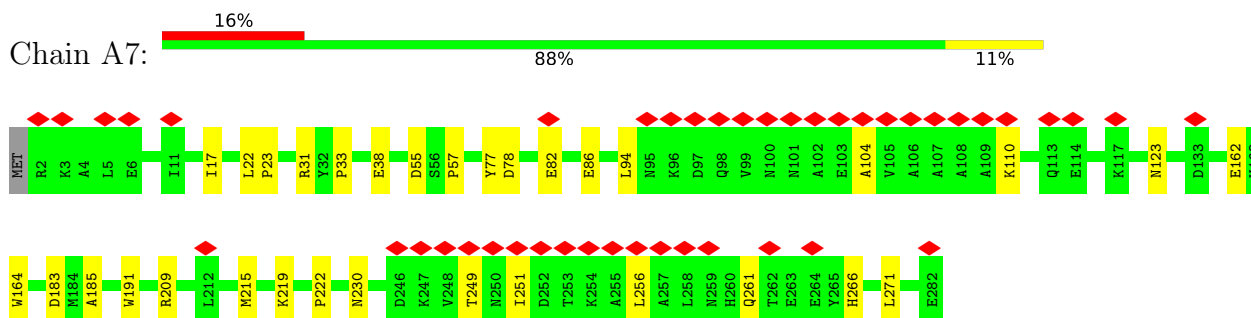




- Molecule 26: NADH dehydrogenase, putative



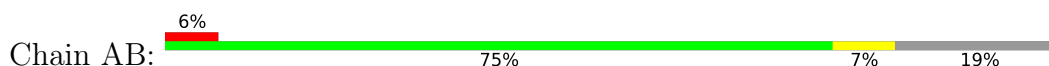
- Molecule 27: NDUA7



- Molecule 28: NAD-dependent epimerase/dehydratase family protein

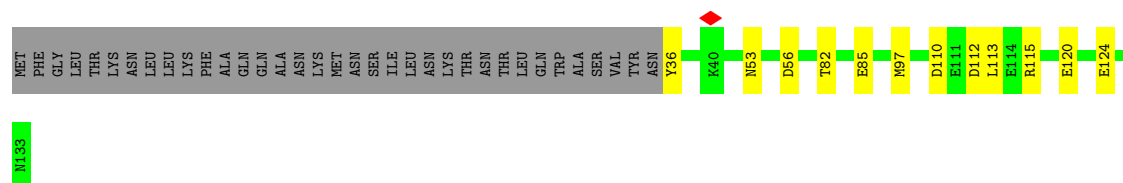


- Molecule 29: Acyl carrier protein



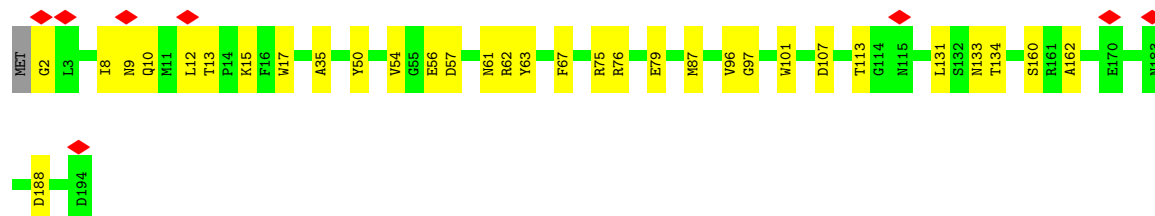
- Molecule 30: Acyl carrier protein





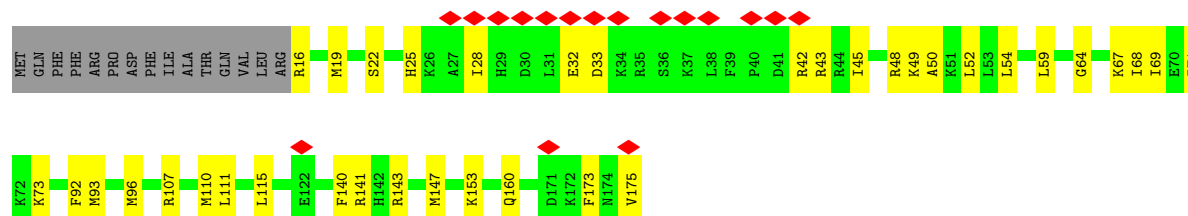
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain AL: 83% 16%



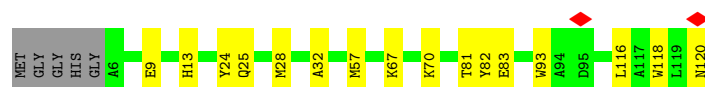
- Molecule 32: NDUA13

Chain AM: 10% 70% 21% 9%



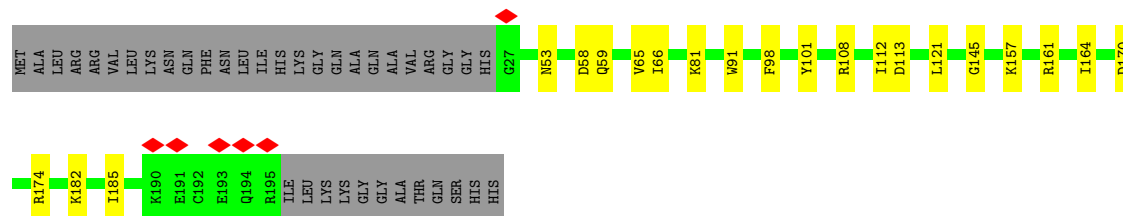
- Molecule 33: NDUB7

Chain B7: 82% 13%



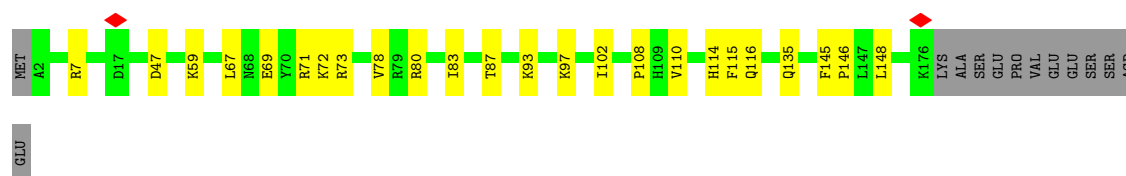
- Molecule 34: NDUB8

Chain B8: 71% 10% 18%

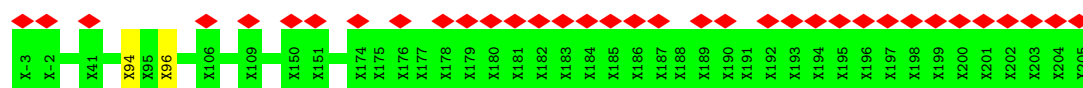


- Molecule 35: NDUB10

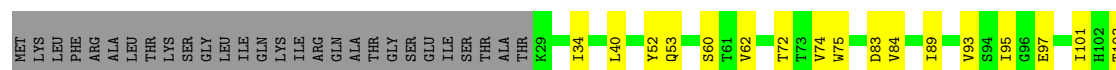
Chain BL: 80% 13% 7%



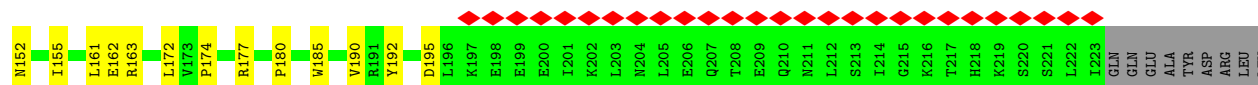
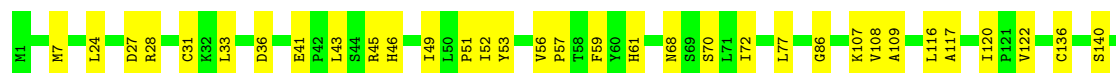
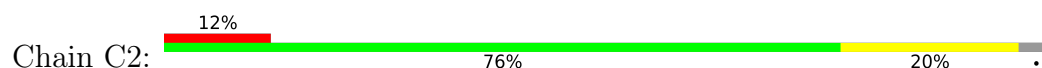
- Molecule 36: UNK4



- Molecule 37: Gamma-carbonic anhydrase

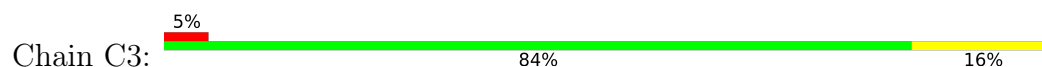


- Molecule 38: Gamma-carbonic anhydrase

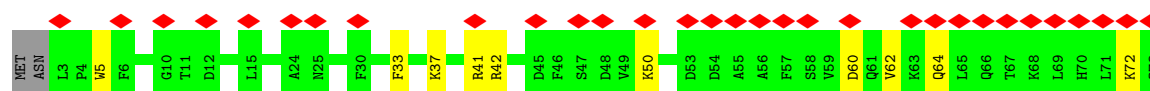
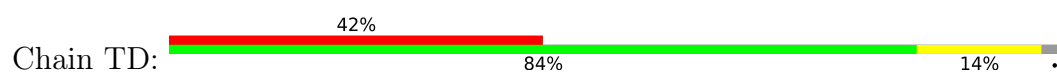


ALA

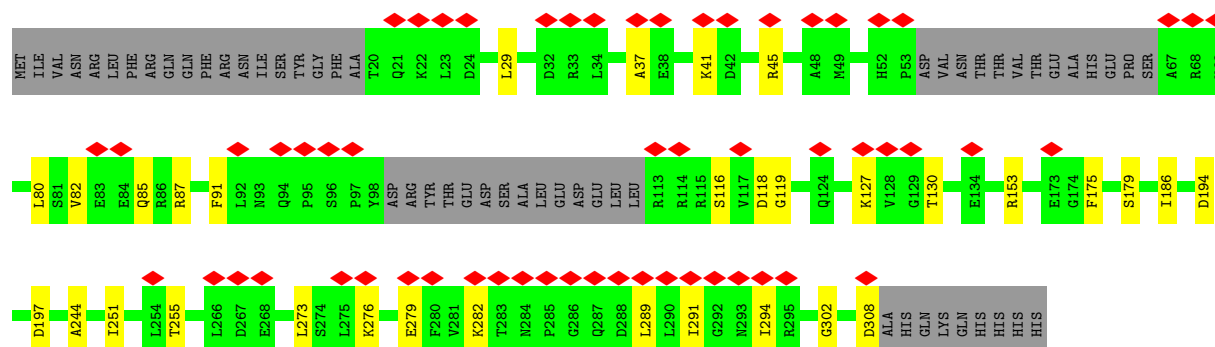
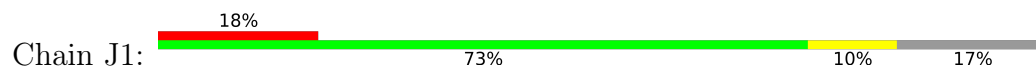
- Molecule 39: Transcription factor apf protein, putative



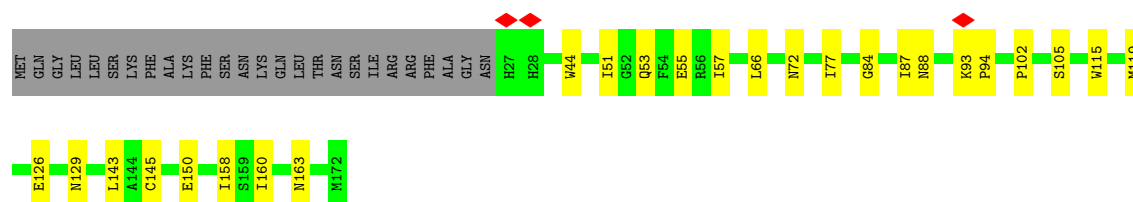
- Molecule 40: Transmembrane protein, putative



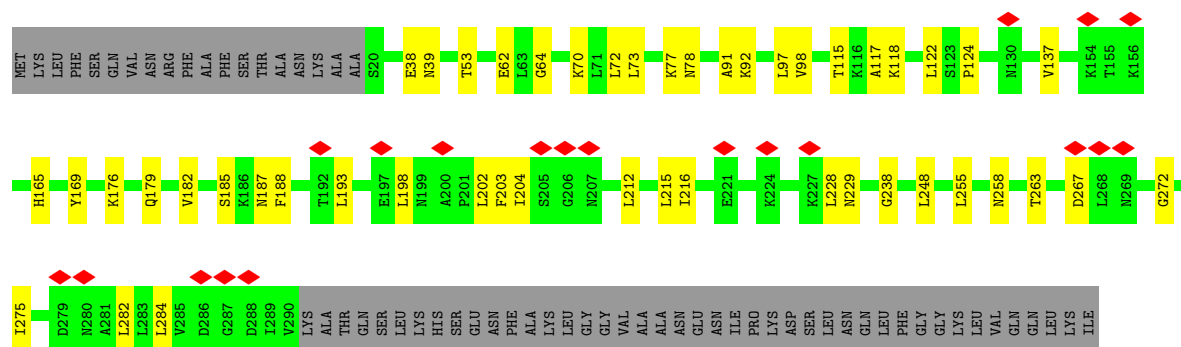
• Molecule 41: DnaJ domain protein



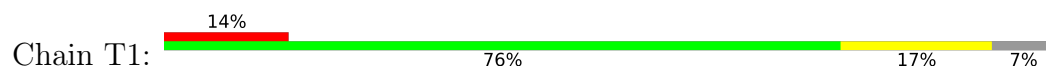
• Molecule 42: 2 iron, 2 sulfur cluster-binding protein



• Molecule 43: Acyl-CoA synthetase (AMP-forming)/AMP-acid ligase II



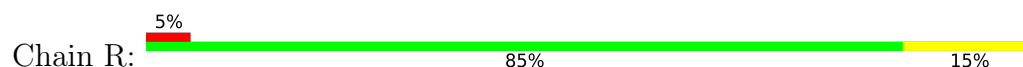
• Molecule 44: Lipid-A-disaccharide synthase



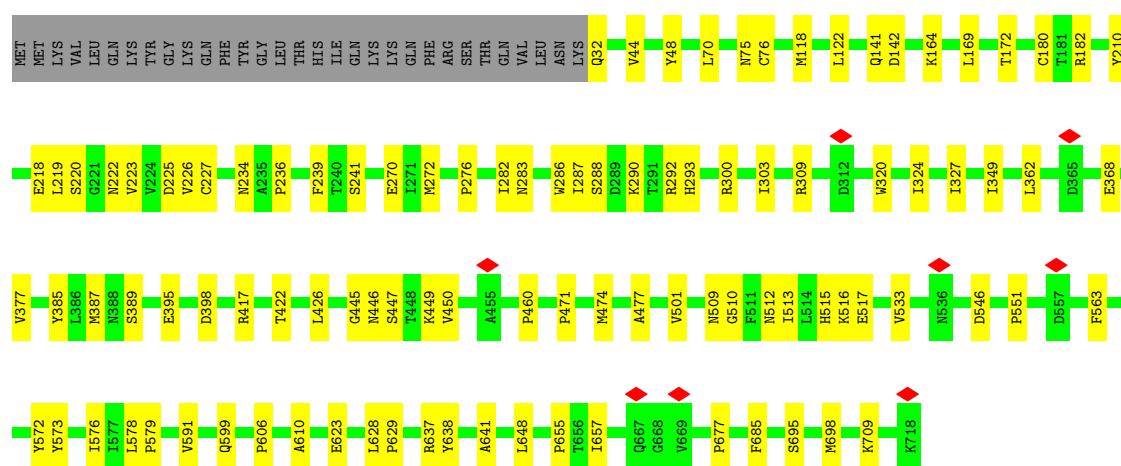
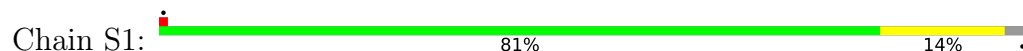




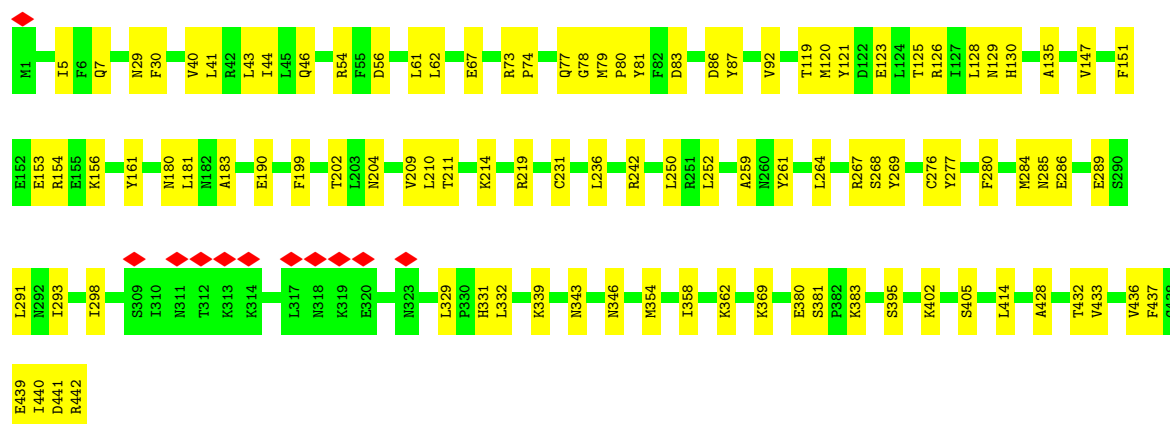
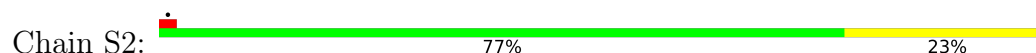
- Molecule 49: UNK5



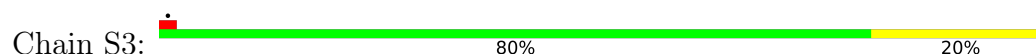
- Molecule 50: NADH-ubiquinone oxidoreductase 75 kDa subunit



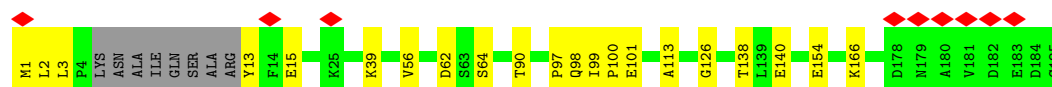
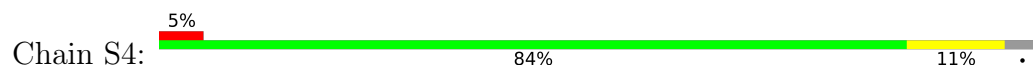
- Molecule 51: NADH dehydrogenase subunit 7



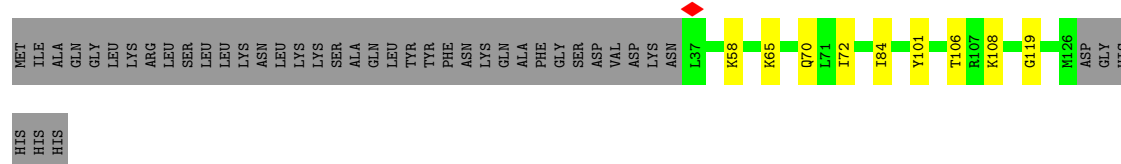
- Molecule 52: NADH dehydrogenase subunit 9



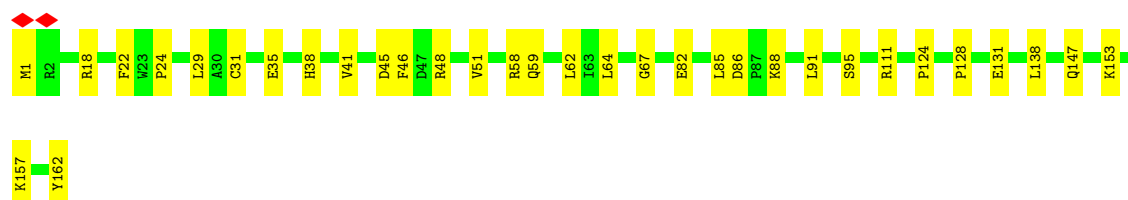
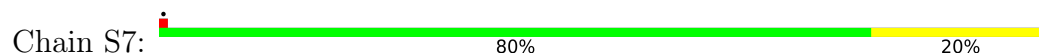
- Molecule 53: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



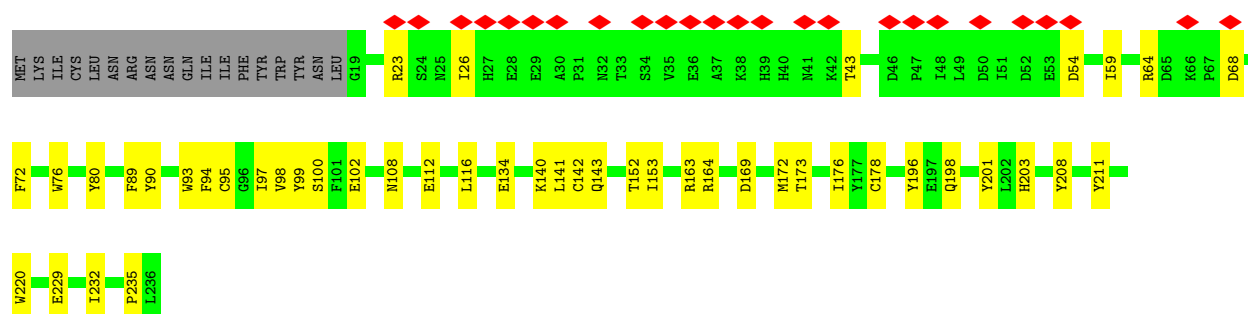
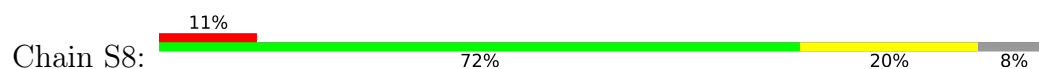
- Molecule 54: Zinc-finger protein



- Molecule 55: NADH dehydrogenase subunit 10



- Molecule 56: NADH-ubiquinone oxidoreductase 1, chain, putative



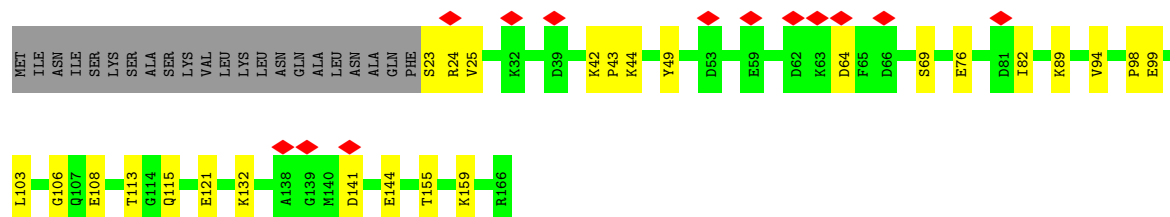
- Molecule 57: NDUB9

Chain B9: 

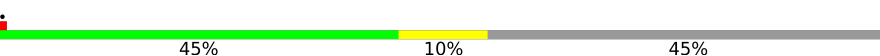


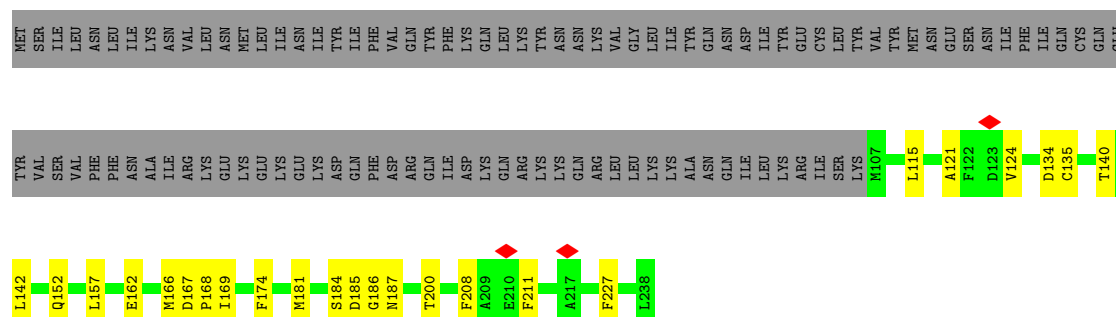
• Molecule 58: Thioredoxin

Chain TX: 



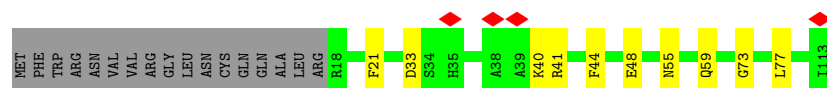
• Molecule 59: NDUA8

Chain A8: 



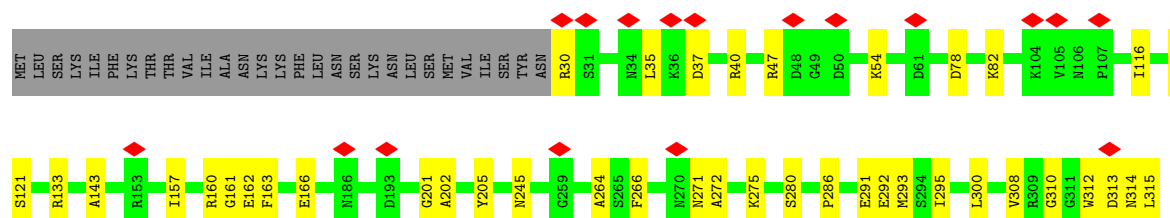
• Molecule 60: Transmembrane protein, putative

Chain TB: 



• Molecule 61: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

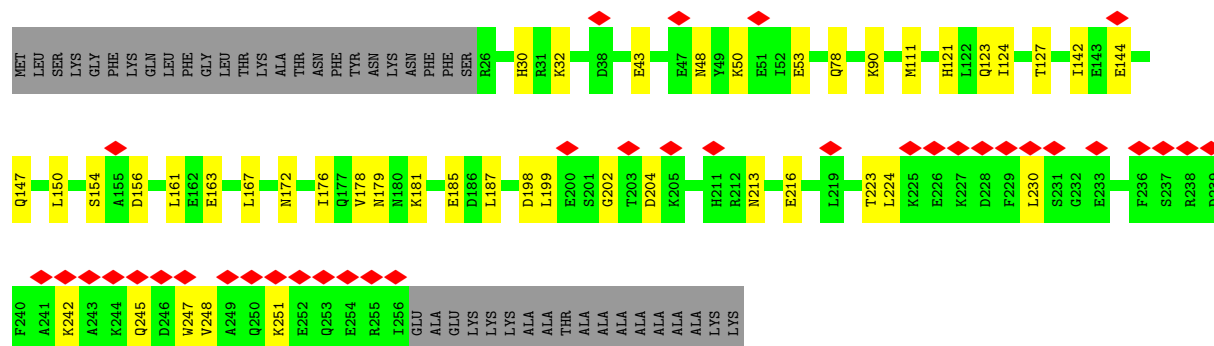
Chain V1: 





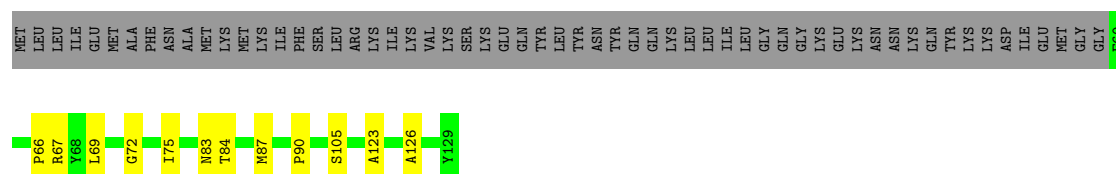
- Molecule 62: NADH-ubiquinone oxidoreductase 24 kDa subunit

Chain V2: 14% 69% 16% 16%



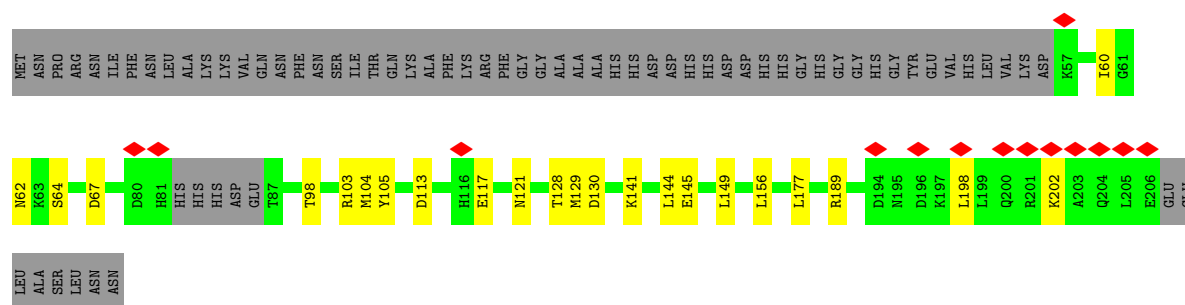
- Molecule 63: NDUB6

Chain B6: 45% 9% 46%



- Molecule 64: Transmembrane protein, putative

Chain BM: 7% 57% 11% 32%

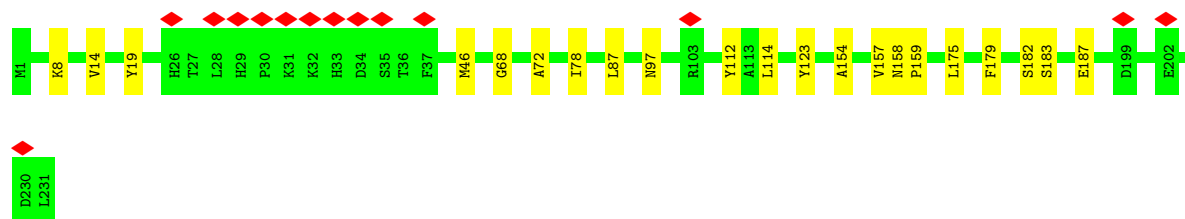


- Molecule 65: NDUC2

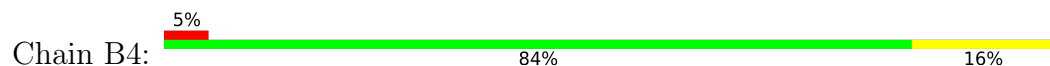
Chain C4: 92% 7%



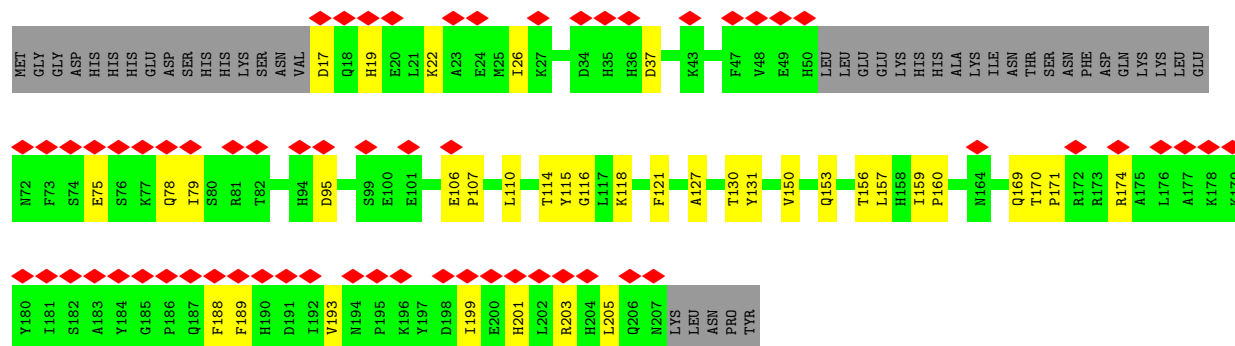
- Molecule 66: Transmembrane protein, putative



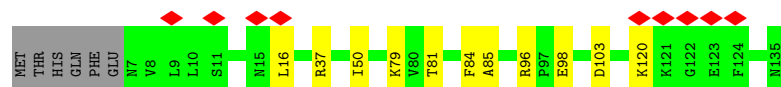
- Molecule 67: NDUB4



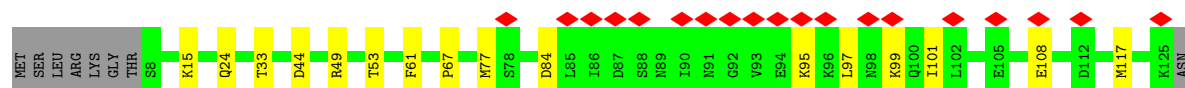
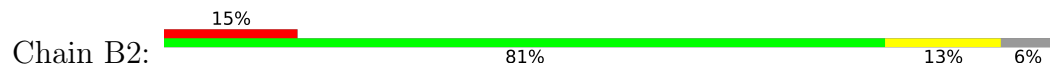
- Molecule 68: NDUTT4



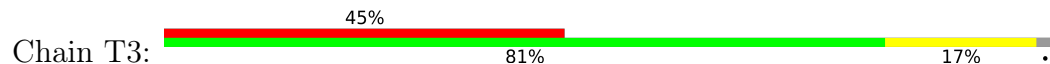
- Molecule 69: NDUTT8

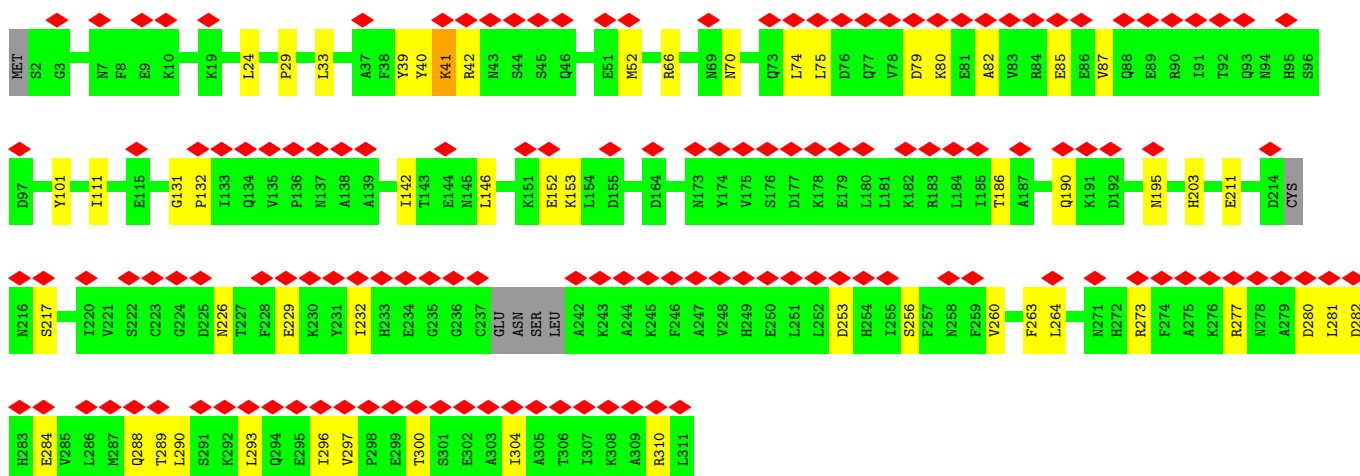


- Molecule 70: NDUB2

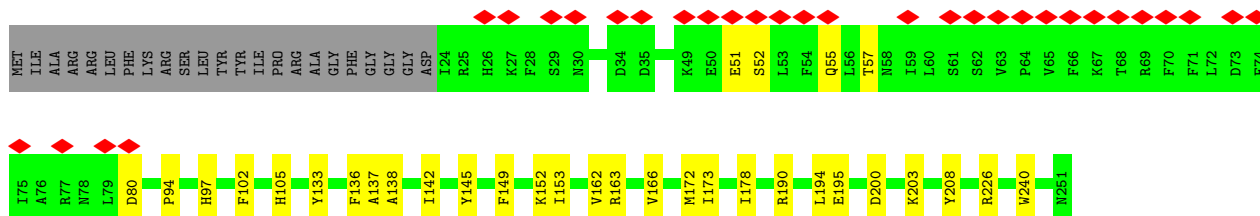
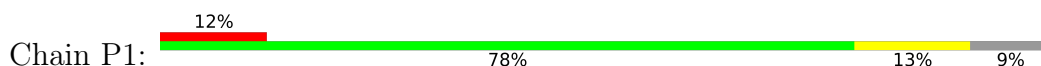


- Molecule 71: NDUTT3





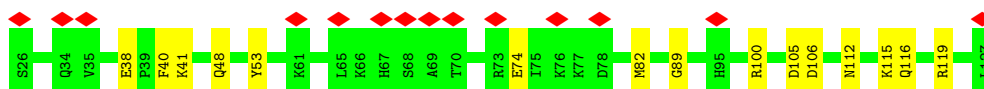
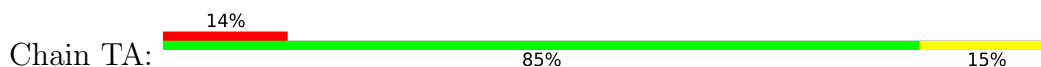
- Molecule 72: Transmembrane protein, putative



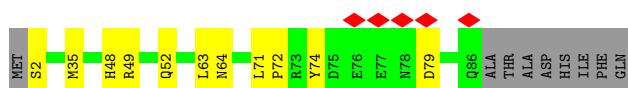
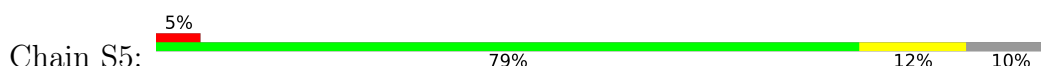
- Molecule 73: Transmembrane protein, putative



- Molecule 74: NDUTT10

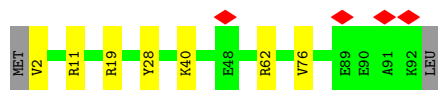


- Molecule 75: GRAM domain protein



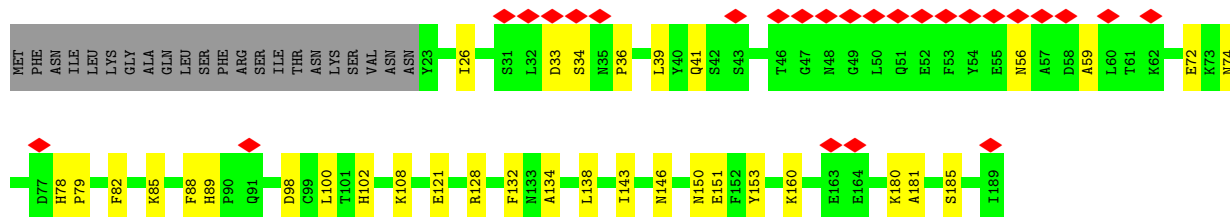
- Molecule 76: NDUTT12

Chain TC:  90% 8%



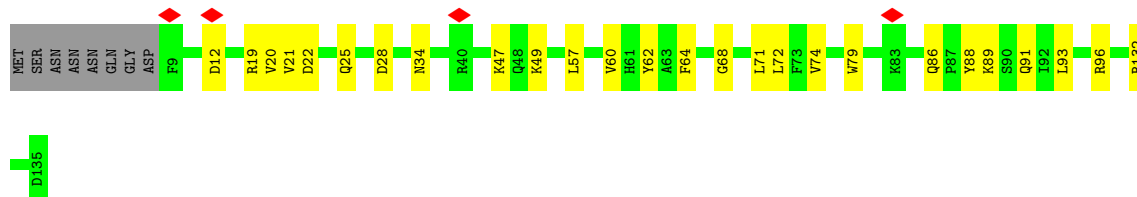
- Molecule 77: NDUPH2

Chain P2:  14% 70% 18% 12%



- Molecule 78: Transmembrane protein, putative

Chain A3:  75% 19% 6%



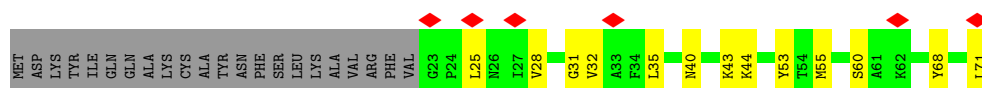
- Molecule 79: NDUTT9

Chain T9:  7% 83% 15%



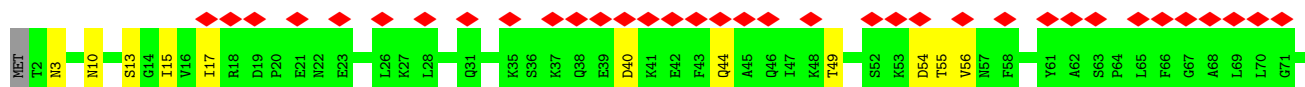
- Molecule 80: Transmembrane protein, putative

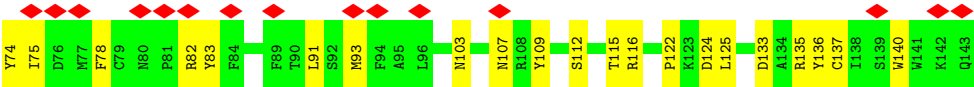
Chain TE:  8% 51% 18% 31%



- Molecule 81: Transmembrane protein, putative

Chain T7:  35% 77% 22%





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 203834                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 66.69                                   | Depositor |
| Minimum defocus (nm)                 | 500                                     | Depositor |
| Maximum defocus (nm)                 | 2500                                    | Depositor |
| Magnification                        | 58616                                   | Depositor |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 32.050                                  | Depositor |
| Minimum map value                    | -15.499                                 | Depositor |
| Average map value                    | 0.004                                   | Depositor |
| Map value standard deviation         | 1.092                                   | Depositor |
| Recommended contour level            | 6                                       | Depositor |
| Map size (Å)                         | 501.0, 501.0, 501.0                     | wwPDB     |
| Map dimensions                       | 600, 600, 600                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.835, 0.835, 0.835                     | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, ZMP, SF4, NDP, 3PE, PC1, ZN, FES, FMN, HEM, HEC, ADP, U10

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

| Mol | Chain | Bond lengths |             | Bond angles |               |
|-----|-------|--------------|-------------|-------------|---------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$   |
| 1   | 1     | 0.14         | 0/2384      | 0.33        | 0/3244        |
| 2   | 1B    | 0.12         | 0/536       | 0.25        | 0/727         |
| 3   | 2     | 0.15         | 0/3165      | 0.33        | 0/4302        |
| 4   | 2B    | 0.14         | 0/1520      | 0.31        | 0/2058        |
| 5   | 3     | 0.14         | 0/1051      | 0.28        | 0/1429        |
| 6   | 3A    | 0.11         | 0/3563      | 0.25        | 0/4827        |
| 6   | 3a    | 0.11         | 0/3547      | 0.26        | 0/4806        |
| 7   | 3B    | 0.13         | 0/3912      | 0.28        | 0/5313        |
| 7   | 3b    | 0.13         | 0/3901      | 0.30        | 0/5299        |
| 8   | 3C    | 0.13         | 0/3716      | 0.29        | 0/5046        |
| 8   | 3c    | 0.13         | 0/3715      | 0.30        | 1/5046 (0.0%) |
| 9   | 3D    | 0.13         | 0/2579      | 0.29        | 0/3491        |
| 9   | 3d    | 0.13         | 0/2491      | 0.28        | 0/3371        |
| 10  | 3E    | 0.13         | 0/1893      | 0.30        | 0/2566        |
| 10  | 3e    | 0.13         | 0/909       | 0.25        | 0/1226        |
| 11  | 3F    | 0.12         | 0/717       | 0.31        | 0/969         |
| 11  | 3f    | 0.15         | 0/608       | 0.35        | 0/823         |
| 12  | 3G    | 0.12         | 0/2670      | 0.28        | 0/3602        |
| 12  | 3g    | 0.12         | 0/2759      | 0.31        | 0/3724        |
| 13  | 3H    | 0.13         | 0/1133      | 0.31        | 0/1524        |
| 13  | 3h    | 0.12         | 0/1077      | 0.30        | 0/1448        |
| 14  | 3I    | 0.12         | 0/1005      | 0.29        | 0/1365        |
| 14  | 3i    | 0.12         | 0/982       | 0.32        | 0/1334        |
| 15  | 3J    | 0.14         | 0/522       | 0.31        | 0/712         |
| 15  | 3j    | 0.17         | 0/463       | 0.35        | 0/634         |
| 16  | 3M    | 0.10         | 0/151       | 0.33        | 0/198         |
| 17  | 3l    | 0.16         | 0/123       | 0.22        | 0/170         |
| 18  | 3m    | 0.09         | 0/122       | 0.24        | 0/162         |
| 19  | 4     | 0.16         | 0/4303      | 0.33        | 0/5844        |
| 20  | 4L    | 0.16         | 0/982       | 0.31        | 0/1335        |
| 21  | 5     | 0.14         | 0/4997      | 0.30        | 0/6794        |
| 22  | 5B    | 0.14         | 0/915       | 0.35        | 0/1224        |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 23  | 6     | 0.13         | 0/2137  | 0.27        | 0/2906  |
| 24  | A2    | 0.10         | 0/780   | 0.26        | 0/1054  |
| 25  | A5    | 0.12         | 0/1336  | 0.28        | 0/1797  |
| 26  | A6    | 0.13         | 0/1459  | 0.26        | 0/1965  |
| 27  | A7    | 0.10         | 0/2400  | 0.24        | 0/3259  |
| 28  | A9    | 0.11         | 0/2789  | 0.26        | 0/3777  |
| 29  | AB    | 0.09         | 0/942   | 0.24        | 0/1272  |
| 30  | AC    | 0.11         | 0/822   | 0.27        | 0/1114  |
| 31  | AL    | 0.11         | 0/1667  | 0.28        | 0/2256  |
| 32  | AM    | 0.13         | 0/1379  | 0.27        | 0/1841  |
| 33  | B7    | 0.13         | 0/964   | 0.30        | 0/1302  |
| 34  | B8    | 0.12         | 0/1445  | 0.26        | 0/1952  |
| 35  | BL    | 0.12         | 0/1489  | 0.27        | 0/2000  |
| 37  | C1    | 0.12         | 0/1806  | 0.28        | 0/2461  |
| 38  | C2    | 0.12         | 0/1653  | 0.29        | 0/2257  |
| 39  | C3    | 0.11         | 0/2865  | 0.27        | 0/3877  |
| 40  | TD    | 0.10         | 0/626   | 0.23        | 0/844   |
| 41  | J1    | 0.09         | 0/2194  | 0.22        | 0/2954  |
| 42  | FX    | 0.11         | 0/1186  | 0.30        | 0/1607  |
| 43  | T2    | 0.10         | 0/2160  | 0.23        | 0/2937  |
| 44  | T1    | 0.12         | 0/3975  | 0.28        | 0/5380  |
| 45  | A1    | 0.12         | 0/827   | 0.27        | 0/1122  |
| 46  | X1    | 0.11         | 0/1261  | 0.25        | 0/1698  |
| 47  | T6    | 0.10         | 0/923   | 0.26        | 0/1239  |
| 48  | T5    | 0.15         | 0/1113  | 0.35        | 0/1507  |
| 49  | R     | 0.14         | 0/962   | 0.32        | 0/1302  |
| 50  | S1    | 0.12         | 0/5502  | 0.30        | 0/7454  |
| 51  | S2    | 0.14         | 0/3681  | 0.31        | 0/4969  |
| 52  | S3    | 0.12         | 0/1718  | 0.30        | 0/2319  |
| 53  | S4    | 0.11         | 0/1505  | 0.28        | 0/2035  |
| 54  | S6    | 0.11         | 0/739   | 0.31        | 0/1000  |
| 55  | S7    | 0.14         | 0/1319  | 0.36        | 0/1789  |
| 56  | S8    | 0.14         | 0/1867  | 0.31        | 0/2538  |
| 57  | B9    | 0.11         | 0/1627  | 0.25        | 0/2203  |
| 58  | TX    | 0.10         | 0/1235  | 0.25        | 0/1662  |
| 59  | A8    | 0.12         | 0/1099  | 0.26        | 0/1477  |
| 60  | TB    | 0.11         | 0/825   | 0.26        | 0/1115  |
| 61  | V1    | 0.11         | 0/3485  | 0.29        | 0/4713  |
| 62  | V2    | 0.11         | 0/1895  | 0.29        | 0/2559  |
| 63  | B6    | 0.13         | 0/623   | 0.26        | 0/850   |
| 64  | BM    | 0.13         | 0/1187  | 0.29        | 0/1605  |
| 65  | C4    | 0.11         | 0/865   | 0.26        | 0/1165  |
| 66  | AN    | 0.09         | 0/1935  | 0.22        | 0/2616  |

| Mol | Chain | Bond lengths |          | Bond angles |                 |
|-----|-------|--------------|----------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5         |
| 67  | B4    | 0.13         | 0/935    | 0.27        | 0/1277          |
| 68  | T4    | 0.10         | 0/1447   | 0.25        | 0/1957          |
| 69  | T8    | 0.12         | 0/1091   | 0.28        | 0/1479          |
| 70  | B2    | 0.13         | 0/980    | 0.29        | 0/1318          |
| 71  | T3    | 0.11         | 0/2488   | 0.29        | 0/3367          |
| 72  | P1    | 0.11         | 0/1951   | 0.30        | 0/2642          |
| 73  | B3    | 0.12         | 0/613    | 0.31        | 0/829           |
| 74  | TA    | 0.10         | 0/877    | 0.28        | 0/1181          |
| 75  | S5    | 0.10         | 0/710    | 0.24        | 0/959           |
| 76  | TC    | 0.09         | 0/803    | 0.22        | 0/1082          |
| 77  | P2    | 0.11         | 0/1454   | 0.26        | 0/1970          |
| 78  | A3    | 0.11         | 0/1103   | 0.26        | 0/1491          |
| 79  | T9    | 0.11         | 0/1088   | 0.27        | 0/1458          |
| 80  | TE    | 0.10         | 0/425    | 0.27        | 0/573           |
| 81  | T7    | 0.11         | 0/1223   | 0.30        | 0/1648          |
| All | All   | 0.12         | 0/151866 | 0.29        | 1/205593 (0.0%) |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 8   | 3c    | 382 | ILE  | N-CA-C | -6.04 | 106.61      | 112.29   |

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 1     | 2313  | 0        | 2361     | 63      | 0            |
| 2   | 1B    | 516   | 0        | 528      | 12      | 0            |
| 3   | 2     | 3065  | 0        | 3141     | 45      | 0            |
| 4   | 2B    | 1483  | 0        | 1554     | 20      | 0            |
| 5   | 3     | 1017  | 0        | 1014     | 18      | 0            |
| 6   | 3A    | 3511  | 0        | 3507     | 37      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6   | 3a    | 3495  | 0        | 3485     | 43      | 0            |
| 7   | 3B    | 3826  | 0        | 3728     | 49      | 0            |
| 7   | 3b    | 3815  | 0        | 3715     | 55      | 0            |
| 8   | 3C    | 3590  | 0        | 3482     | 70      | 0            |
| 8   | 3c    | 3589  | 0        | 3483     | 67      | 0            |
| 9   | 3D    | 2488  | 0        | 2343     | 40      | 0            |
| 9   | 3d    | 2403  | 0        | 2265     | 48      | 0            |
| 10  | 3E    | 1846  | 0        | 1806     | 46      | 0            |
| 10  | 3e    | 882   | 0        | 843      | 20      | 0            |
| 11  | 3F    | 703   | 0        | 702      | 5       | 0            |
| 11  | 3f    | 597   | 0        | 599      | 17      | 0            |
| 12  | 3G    | 2595  | 0        | 2520     | 38      | 0            |
| 12  | 3g    | 2682  | 0        | 2611     | 48      | 0            |
| 13  | 3H    | 1098  | 0        | 1040     | 17      | 0            |
| 13  | 3h    | 1046  | 0        | 999      | 20      | 0            |
| 14  | 3I    | 971   | 0        | 986      | 3       | 0            |
| 14  | 3i    | 948   | 0        | 967      | 12      | 0            |
| 15  | 3J    | 501   | 0        | 503      | 11      | 0            |
| 15  | 3j    | 443   | 0        | 439      | 6       | 0            |
| 16  | 3M    | 150   | 0        | 160      | 6       | 0            |
| 17  | 3l    | 124   | 0        | 120      | 0       | 0            |
| 18  | 3m    | 121   | 0        | 133      | 2       | 0            |
| 19  | 4     | 4170  | 0        | 4223     | 71      | 0            |
| 20  | 4L    | 957   | 0        | 987      | 17      | 0            |
| 21  | 5     | 4844  | 0        | 4892     | 84      | 0            |
| 22  | 5B    | 888   | 0        | 917      | 17      | 0            |
| 23  | 6     | 2076  | 0        | 2071     | 46      | 0            |
| 24  | A2    | 765   | 0        | 755      | 7       | 0            |
| 25  | A5    | 1307  | 0        | 1317     | 21      | 0            |
| 26  | A6    | 1421  | 0        | 1382     | 21      | 0            |
| 27  | A7    | 2339  | 0        | 2237     | 25      | 0            |
| 28  | A9    | 2718  | 0        | 2649     | 25      | 0            |
| 29  | AB    | 926   | 0        | 902      | 6       | 0            |
| 30  | AC    | 806   | 0        | 784      | 7       | 0            |
| 31  | AL    | 1612  | 0        | 1511     | 23      | 0            |
| 32  | AM    | 1349  | 0        | 1375     | 40      | 0            |
| 33  | B7    | 937   | 0        | 881      | 13      | 0            |
| 34  | B8    | 1408  | 0        | 1357     | 21      | 0            |
| 35  | BL    | 1461  | 0        | 1467     | 22      | 0            |
| 36  | C     | 1045  | 0        | 216      | 1       | 0            |
| 37  | C1    | 1769  | 0        | 1721     | 34      | 0            |
| 38  | C2    | 1624  | 0        | 1566     | 36      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 39  | C3    | 2804  | 0        | 2727     | 40      | 0            |
| 40  | TD    | 608   | 0        | 605      | 10      | 0            |
| 41  | J1    | 2146  | 0        | 2110     | 25      | 0            |
| 42  | FX    | 1162  | 0        | 1120     | 18      | 0            |
| 43  | T2    | 2117  | 0        | 2109     | 29      | 0            |
| 44  | T1    | 3884  | 0        | 3827     | 54      | 0            |
| 45  | A1    | 799   | 0        | 792      | 16      | 0            |
| 46  | X1    | 1227  | 0        | 1208     | 13      | 0            |
| 47  | T6    | 903   | 0        | 851      | 12      | 0            |
| 48  | T5    | 1088  | 0        | 1107     | 22      | 0            |
| 49  | R     | 943   | 0        | 950      | 18      | 0            |
| 50  | S1    | 5394  | 0        | 5345     | 69      | 0            |
| 51  | S2    | 3599  | 0        | 3552     | 72      | 0            |
| 52  | S3    | 1681  | 0        | 1679     | 27      | 0            |
| 53  | S4    | 1463  | 0        | 1397     | 17      | 0            |
| 54  | S6    | 722   | 0        | 714      | 6       | 0            |
| 55  | S7    | 1286  | 0        | 1283     | 27      | 0            |
| 56  | S8    | 1812  | 0        | 1688     | 39      | 0            |
| 57  | B9    | 1579  | 0        | 1482     | 17      | 0            |
| 58  | TX    | 1206  | 0        | 1155     | 18      | 0            |
| 59  | A8    | 1075  | 0        | 1022     | 16      | 0            |
| 60  | TB    | 801   | 0        | 763      | 8       | 0            |
| 61  | V1    | 3410  | 0        | 3357     | 42      | 0            |
| 62  | V2    | 1858  | 0        | 1842     | 28      | 0            |
| 63  | B6    | 596   | 0        | 583      | 9       | 0            |
| 64  | BM    | 1163  | 0        | 1120     | 18      | 0            |
| 65  | C4    | 842   | 0        | 828      | 7       | 0            |
| 66  | AN    | 1879  | 0        | 1818     | 17      | 0            |
| 67  | B4    | 898   | 0        | 819      | 13      | 0            |
| 68  | T4    | 1408  | 0        | 1392     | 27      | 0            |
| 69  | T8    | 1064  | 0        | 1095     | 13      | 0            |
| 70  | B2    | 955   | 0        | 930      | 14      | 0            |
| 71  | T3    | 2442  | 0        | 2438     | 37      | 0            |
| 72  | P1    | 1896  | 0        | 1854     | 25      | 0            |
| 73  | B3    | 594   | 0        | 589      | 9       | 0            |
| 74  | TA    | 854   | 0        | 839      | 15      | 0            |
| 75  | S5    | 693   | 0        | 669      | 14      | 0            |
| 76  | TC    | 781   | 0        | 734      | 9       | 0            |
| 77  | P2    | 1414  | 0        | 1378     | 23      | 0            |
| 78  | A3    | 1065  | 0        | 997      | 23      | 0            |
| 79  | T9    | 1066  | 0        | 1023     | 16      | 0            |
| 80  | TE    | 413   | 0        | 418      | 9       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 81  | T7    | 1187  | 0        | 1137     | 23      | 0            |
| 82  | 1     | 50    | 0        | 44       | 1       | 0            |
| 82  | 2B    | 53    | 0        | 50       | 0       | 0            |
| 82  | 3     | 44    | 0        | 32       | 0       | 0            |
| 82  | 3B    | 78    | 0        | 103      | 5       | 0            |
| 82  | 3C    | 65    | 0        | 74       | 4       | 0            |
| 82  | 3G    | 66    | 0        | 79       | 2       | 0            |
| 82  | 3H    | 128   | 0        | 144      | 3       | 0            |
| 82  | 3I    | 108   | 0        | 104      | 2       | 0            |
| 82  | 3b    | 68    | 0        | 80       | 3       | 0            |
| 82  | 3c    | 120   | 0        | 128      | 2       | 0            |
| 82  | 3i    | 71    | 0        | 86       | 3       | 0            |
| 82  | 5     | 186   | 0        | 272      | 14      | 0            |
| 82  | A1    | 53    | 0        | 50       | 0       | 0            |
| 82  | AL    | 53    | 0        | 50       | 3       | 0            |
| 82  | AM    | 62    | 0        | 68       | 7       | 0            |
| 82  | AN    | 53    | 0        | 50       | 3       | 0            |
| 82  | B4    | 40    | 0        | 20       | 1       | 0            |
| 82  | B8    | 45    | 0        | 34       | 1       | 0            |
| 82  | BM    | 86    | 0        | 119      | 9       | 0            |
| 82  | C4    | 98    | 0        | 149      | 6       | 0            |
| 82  | P2    | 82    | 0        | 111      | 3       | 0            |
| 82  | R     | 84    | 0        | 115      | 3       | 0            |
| 82  | T1    | 55    | 0        | 54       | 3       | 0            |
| 82  | T7    | 48    | 0        | 40       | 1       | 0            |
| 82  | TD    | 66    | 0        | 76       | 2       | 0            |
| 83  | 1     | 36    | 0        | 46       | 0       | 0            |
| 83  | 3     | 31    | 0        | 36       | 0       | 0            |
| 83  | 3C    | 119   | 0        | 166      | 6       | 0            |
| 83  | 3E    | 78    | 0        | 110      | 8       | 0            |
| 83  | 3F    | 22    | 0        | 18       | 0       | 0            |
| 83  | 3I    | 78    | 0        | 107      | 0       | 0            |
| 83  | 3J    | 37    | 0        | 48       | 4       | 0            |
| 83  | 3b    | 30    | 0        | 34       | 1       | 0            |
| 83  | 3c    | 69    | 0        | 86       | 2       | 0            |
| 83  | 3e    | 50    | 0        | 77       | 2       | 0            |
| 83  | 3g    | 33    | 0        | 40       | 2       | 0            |
| 83  | 3j    | 36    | 0        | 46       | 1       | 0            |
| 83  | 5     | 147   | 0        | 228      | 10      | 0            |
| 83  | 6     | 93    | 0        | 140      | 6       | 0            |
| 83  | AM    | 30    | 0        | 34       | 2       | 0            |
| 83  | AN    | 36    | 0        | 46       | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 83  | B2    | 48    | 0        | 73       | 7       | 0            |
| 83  | B6    | 52    | 0        | 81       | 3       | 0            |
| 83  | C4    | 32    | 0        | 38       | 1       | 0            |
| 83  | J1    | 40    | 0        | 54       | 1       | 0            |
| 83  | P1    | 40    | 0        | 54       | 0       | 0            |
| 83  | T1    | 26    | 0        | 26       | 0       | 0            |
| 83  | TC    | 42    | 0        | 61       | 4       | 0            |
| 83  | X1    | 49    | 0        | 75       | 2       | 0            |
| 84  | 3C    | 86    | 0        | 60       | 2       | 0            |
| 84  | 3c    | 86    | 0        | 60       | 7       | 0            |
| 85  | 3C    | 26    | 0        | 35       | 4       | 0            |
| 85  | 3H    | 29    | 0        | 33       | 0       | 0            |
| 85  | 5B    | 63    | 0        | 90       | 7       | 0            |
| 86  | 3D    | 43    | 0        | 30       | 0       | 0            |
| 86  | 3d    | 43    | 0        | 30       | 1       | 0            |
| 87  | 3E    | 4     | 0        | 0        | 0       | 0            |
| 87  | FX    | 4     | 0        | 0        | 0       | 0            |
| 87  | S1    | 4     | 0        | 0        | 0       | 0            |
| 87  | V2    | 4     | 0        | 0        | 1       | 0            |
| 88  | 3E    | 34    | 0        | 42       | 0       | 0            |
| 88  | 3d    | 47    | 0        | 68       | 3       | 0            |
| 88  | 4     | 83    | 0        | 114      | 2       | 0            |
| 88  | 5     | 72    | 0        | 92       | 2       | 0            |
| 88  | 5B    | 24    | 0        | 22       | 0       | 0            |
| 88  | A3    | 45    | 0        | 64       | 4       | 0            |
| 88  | AN    | 80    | 0        | 111      | 5       | 0            |
| 88  | B8    | 36    | 0        | 46       | 3       | 0            |
| 88  | C4    | 51    | 0        | 82       | 3       | 0            |
| 88  | P1    | 47    | 0        | 71       | 4       | 0            |
| 88  | S8    | 41    | 0        | 59       | 1       | 0            |
| 88  | T4    | 25    | 0        | 24       | 3       | 0            |
| 88  | T8    | 39    | 0        | 55       | 0       | 0            |
| 88  | TA    | 26    | 0        | 26       | 0       | 0            |
| 89  | 3F    | 1     | 0        | 0        | 0       | 0            |
| 89  | A9    | 1     | 0        | 0        | 0       | 0            |
| 89  | S6    | 1     | 0        | 0        | 0       | 0            |
| 90  | A9    | 48    | 0        | 26       | 1       | 0            |
| 91  | AB    | 34    | 0        | 40       | 4       | 0            |
| 92  | B8    | 27    | 0        | 12       | 1       | 0            |
| 93  | S1    | 16    | 0        | 0        | 2       | 0            |
| 93  | S7    | 8     | 0        | 0        | 1       | 0            |
| 93  | S8    | 16    | 0        | 0        | 3       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 93  | V1    | 8      | 0        | 0        | 0       | 0            |
| 94  | V1    | 31     | 0        | 19       | 1       | 0            |
| All | All   | 153366 | 0        | 150757   | 1931    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 1931 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:AM:16:ARG:N    | 32:AM:22:SER:HG   | 1.46                     | 1.14              |
| 7:3b:418:TYR:HD2  | 7:3b:455:ILE:HD13 | 1.39                     | 0.87              |
| 53:S4:98:GLN:HG3  | 53:S4:99:ILE:HD12 | 1.58                     | 0.85              |
| 10:3E:202:CYS:CB  | 10:3E:216:CYS:SG  | 2.64                     | 0.84              |
| 12:3g:80:LEU:HD12 | 12:3g:84:ASP:HB2  | 1.60                     | 0.83              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | 1     | 282/284 (99%) | 272 (96%) | 10 (4%) | 0        | 100         | 100 |
| 2   | 1B    | 57/59 (97%)   | 56 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 3   | 2     | 357/360 (99%) | 349 (98%) | 8 (2%)  | 0        | 100         | 100 |
| 4   | 2B    | 176/178 (99%) | 172 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 5   | 3     | 118/121 (98%) | 115 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 6   | 3A    | 449/482 (93%) | 437 (97%) | 12 (3%) | 0        | 100         | 100 |
| 6   | 3a    | 447/482 (93%) | 435 (97%) | 12 (3%) | 0        | 100         | 100 |
| 7   | 3B    | 477/513 (93%) | 468 (98%) | 9 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|----------|-------------|-----|
| 7   | 3b    | 476/513 (93%)  | 461 (97%)  | 15 (3%)  | 0        | 100         | 100 |
| 8   | 3C    | 424/426 (100%) | 415 (98%)  | 9 (2%)   | 0        | 100         | 100 |
| 8   | 3c    | 424/426 (100%) | 404 (95%)  | 20 (5%)  | 0        | 100         | 100 |
| 9   | 3D    | 293/319 (92%)  | 275 (94%)  | 18 (6%)  | 0        | 100         | 100 |
| 9   | 3d    | 283/319 (89%)  | 267 (94%)  | 16 (6%)  | 0        | 100         | 100 |
| 10  | 3E    | 226/269 (84%)  | 215 (95%)  | 10 (4%)  | 1 (0%)   | 30          | 51  |
| 10  | 3e    | 100/269 (37%)  | 91 (91%)   | 9 (9%)   | 0        | 100         | 100 |
| 11  | 3F    | 87/90 (97%)    | 86 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 11  | 3f    | 73/90 (81%)    | 73 (100%)  | 0        | 0        | 100         | 100 |
| 12  | 3G    | 305/328 (93%)  | 291 (95%)  | 14 (5%)  | 0        | 100         | 100 |
| 12  | 3g    | 313/328 (95%)  | 298 (95%)  | 15 (5%)  | 0        | 100         | 100 |
| 13  | 3H    | 127/130 (98%)  | 111 (87%)  | 16 (13%) | 0        | 100         | 100 |
| 13  | 3h    | 122/130 (94%)  | 108 (88%)  | 14 (12%) | 0        | 100         | 100 |
| 14  | 3I    | 112/119 (94%)  | 106 (95%)  | 6 (5%)   | 0        | 100         | 100 |
| 14  | 3i    | 109/119 (92%)  | 101 (93%)  | 8 (7%)   | 0        | 100         | 100 |
| 15  | 3J    | 56/62 (90%)    | 54 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 15  | 3j    | 49/62 (79%)    | 47 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 16  | 3M    | 17/19 (90%)    | 14 (82%)   | 3 (18%)  | 0        | 100         | 100 |
| 17  | 3l    | 22/24 (92%)    | 22 (100%)  | 0        | 0        | 100         | 100 |
| 18  | 3m    | 15/17 (88%)    | 14 (93%)   | 1 (7%)   | 0        | 100         | 100 |
| 19  | 4     | 503/505 (100%) | 481 (96%)  | 22 (4%)  | 0        | 100         | 100 |
| 20  | 4L    | 114/116 (98%)  | 114 (100%) | 0        | 0        | 100         | 100 |
| 21  | 5     | 585/750 (78%)  | 576 (98%)  | 9 (2%)   | 0        | 100         | 100 |
| 22  | 5B    | 98/100 (98%)   | 86 (88%)   | 12 (12%) | 0        | 100         | 100 |
| 23  | 6     | 242/255 (95%)  | 228 (94%)  | 14 (6%)  | 0        | 100         | 100 |
| 24  | A2    | 90/103 (87%)   | 90 (100%)  | 0        | 0        | 100         | 100 |
| 25  | A5    | 153/206 (74%)  | 150 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 26  | A6    | 170/172 (99%)  | 163 (96%)  | 7 (4%)   | 0        | 100         | 100 |
| 27  | A7    | 279/282 (99%)  | 274 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 28  | A9    | 336/362 (93%)  | 329 (98%)  | 7 (2%)   | 0        | 100         | 100 |
| 29  | AB    | 110/138 (80%)  | 108 (98%)  | 2 (2%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 30  | AC    | 96/133 (72%)   | 95 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 31  | AL    | 191/194 (98%)  | 184 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 32  | AM    | 158/175 (90%)  | 152 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 33  | B7    | 113/120 (94%)  | 109 (96%) | 4 (4%)  | 0        | 100         | 100 |
| 34  | B8    | 167/207 (81%)  | 166 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 35  | BL    | 173/188 (92%)  | 167 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 37  | C1    | 227/257 (88%)  | 213 (94%) | 14 (6%) | 0        | 100         | 100 |
| 38  | C2    | 221/233 (95%)  | 209 (95%) | 12 (5%) | 0        | 100         | 100 |
| 39  | C3    | 344/346 (99%)  | 337 (98%) | 7 (2%)  | 0        | 100         | 100 |
| 40  | TD    | 69/73 (94%)    | 68 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 41  | J1    | 256/317 (81%)  | 253 (99%) | 3 (1%)  | 0        | 100         | 100 |
| 42  | FX    | 144/172 (84%)  | 142 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 43  | T2    | 269/333 (81%)  | 259 (96%) | 10 (4%) | 0        | 100         | 100 |
| 44  | T1    | 479/516 (93%)  | 465 (97%) | 14 (3%) | 0        | 100         | 100 |
| 45  | A1    | 90/94 (96%)    | 87 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 46  | X1    | 147/150 (98%)  | 141 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 47  | T6    | 107/144 (74%)  | 104 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 48  | T5    | 132/205 (64%)  | 129 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 49  | R     | 122/124 (98%)  | 118 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 50  | S1    | 685/718 (95%)  | 667 (97%) | 18 (3%) | 0        | 100         | 100 |
| 51  | S2    | 440/442 (100%) | 427 (97%) | 13 (3%) | 0        | 100         | 100 |
| 52  | S3    | 196/198 (99%)  | 191 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 53  | S4    | 173/185 (94%)  | 166 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 54  | S6    | 88/132 (67%)   | 87 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 55  | S7    | 160/162 (99%)  | 156 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 56  | S8    | 216/236 (92%)  | 212 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 57  | B9    | 184/189 (97%)  | 177 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 58  | TX    | 142/166 (86%)  | 140 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 59  | A8    | 130/238 (55%)  | 129 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 60  | TB    | 94/113 (83%)   | 89 (95%)  | 5 (5%)  | 0        | 100         | 100 |
| 61  | V1    | 440/474 (93%)  | 426 (97%) | 14 (3%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 62  | V2    | 229/274 (84%)     | 222 (97%)   | 7 (3%)   | 0        | 100         | 100 |
| 63  | B6    | 68/129 (53%)      | 64 (94%)    | 4 (6%)   | 0        | 100         | 100 |
| 64  | BM    | 141/214 (66%)     | 139 (99%)   | 2 (1%)   | 0        | 100         | 100 |
| 65  | C4    | 99/102 (97%)      | 98 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 66  | AN    | 229/231 (99%)     | 226 (99%)   | 3 (1%)   | 0        | 100         | 100 |
| 67  | B4    | 106/108 (98%)     | 103 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 68  | T4    | 166/212 (78%)     | 164 (99%)   | 2 (1%)   | 0        | 100         | 100 |
| 69  | T8    | 127/135 (94%)     | 124 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| 70  | B2    | 116/126 (92%)     | 112 (97%)   | 4 (3%)   | 0        | 100         | 100 |
| 71  | T3    | 299/311 (96%)     | 294 (98%)   | 4 (1%)   | 1 (0%)   | 36          | 58  |
| 72  | P1    | 226/251 (90%)     | 218 (96%)   | 8 (4%)   | 0        | 100         | 100 |
| 73  | B3    | 66/83 (80%)       | 63 (96%)    | 3 (4%)   | 0        | 100         | 100 |
| 74  | TA    | 100/102 (98%)     | 96 (96%)    | 4 (4%)   | 0        | 100         | 100 |
| 75  | S5    | 83/94 (88%)       | 80 (96%)    | 3 (4%)   | 0        | 100         | 100 |
| 76  | TC    | 89/93 (96%)       | 87 (98%)    | 2 (2%)   | 0        | 100         | 100 |
| 77  | P2    | 165/189 (87%)     | 164 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 78  | A3    | 125/135 (93%)     | 122 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| 79  | T9    | 130/135 (96%)     | 126 (97%)   | 4 (3%)   | 0        | 100         | 100 |
| 80  | TE    | 47/71 (66%)       | 47 (100%)   | 0        | 0        | 100         | 100 |
| 81  | T7    | 140/143 (98%)     | 135 (96%)   | 5 (4%)   | 0        | 100         | 100 |
| All | All   | 17880/19899 (90%) | 17305 (97%) | 573 (3%) | 2 (0%)   | 100         | 100 |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 71  | T3    | 41  | LYS  |
| 10  | 3E    | 229 | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | 1     | 250/250 (100%) | 250 (100%) | 0        | 100         | 100 |
| 2   | 1B    | 55/55 (100%)   | 55 (100%)  | 0        | 100         | 100 |
| 3   | 2     | 345/346 (100%) | 345 (100%) | 0        | 100         | 100 |
| 4   | 2B    | 170/170 (100%) | 170 (100%) | 0        | 100         | 100 |
| 5   | 3     | 111/112 (99%)  | 111 (100%) | 0        | 100         | 100 |
| 6   | 3A    | 384/409 (94%)  | 384 (100%) | 0        | 100         | 100 |
| 6   | 3a    | 382/409 (93%)  | 382 (100%) | 0        | 100         | 100 |
| 7   | 3B    | 410/440 (93%)  | 410 (100%) | 0        | 100         | 100 |
| 7   | 3b    | 409/440 (93%)  | 409 (100%) | 0        | 100         | 100 |
| 8   | 3C    | 386/386 (100%) | 386 (100%) | 0        | 100         | 100 |
| 8   | 3c    | 386/386 (100%) | 386 (100%) | 0        | 100         | 100 |
| 9   | 3D    | 255/274 (93%)  | 255 (100%) | 0        | 100         | 100 |
| 9   | 3d    | 247/274 (90%)  | 247 (100%) | 0        | 100         | 100 |
| 10  | 3E    | 200/237 (84%)  | 200 (100%) | 0        | 100         | 100 |
| 10  | 3e    | 92/237 (39%)   | 92 (100%)  | 0        | 100         | 100 |
| 11  | 3F    | 80/81 (99%)    | 80 (100%)  | 0        | 100         | 100 |
| 11  | 3f    | 69/81 (85%)    | 69 (100%)  | 0        | 100         | 100 |
| 12  | 3G    | 269/289 (93%)  | 269 (100%) | 0        | 100         | 100 |
| 12  | 3g    | 278/289 (96%)  | 278 (100%) | 0        | 100         | 100 |
| 13  | 3H    | 117/118 (99%)  | 117 (100%) | 0        | 100         | 100 |
| 13  | 3h    | 112/118 (95%)  | 112 (100%) | 0        | 100         | 100 |
| 14  | 3I    | 104/109 (95%)  | 104 (100%) | 0        | 100         | 100 |
| 14  | 3i    | 102/109 (94%)  | 102 (100%) | 0        | 100         | 100 |
| 15  | 3J    | 53/56 (95%)    | 53 (100%)  | 0        | 100         | 100 |
| 15  | 3j    | 47/56 (84%)    | 47 (100%)  | 0        | 100         | 100 |
| 16  | 3M    | 16/16 (100%)   | 16 (100%)  | 0        | 100         | 100 |
| 17  | 3l    | 1/1 (100%)     | 1 (100%)   | 0        | 100         | 100 |
| 18  | 3m    | 7/7 (100%)     | 7 (100%)   | 0        | 100         | 100 |
| 19  | 4     | 463/463 (100%) | 463 (100%) | 0        | 100         | 100 |
| 20  | 4L    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 21  | 5     | 533/694 (77%)  | 533 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 22  | 5B    | 98/98 (100%)   | 98 (100%)  | 0        | 100         | 100 |
| 23  | 6     | 233/244 (96%)  | 233 (100%) | 0        | 100         | 100 |
| 24  | A2    | 82/93 (88%)    | 82 (100%)  | 0        | 100         | 100 |
| 25  | A5    | 144/186 (77%)  | 144 (100%) | 0        | 100         | 100 |
| 26  | A6    | 154/154 (100%) | 154 (100%) | 0        | 100         | 100 |
| 27  | A7    | 256/257 (100%) | 256 (100%) | 0        | 100         | 100 |
| 28  | A9    | 288/311 (93%)  | 288 (100%) | 0        | 100         | 100 |
| 29  | AB    | 104/129 (81%)  | 104 (100%) | 0        | 100         | 100 |
| 30  | AC    | 88/119 (74%)   | 88 (100%)  | 0        | 100         | 100 |
| 31  | AL    | 169/170 (99%)  | 169 (100%) | 0        | 100         | 100 |
| 32  | AM    | 142/156 (91%)  | 142 (100%) | 0        | 100         | 100 |
| 33  | B7    | 97/99 (98%)    | 97 (100%)  | 0        | 100         | 100 |
| 34  | B8    | 151/180 (84%)  | 151 (100%) | 0        | 100         | 100 |
| 35  | BL    | 160/172 (93%)  | 160 (100%) | 0        | 100         | 100 |
| 37  | C1    | 194/218 (89%)  | 194 (100%) | 0        | 100         | 100 |
| 38  | C2    | 165/197 (84%)  | 165 (100%) | 0        | 100         | 100 |
| 39  | C3    | 309/309 (100%) | 309 (100%) | 0        | 100         | 100 |
| 40  | TD    | 63/65 (97%)    | 63 (100%)  | 0        | 100         | 100 |
| 41  | J1    | 220/270 (82%)  | 220 (100%) | 0        | 100         | 100 |
| 42  | FX    | 130/152 (86%)  | 130 (100%) | 0        | 100         | 100 |
| 43  | T2    | 230/280 (82%)  | 230 (100%) | 0        | 100         | 100 |
| 44  | T1    | 421/454 (93%)  | 421 (100%) | 0        | 100         | 100 |
| 45  | A1    | 87/89 (98%)    | 87 (100%)  | 0        | 100         | 100 |
| 46  | X1    | 132/133 (99%)  | 132 (100%) | 0        | 100         | 100 |
| 47  | T6    | 97/131 (74%)   | 97 (100%)  | 0        | 100         | 100 |
| 48  | T5    | 115/179 (64%)  | 115 (100%) | 0        | 100         | 100 |
| 49  | R     | 98/98 (100%)   | 98 (100%)  | 0        | 100         | 100 |
| 50  | S1    | 588/617 (95%)  | 588 (100%) | 0        | 100         | 100 |
| 51  | S2    | 399/399 (100%) | 399 (100%) | 0        | 100         | 100 |
| 52  | S3    | 191/191 (100%) | 190 (100%) | 1 (0%)   | 81          | 92  |
| 53  | S4    | 157/163 (96%)  | 157 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Rotameric    | Outliers | Percentiles |     |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 54  | S6    | 80/116 (69%)      | 80 (100%)    | 0        | 100         | 100 |
| 55  | S7    | 137/137 (100%)    | 137 (100%)   | 0        | 100         | 100 |
| 56  | S8    | 197/215 (92%)     | 197 (100%)   | 0        | 100         | 100 |
| 57  | B9    | 169/172 (98%)     | 169 (100%)   | 0        | 100         | 100 |
| 58  | TX    | 128/147 (87%)     | 128 (100%)   | 0        | 100         | 100 |
| 59  | A8    | 121/224 (54%)     | 120 (99%)    | 1 (1%)   | 73          | 88  |
| 60  | TB    | 82/97 (84%)       | 82 (100%)    | 0        | 100         | 100 |
| 61  | V1    | 362/392 (92%)     | 362 (100%)   | 0        | 100         | 100 |
| 62  | V2    | 205/236 (87%)     | 205 (100%)   | 0        | 100         | 100 |
| 63  | B6    | 64/117 (55%)      | 64 (100%)    | 0        | 100         | 100 |
| 64  | BM    | 125/182 (69%)     | 125 (100%)   | 0        | 100         | 100 |
| 65  | C4    | 88/89 (99%)       | 88 (100%)    | 0        | 100         | 100 |
| 66  | AN    | 199/199 (100%)    | 199 (100%)   | 0        | 100         | 100 |
| 67  | B4    | 94/94 (100%)      | 94 (100%)    | 0        | 100         | 100 |
| 68  | T4    | 151/190 (80%)     | 151 (100%)   | 0        | 100         | 100 |
| 69  | T8    | 116/122 (95%)     | 116 (100%)   | 0        | 100         | 100 |
| 70  | B2    | 102/109 (94%)     | 102 (100%)   | 0        | 100         | 100 |
| 71  | T3    | 267/275 (97%)     | 267 (100%)   | 0        | 100         | 100 |
| 72  | P1    | 206/223 (92%)     | 206 (100%)   | 0        | 100         | 100 |
| 73  | B3    | 63/74 (85%)       | 63 (100%)    | 0        | 100         | 100 |
| 74  | TA    | 94/94 (100%)      | 94 (100%)    | 0        | 100         | 100 |
| 75  | S5    | 76/83 (92%)       | 76 (100%)    | 0        | 100         | 100 |
| 76  | TC    | 82/84 (98%)       | 82 (100%)    | 0        | 100         | 100 |
| 77  | P2    | 158/178 (89%)     | 158 (100%)   | 0        | 100         | 100 |
| 78  | A3    | 107/114 (94%)     | 107 (100%)   | 0        | 100         | 100 |
| 79  | T9    | 118/121 (98%)     | 118 (100%)   | 0        | 100         | 100 |
| 80  | TE    | 44/63 (70%)       | 44 (100%)    | 0        | 100         | 100 |
| 81  | T7    | 124/125 (99%)     | 124 (100%)   | 0        | 100         | 100 |
| All | All   | 15962/17605 (91%) | 15960 (100%) | 2 (0%)   | 100         | 100 |

All (2) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 52  | S3    | 3   | ASN  |
| 59  | A8    | 187 | ASN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 196 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44  | T1    | 359 | ASN  |
| 58  | TX    | 119 | ASN  |
| 44  | T1    | 450 | GLN  |
| 50  | S1    | 371 | GLN  |
| 61  | V1    | 168 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 104 ligands modelled in this entry, 3 are monoatomic - leaving 101 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 | $\# Z  > 2$ |
| 82  | CDL  | C4    | 401 | -    | 97,97,99     | 0.30 | 0           | 103,109,111 | 0.33 | 0           |
| 82  | CDL  | TD    | 101 | -    | 65,65,99     | 0.36 | 0           | 71,77,111   | 0.36 | 0           |
| 83  | PC1  | 3I    | 602 | -    | 45,45,53     | 0.32 | 0           | 51,53,61    | 0.30 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 83  | PC1  | X1    | 201 | -    | 48,48,53     | 0.30 | 0        | 54,56,61    | 0.35 | 0        |
| 83  | PC1  | 3j    | 101 | -    | 35,35,53     | 0.34 | 0        | 41,43,61    | 0.33 | 0        |
| 82  | CDL  | 1     | 301 | -    | 49,49,99     | 0.41 | 0        | 55,61,111   | 0.35 | 0        |
| 82  | CDL  | 3H    | 202 | -    | 61,61,99     | 0.37 | 0        | 67,73,111   | 0.36 | 0        |
| 88  | 3PE  | T4    | 301 | -    | 24,24,50     | 0.42 | 0        | 27,29,55    | 0.37 | 0        |
| 83  | PC1  | 3I    | 601 | -    | 31,31,53     | 0.38 | 0        | 37,39,61    | 0.36 | 0        |
| 82  | CDL  | 5     | 803 | -    | 89,89,99     | 0.31 | 0        | 95,101,111  | 0.26 | 0        |
| 88  | 3PE  | 4     | 602 | -    | 35,35,50     | 0.35 | 0        | 38,40,55    | 0.33 | 0        |
| 85  | U10  | 5B    | 202 | -    | 63,63,63     | 2.19 | 24 (38%) | 78,79,79    | 1.72 | 22 (28%) |
| 93  | SF4  | S8    | 302 | 56   | 0,12,12      | -    | -        | -           | -    | -        |
| 82  | CDL  | T7    | 201 | -    | 47,47,99     | 0.42 | 0        | 53,59,111   | 0.35 | 0        |
| 82  | CDL  | 3I    | 604 | -    | 36,36,99     | 0.43 | 0        | 42,48,111   | 0.39 | 0        |
| 82  | CDL  | 5     | 805 | -    | 95,95,99     | 0.31 | 0        | 101,107,111 | 0.36 | 0        |
| 82  | CDL  | B4    | 201 | -    | 38,38,99     | 0.42 | 0        | 43,49,111   | 0.40 | 0        |
| 83  | PC1  | C4    | 403 | -    | 31,31,53     | 0.37 | 0        | 37,39,61    | 0.41 | 0        |
| 91  | ZMP  | AB    | 201 | 29   | 28,33,36     | 0.72 | 1 (3%)   | 32,40,45    | 3.80 | 6 (18%)  |
| 92  | ADP  | B8    | 602 | -    | 28,29,29     | 1.40 | 4 (14%)  | 43,45,45    | 1.84 | 9 (20%)  |
| 87  | FES  | FX    | 201 | 42   | 0,4,4        | -    | -        | -           | -    | -        |
| 93  | SF4  | S7    | 201 | 55   | 0,12,12      | -    | -        | -           | -    | -        |
| 87  | FES  | 3E    | 301 | 10   | 0,4,4        | -    | -        | -           | -    | -        |
| 82  | CDL  | B8    | 603 | -    | 44,44,99     | 0.43 | 0        | 50,56,111   | 0.36 | 0        |
| 84  | HEM  | 3C    | 602 | 8    | 50,50,50     | 1.30 | 7 (14%)  | 67,82,82    | 1.56 | 11 (16%) |
| 88  | 3PE  | T8    | 201 | -    | 38,38,50     | 0.33 | 0        | 41,43,55    | 0.31 | 0        |
| 85  | U10  | 3C    | 605 | -    | 25,25,63     | 2.84 | 9 (36%)  | 24,29,79    | 1.99 | 8 (33%)  |
| 82  | CDL  | 3G    | 401 | -    | 65,65,99     | 0.36 | 0        | 71,77,111   | 0.32 | 0        |
| 82  | CDL  | A1    | 101 | -    | 52,52,99     | 0.40 | 0        | 58,64,111   | 0.34 | 0        |
| 82  | CDL  | 2B    | 201 | -    | 52,52,99     | 0.40 | 0        | 58,64,111   | 0.33 | 0        |
| 82  | CDL  | 3I    | 603 | -    | 70,70,99     | 0.35 | 0        | 76,82,111   | 0.35 | 0        |
| 83  | PC1  | 3C    | 604 | -    | 45,45,53     | 0.31 | 0        | 51,53,61    | 0.31 | 0        |
| 82  | CDL  | T1    | 602 | -    | 54,54,99     | 0.39 | 0        | 60,66,111   | 0.41 | 0        |
| 82  | CDL  | 3i    | 201 | -    | 70,70,99     | 0.35 | 0        | 76,82,111   | 0.34 | 0        |
| 93  | SF4  | V1    | 500 | 61   | 0,12,12      | -    | -        | -           | -    | -        |
| 83  | PC1  | TC    | 101 | -    | 41,41,53     | 0.32 | 0        | 47,49,61    | 0.31 | 0        |
| 88  | 3PE  | 4     | 601 | -    | 46,46,50     | 0.32 | 0        | 49,51,55    | 0.37 | 0        |
| 83  | PC1  | T1    | 601 | -    | 25,25,53     | 0.40 | 0        | 31,33,61    | 0.38 | 0        |
| 87  | FES  | V2    | 300 | 62   | 0,4,4        | -    | -        | -           | -    | -        |
| 86  | HEC  | 3d    | 401 | 9    | 46,50,50     | 1.92 | 10 (21%) | 58,82,82    | 1.83 | 8 (13%)  |
| 88  | 3PE  | A3    | 201 | -    | 44,44,50     | 0.33 | 0        | 47,49,55    | 0.40 | 0        |
| 88  | 3PE  | 3E    | 303 | -    | 33,33,50     | 0.37 | 0        | 36,38,55    | 0.34 | 0        |
| 88  | 3PE  | B8    | 601 | -    | 35,35,50     | 0.35 | 0        | 38,40,55    | 0.33 | 0        |
| 83  | PC1  | 3E    | 304 | -    | 23,23,53     | 0.41 | 0        | 29,31,61    | 0.38 | 0        |
| 83  | PC1  | 5     | 807 | -    | 53,53,53     | 0.29 | 0        | 59,61,61    | 0.30 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 83  | PC1  | 3c    | 506 | -    | 37,37,53     | 0.34 | 0        | 43,45,61    | 0.32 | 0        |
| 82  | CDL  | BM    | 301 | -    | 85,85,99     | 0.32 | 0        | 91,97,111   | 0.31 | 0        |
| 88  | 3PE  | 5     | 804 | -    | 36,36,50     | 0.34 | 0        | 39,41,55    | 0.31 | 0        |
| 83  | PC1  | 3C    | 606 | -    | 43,43,53     | 0.31 | 0        | 49,51,61    | 0.30 | 0        |
| 83  | PC1  | 3g    | 401 | -    | 32,32,53     | 0.36 | 0        | 38,40,61    | 0.36 | 0        |
| 93  | SF4  | S1    | 802 | 50   | 0,12,12      | -    | -        | -           | -    | -        |
| 82  | CDL  | 3c    | 504 | -    | 63,63,99     | 0.36 | 0        | 69,75,111   | 0.31 | 0        |
| 82  | CDL  | 3c    | 505 | -    | 55,55,99     | 0.38 | 0        | 61,67,111   | 0.33 | 0        |
| 85  | U10  | 3H    | 201 | -    | 29,29,63     | 2.72 | 13 (44%) | 36,38,79    | 1.60 | 8 (22%)  |
| 88  | 3PE  | P1    | 402 | -    | 46,46,50     | 0.32 | 0        | 49,51,55    | 0.32 | 0        |
| 82  | CDL  | 3C    | 603 | -    | 64,64,99     | 0.36 | 0        | 70,76,111   | 0.35 | 0        |
| 84  | HEM  | 3C    | 601 | 8    | 50,50,50     | 1.29 | 8 (16%)  | 67,82,82    | 1.68 | 12 (17%) |
| 90  | NDP  | A9    | 401 | -    | 51,52,52     | 0.35 | 0        | 71,80,80    | 0.37 | 0        |
| 88  | 3PE  | 5B    | 201 | -    | 23,23,50     | 0.43 | 0        | 26,28,55    | 0.36 | 0        |
| 82  | CDL  | 3B    | 701 | -    | 77,77,99     | 0.33 | 0        | 83,89,111   | 0.31 | 0        |
| 94  | FMN  | V1    | 501 | -    | 33,33,33     | 0.21 | 0        | 48,50,50    | 0.34 | 0        |
| 83  | PC1  | 3J    | 101 | -    | 36,36,53     | 0.36 | 0        | 42,44,61    | 0.40 | 0        |
| 87  | FES  | S1    | 803 | 50   | 0,4,4        | -    | -        | -           | -    | -        |
| 88  | 3PE  | 3d    | 402 | -    | 46,46,50     | 0.32 | 0        | 49,51,55    | 0.39 | 0        |
| 83  | PC1  | AM    | 201 | -    | 29,29,53     | 0.38 | 0        | 35,37,61    | 0.34 | 0        |
| 88  | 3PE  | AN    | 301 | -    | 44,44,50     | 0.32 | 0        | 47,49,55    | 0.32 | 0        |
| 88  | 3PE  | 5     | 806 | -    | 34,34,50     | 0.35 | 0        | 37,39,55    | 0.32 | 0        |
| 82  | CDL  | P2    | 201 | -    | 81,81,99     | 0.33 | 0        | 87,93,111   | 0.28 | 0        |
| 83  | PC1  | 5     | 802 | -    | 38,38,53     | 0.33 | 0        | 44,46,61    | 0.33 | 0        |
| 83  | PC1  | AN    | 303 | -    | 35,35,53     | 0.35 | 0        | 41,43,61    | 0.39 | 0        |
| 88  | 3PE  | TA    | 201 | -    | 25,25,50     | 0.41 | 0        | 28,30,55    | 0.37 | 0        |
| 83  | PC1  | B6    | 201 | -    | 51,51,53     | 0.29 | 0        | 57,59,61    | 0.30 | 0        |
| 82  | CDL  | 3H    | 203 | -    | 65,65,99     | 0.36 | 0        | 71,77,111   | 0.31 | 0        |
| 82  | CDL  | 3b    | 602 | -    | 67,67,99     | 0.36 | 0        | 73,79,111   | 0.37 | 0        |
| 84  | HEM  | 3c    | 502 | 8    | 50,50,50     | 1.30 | 8 (16%)  | 67,82,82    | 1.60 | 10 (14%) |
| 82  | CDL  | 3     | 202 | -    | 43,43,99     | 0.43 | 0        | 49,55,111   | 0.37 | 0        |
| 93  | SF4  | S1    | 801 | 50   | 0,12,12      | -    | -        | -           | -    | -        |
| 83  | PC1  | B2    | 201 | -    | 47,47,53     | 0.31 | 0        | 53,55,61    | 0.35 | 0        |
| 83  | PC1  | 3E    | 302 | -    | 53,53,53     | 0.29 | 0        | 59,61,61    | 0.32 | 0        |
| 86  | HEC  | 3D    | 401 | 9    | 46,50,50     | 1.93 | 10 (21%) | 58,82,82    | 1.80 | 8 (13%)  |
| 83  | PC1  | 3e    | 301 | -    | 49,49,53     | 0.31 | 0        | 55,57,61    | 0.30 | 0        |
| 83  | PC1  | 6     | 302 | -    | 53,53,53     | 0.29 | 0        | 59,61,61    | 0.31 | 0        |
| 88  | 3PE  | C4    | 402 | -    | 50,50,50     | 0.30 | 0        | 53,55,55    | 0.34 | 0        |
| 83  | PC1  | 3c    | 501 | -    | 30,30,53     | 0.38 | 0        | 36,38,61    | 0.45 | 0        |
| 83  | PC1  | 3C    | 607 | -    | 28,28,53     | 0.38 | 0        | 34,36,61    | 0.37 | 0        |
| 93  | SF4  | S8    | 301 | 56   | 0,12,12      | -    | -        | -           | -    | -        |
| 82  | CDL  | R     | 201 | -    | 83,83,99     | 0.32 | 0        | 89,95,111   | 0.31 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 84  | HEM  | 3c    | 503 | 8    | 50,50,50     | 1.30 | 7 (14%)  | 67,82,82    | 1.61 | 15 (22%) |
| 83  | PC1  | 3b    | 601 | -    | 29,29,53     | 0.39 | 0        | 35,37,61    | 0.48 | 0        |
| 83  | PC1  | 3     | 201 | -    | 30,30,53     | 0.37 | 0        | 36,38,61    | 0.36 | 0        |
| 83  | PC1  | 6     | 301 | -    | 38,38,53     | 0.33 | 0        | 44,46,61    | 0.33 | 0        |
| 88  | 3PE  | S8    | 303 | -    | 40,40,50     | 0.34 | 0        | 43,45,55    | 0.32 | 0        |
| 83  | PC1  | J1    | 400 | -    | 39,39,53     | 0.33 | 0        | 45,47,61    | 0.35 | 0        |
| 88  | 3PE  | AN    | 302 | -    | 34,34,50     | 0.36 | 0        | 37,39,55    | 0.33 | 0        |
| 83  | PC1  | 1     | 302 | -    | 35,35,53     | 0.35 | 0        | 41,43,61    | 0.35 | 0        |
| 82  | CDL  | AN    | 304 | -    | 52,52,99     | 0.39 | 0        | 58,64,111   | 0.35 | 0        |
| 83  | PC1  | 3F    | 102 | -    | 21,21,53     | 0.39 | 0        | 27,29,61    | 0.43 | 0        |
| 82  | CDL  | AM    | 202 | -    | 61,61,99     | 0.37 | 0        | 67,73,111   | 0.31 | 0        |
| 83  | PC1  | 5     | 801 | -    | 53,53,53     | 0.29 | 0        | 59,61,61    | 0.28 | 0        |
| 83  | PC1  | P1    | 401 | -    | 39,39,53     | 0.33 | 0        | 45,47,61    | 0.30 | 0        |
| 82  | CDL  | AL    | 301 | -    | 52,52,99     | 0.40 | 0        | 58,64,111   | 0.33 | 0        |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions       | Rings   |
|-----|------|-------|-----|------|---------|----------------|---------|
| 82  | CDL  | C4    | 401 | -    | -       | 21/108/108/110 | -       |
| 82  | CDL  | TD    | 101 | -    | -       | 14/76/76/110   | -       |
| 83  | PC1  | 3I    | 602 | -    | -       | 7/49/49/57     | -       |
| 83  | PC1  | X1    | 201 | -    | -       | 12/52/52/57    | -       |
| 83  | PC1  | 3j    | 101 | -    | -       | 5/39/39/57     | -       |
| 82  | CDL  | 1     | 301 | -    | -       | 11/60/60/110   | -       |
| 82  | CDL  | 3H    | 202 | -    | -       | 17/72/72/110   | -       |
| 88  | 3PE  | T4    | 301 | -    | -       | 4/28/28/54     | -       |
| 83  | PC1  | 3I    | 601 | -    | -       | 9/35/35/57     | -       |
| 82  | CDL  | 5     | 803 | -    | -       | 22/100/100/110 | -       |
| 88  | 3PE  | 4     | 602 | -    | -       | 7/39/39/54     | -       |
| 85  | U10  | 5B    | 202 | -    | -       | 18/63/87/87    | 0/1/1/1 |
| 93  | SF4  | S8    | 302 | 56   | -       | -              | 0/6/5/5 |
| 82  | CDL  | T7    | 201 | -    | -       | 14/58/58/110   | -       |
| 82  | CDL  | 3I    | 604 | -    | -       | 6/44/44/110    | -       |
| 82  | CDL  | 5     | 805 | -    | -       | 20/106/106/110 | -       |
| 82  | CDL  | B4    | 201 | -    | -       | 10/44/44/110   | -       |
| 83  | PC1  | C4    | 403 | -    | -       | 13/35/35/57    | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions     | Rings   |
|-----|------|-------|-----|------|---------|--------------|---------|
| 91  | ZMP  | AB    | 201 | 29   | -       | 8/38/40/43   | -       |
| 92  | ADP  | B8    | 602 | -    | -       | 1/16/32/32   | 0/3/3/3 |
| 87  | FES  | FX    | 201 | 42   | -       | -            | 0/1/1/1 |
| 93  | SF4  | S7    | 201 | 55   | -       | -            | 0/6/5/5 |
| 87  | FES  | 3E    | 301 | 10   | -       | -            | 0/1/1/1 |
| 82  | CDL  | B8    | 603 | -    | -       | 4/55/55/110  | -       |
| 84  | HEM  | 3C    | 602 | 8    | -       | 5/14/54/54   | -       |
| 88  | 3PE  | T8    | 201 | -    | -       | 9/42/42/54   | -       |
| 85  | U10  | 3C    | 605 | -    | -       | 12/28/28/87  | -       |
| 82  | CDL  | 3G    | 401 | -    | -       | 19/76/76/110 | -       |
| 82  | CDL  | A1    | 101 | -    | -       | 15/63/63/110 | -       |
| 82  | CDL  | 2B    | 201 | -    | -       | 9/63/63/110  | -       |
| 82  | CDL  | 3I    | 603 | -    | -       | 23/81/81/110 | -       |
| 83  | PC1  | 3C    | 604 | -    | -       | 14/49/49/57  | -       |
| 82  | CDL  | T1    | 602 | -    | -       | 10/65/65/110 | -       |
| 82  | CDL  | 3i    | 201 | -    | -       | 15/81/81/110 | -       |
| 93  | SF4  | V1    | 500 | 61   | -       | -            | 0/6/5/5 |
| 83  | PC1  | TC    | 101 | -    | -       | 7/45/45/57   | -       |
| 88  | 3PE  | 4     | 601 | -    | -       | 6/50/50/54   | -       |
| 83  | PC1  | T1    | 601 | -    | -       | 11/29/29/57  | -       |
| 87  | FES  | V2    | 300 | 62   | -       | -            | 0/1/1/1 |
| 86  | HEC  | 3d    | 401 | 9    | -       | 7/14/54/54   | -       |
| 88  | 3PE  | A3    | 201 | -    | -       | 6/48/48/54   | -       |
| 88  | 3PE  | 3E    | 303 | -    | -       | 7/37/37/54   | -       |
| 88  | 3PE  | B8    | 601 | -    | -       | 8/39/39/54   | -       |
| 83  | PC1  | 3E    | 304 | -    | -       | 9/26/26/57   | -       |
| 83  | PC1  | 5     | 807 | -    | -       | 10/57/57/57  | -       |
| 83  | PC1  | 3c    | 506 | -    | -       | 13/41/41/57  | -       |
| 82  | CDL  | BM    | 301 | -    | -       | 19/96/96/110 | -       |
| 88  | 3PE  | 5     | 804 | -    | -       | 5/40/40/54   | -       |
| 83  | PC1  | 3C    | 606 | -    | -       | 6/47/47/57   | -       |
| 83  | PC1  | 3g    | 401 | -    | -       | 2/36/36/57   | -       |
| 93  | SF4  | S1    | 802 | 50   | -       | -            | 0/6/5/5 |
| 82  | CDL  | 3c    | 504 | -    | -       | 15/74/74/110 | -       |
| 82  | CDL  | 3c    | 505 | -    | -       | 16/66/66/110 | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions     | Rings   |
|-----|------|-------|-----|------|---------|--------------|---------|
| 85  | U10  | 3H    | 201 | -    | -       | 6/23/47/87   | 0/1/1/1 |
| 88  | 3PE  | P1    | 402 | -    | -       | 11/50/50/54  | -       |
| 82  | CDL  | 3C    | 603 | -    | -       | 20/75/75/110 | -       |
| 84  | HEM  | 3C    | 601 | 8    | -       | 5/14/54/54   | -       |
| 90  | NDP  | A9    | 401 | -    | -       | 3/34/77/77   | 0/5/5/5 |
| 88  | 3PE  | 5B    | 201 | -    | -       | 7/27/27/54   | -       |
| 82  | CDL  | 3B    | 701 | -    | -       | 23/88/88/110 | -       |
| 94  | FMN  | V1    | 501 | -    | -       | 1/18/18/18   | 0/3/3/3 |
| 83  | PC1  | 3J    | 101 | -    | -       | 16/40/40/57  | -       |
| 87  | FES  | S1    | 803 | 50   | -       | -            | 0/1/1/1 |
| 88  | 3PE  | 3d    | 402 | -    | -       | 11/50/50/54  | -       |
| 83  | PC1  | AM    | 201 | -    | -       | 12/33/33/57  | -       |
| 88  | 3PE  | AN    | 301 | -    | -       | 6/48/48/54   | -       |
| 88  | 3PE  | 5     | 806 | -    | -       | 6/38/38/54   | -       |
| 82  | CDL  | P2    | 201 | -    | -       | 20/92/92/110 | -       |
| 83  | PC1  | 5     | 802 | -    | -       | 7/42/42/57   | -       |
| 83  | PC1  | AN    | 303 | -    | -       | 7/39/39/57   | -       |
| 88  | 3PE  | TA    | 201 | -    | -       | 5/29/29/54   | -       |
| 83  | PC1  | B6    | 201 | -    | -       | 9/55/55/57   | -       |
| 82  | CDL  | 3H    | 203 | -    | -       | 11/76/76/110 | -       |
| 82  | CDL  | 3b    | 602 | -    | -       | 24/78/78/110 | -       |
| 84  | HEM  | 3c    | 502 | 8    | -       | 7/14/54/54   | -       |
| 82  | CDL  | 3     | 202 | -    | -       | 7/54/54/110  | -       |
| 93  | SF4  | S1    | 801 | 50   | -       | -            | 0/6/5/5 |
| 83  | PC1  | B2    | 201 | -    | -       | 15/51/51/57  | -       |
| 83  | PC1  | 3E    | 302 | -    | -       | 21/57/57/57  | -       |
| 86  | HEC  | 3D    | 401 | 9    | -       | 7/14/54/54   | -       |
| 83  | PC1  | 3e    | 301 | -    | -       | 6/53/53/57   | -       |
| 83  | PC1  | 6     | 302 | -    | -       | 11/57/57/57  | -       |
| 88  | 3PE  | C4    | 402 | -    | -       | 14/54/54/54  | -       |
| 83  | PC1  | 3c    | 501 | -    | -       | 7/34/34/57   | -       |
| 83  | PC1  | 3C    | 607 | -    | -       | 9/32/32/57   | -       |
| 93  | SF4  | S8    | 301 | 56   | -       | -            | 0/6/5/5 |
| 82  | CDL  | R     | 201 | -    | -       | 17/94/94/110 | -       |
| 84  | HEM  | 3c    | 503 | 8    | -       | 9/14/54/54   | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions     | Rings |
|-----|------|-------|-----|------|---------|--------------|-------|
| 83  | PC1  | 3b    | 601 | -    | -       | 15/33/33/57  | -     |
| 83  | PC1  | 3     | 201 | -    | -       | 6/34/34/57   | -     |
| 83  | PC1  | 6     | 301 | -    | -       | 6/42/42/57   | -     |
| 88  | 3PE  | S8    | 303 | -    | -       | 8/44/44/54   | -     |
| 83  | PC1  | J1    | 400 | -    | -       | 9/43/43/57   | -     |
| 88  | 3PE  | AN    | 302 | -    | -       | 8/38/38/54   | -     |
| 83  | PC1  | 1     | 302 | -    | -       | 12/39/39/57  | -     |
| 82  | CDL  | AN    | 304 | -    | -       | 20/62/62/110 | -     |
| 83  | PC1  | 3F    | 102 | -    | -       | 8/23/23/57   | -     |
| 82  | CDL  | AM    | 202 | -    | -       | 14/72/72/110 | -     |
| 83  | PC1  | 5     | 801 | -    | -       | 6/57/57/57   | -     |
| 83  | PC1  | P1    | 401 | -    | -       | 15/43/43/57  | -     |
| 82  | CDL  | AL    | 301 | -    | -       | 15/63/63/110 | -     |

The worst 5 of 101 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 85  | 3H    | 201 | U10  | C6-C1   | 10.27 | 1.53        | 1.35     |
| 85  | 3C    | 605 | U10  | C6-C1   | 10.27 | 1.56        | 1.33     |
| 85  | 5B    | 202 | U10  | C6-C1   | 10.25 | 1.53        | 1.35     |
| 86  | 3D    | 401 | HEC  | CAC-C3C | 7.19  | 1.58        | 1.35     |
| 86  | 3d    | 401 | HEC  | CAC-C3C | 7.18  | 1.58        | 1.35     |

The worst 5 of 117 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 91  | AB    | 201 | ZMP  | C19-C18-C17 | -12.73 | 87.07       | 108.77   |
| 91  | AB    | 201 | ZMP  | C20-C18-C17 | -11.76 | 88.73       | 108.77   |
| 86  | 3d    | 401 | HEC  | CBB-CAB-C3B | -8.72  | 110.00      | 127.43   |
| 86  | 3D    | 401 | HEC  | CBB-CAB-C3B | -8.54  | 110.37      | 127.43   |
| 91  | AB    | 201 | ZMP  | C20-C18-C21 | 8.27   | 121.88      | 108.22   |

There are no chirality outliers.

5 of 983 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 82  | 1     | 301 | CDL  | CB2-OB2-PB2-OB3 |
| 82  | 1     | 301 | CDL  | OB5-CB3-CB4-OB6 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 82  | 2B    | 201 | CDL  | CA2-OA2-PA1-OA3 |
| 82  | 2B    | 201 | CDL  | CA2-OA2-PA1-OA5 |
| 82  | 2B    | 201 | CDL  | CB2-OB2-PB2-OB4 |

There are no ring outliers.

75 monomers are involved in 191 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 82  | C4    | 401 | CDL  | 6       | 0            |
| 82  | TD    | 101 | CDL  | 2       | 0            |
| 83  | X1    | 201 | PC1  | 2       | 0            |
| 83  | 3j    | 101 | PC1  | 1       | 0            |
| 82  | 1     | 301 | CDL  | 1       | 0            |
| 82  | 3H    | 202 | CDL  | 3       | 0            |
| 88  | T4    | 301 | 3PE  | 3       | 0            |
| 82  | 5     | 803 | CDL  | 6       | 0            |
| 85  | 5B    | 202 | U10  | 7       | 0            |
| 93  | S8    | 302 | SF4  | 2       | 0            |
| 82  | T7    | 201 | CDL  | 1       | 0            |
| 82  | 3I    | 604 | CDL  | 1       | 0            |
| 82  | 5     | 805 | CDL  | 8       | 0            |
| 82  | B4    | 201 | CDL  | 1       | 0            |
| 83  | C4    | 403 | PC1  | 1       | 0            |
| 91  | AB    | 201 | ZMP  | 4       | 0            |
| 92  | B8    | 602 | ADP  | 1       | 0            |
| 93  | S7    | 201 | SF4  | 1       | 0            |
| 82  | B8    | 603 | CDL  | 1       | 0            |
| 84  | 3C    | 602 | HEM  | 1       | 0            |
| 85  | 3C    | 605 | U10  | 4       | 0            |
| 82  | 3G    | 401 | CDL  | 2       | 0            |
| 82  | 3I    | 603 | CDL  | 1       | 0            |
| 83  | 3C    | 604 | PC1  | 2       | 0            |
| 82  | T1    | 602 | CDL  | 3       | 0            |
| 82  | 3i    | 201 | CDL  | 3       | 0            |
| 83  | TC    | 101 | PC1  | 4       | 0            |
| 88  | 4     | 601 | 3PE  | 2       | 0            |
| 87  | V2    | 300 | FES  | 1       | 0            |
| 86  | 3d    | 401 | HEC  | 1       | 0            |
| 88  | A3    | 201 | 3PE  | 4       | 0            |
| 88  | B8    | 601 | 3PE  | 3       | 0            |
| 83  | 3E    | 304 | PC1  | 1       | 0            |
| 83  | 5     | 807 | PC1  | 5       | 0            |

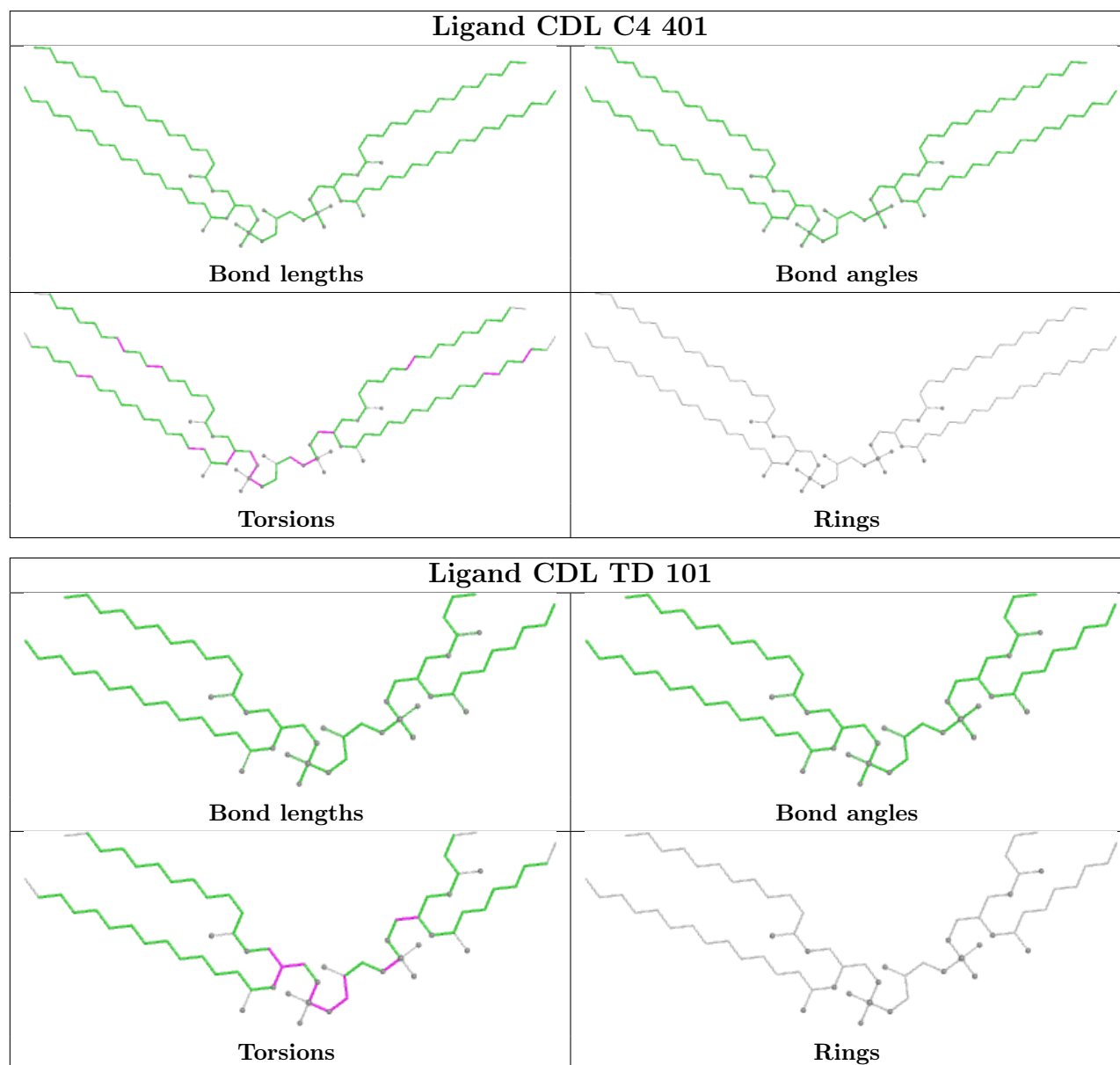
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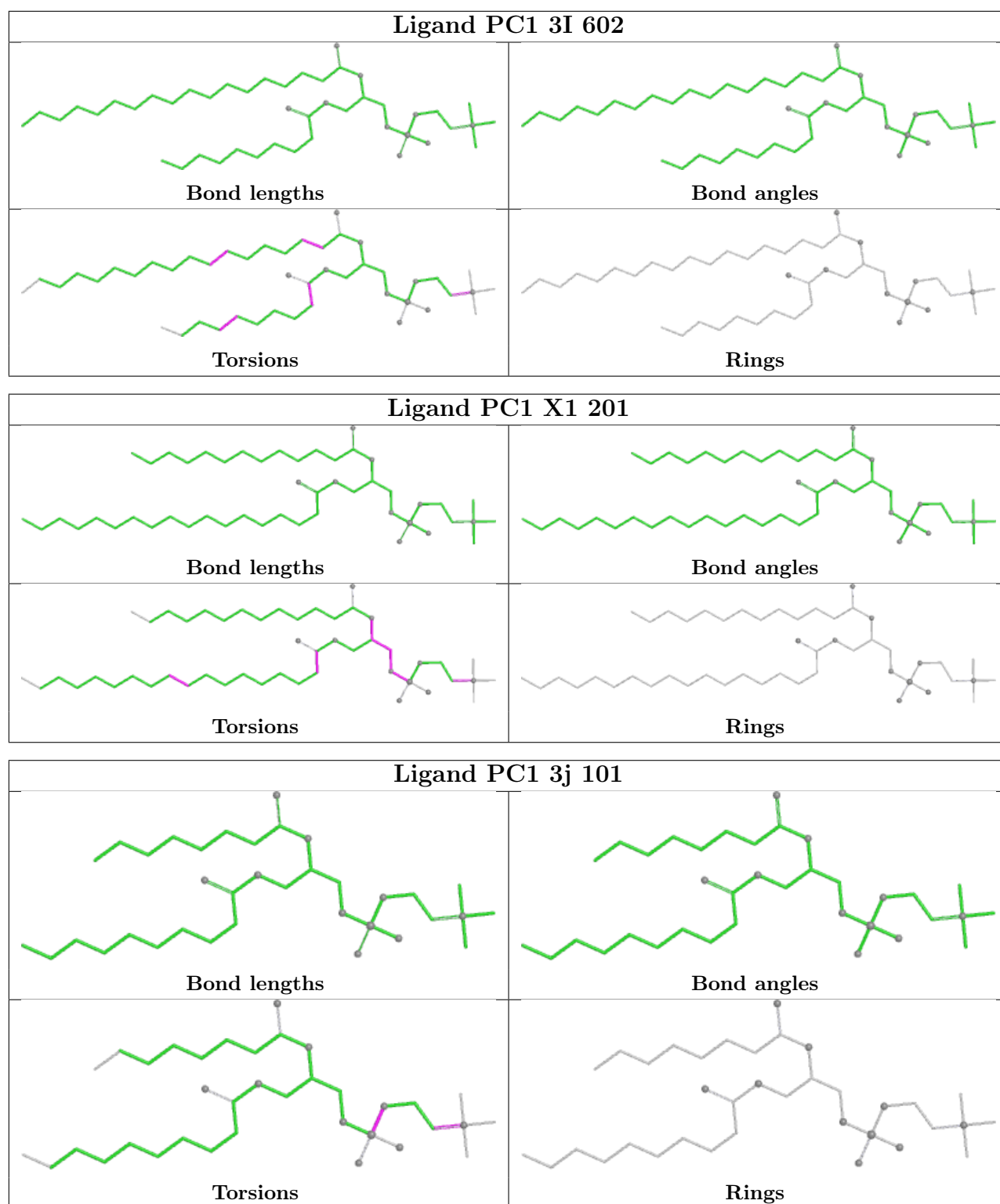
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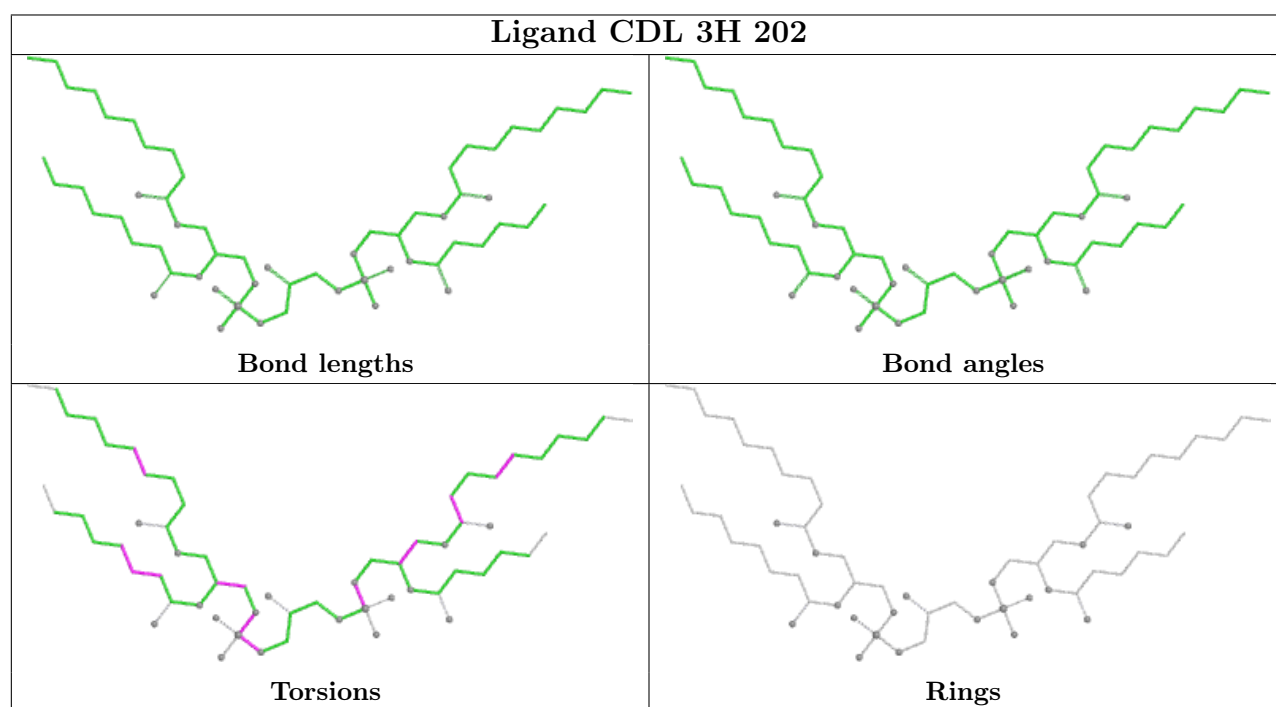
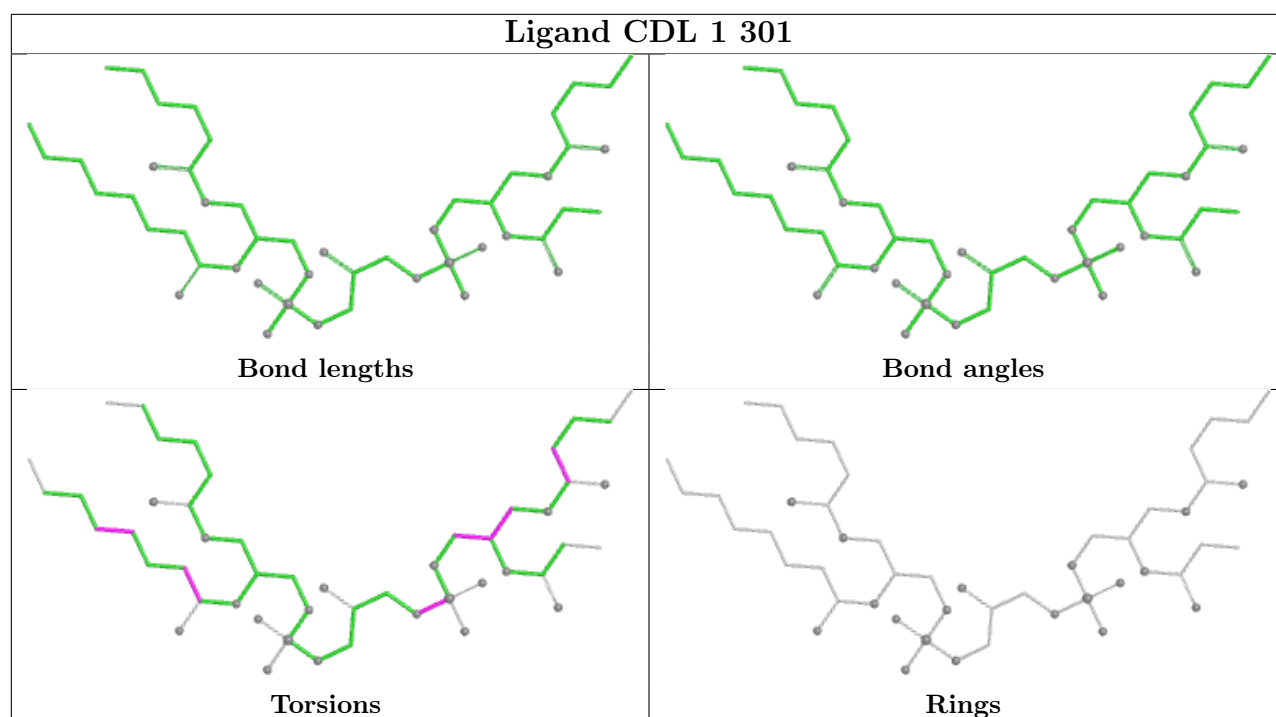
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 83  | 3c    | 506 | PC1  | 1       | 0            |
| 82  | BM    | 301 | CDL  | 9       | 0            |
| 88  | 5     | 804 | 3PE  | 2       | 0            |
| 83  | 3C    | 606 | PC1  | 4       | 0            |
| 83  | 3g    | 401 | PC1  | 2       | 0            |
| 93  | S1    | 802 | SF4  | 2       | 0            |
| 82  | 3c    | 505 | CDL  | 2       | 0            |
| 88  | P1    | 402 | 3PE  | 4       | 0            |
| 82  | 3C    | 603 | CDL  | 4       | 0            |
| 84  | 3C    | 601 | HEM  | 1       | 0            |
| 90  | A9    | 401 | NDP  | 1       | 0            |
| 82  | 3B    | 701 | CDL  | 5       | 0            |
| 94  | V1    | 501 | FMN  | 1       | 0            |
| 83  | 3J    | 101 | PC1  | 4       | 0            |
| 88  | 3d    | 402 | 3PE  | 3       | 0            |
| 83  | AM    | 201 | PC1  | 2       | 0            |
| 88  | AN    | 301 | 3PE  | 4       | 0            |
| 82  | P2    | 201 | CDL  | 3       | 0            |
| 83  | 5     | 802 | PC1  | 2       | 0            |
| 83  | AN    | 303 | PC1  | 1       | 0            |
| 83  | B6    | 201 | PC1  | 3       | 0            |
| 82  | 3b    | 602 | CDL  | 3       | 0            |
| 84  | 3c    | 502 | HEM  | 3       | 0            |
| 83  | B2    | 201 | PC1  | 7       | 0            |
| 83  | 3E    | 302 | PC1  | 7       | 0            |
| 83  | 3e    | 301 | PC1  | 2       | 0            |
| 83  | 6     | 302 | PC1  | 3       | 0            |
| 88  | C4    | 402 | 3PE  | 3       | 0            |
| 83  | 3c    | 501 | PC1  | 1       | 0            |
| 93  | S8    | 301 | SF4  | 1       | 0            |
| 82  | R     | 201 | CDL  | 3       | 0            |
| 84  | 3c    | 503 | HEM  | 4       | 0            |
| 83  | 3b    | 601 | PC1  | 1       | 0            |
| 83  | 6     | 301 | PC1  | 3       | 0            |
| 88  | S8    | 303 | 3PE  | 1       | 0            |
| 83  | J1    | 400 | PC1  | 1       | 0            |
| 88  | AN    | 302 | 3PE  | 1       | 0            |
| 82  | AN    | 304 | CDL  | 3       | 0            |
| 82  | AM    | 202 | CDL  | 7       | 0            |
| 83  | 5     | 801 | PC1  | 3       | 0            |
| 82  | AL    | 301 | CDL  | 3       | 0            |

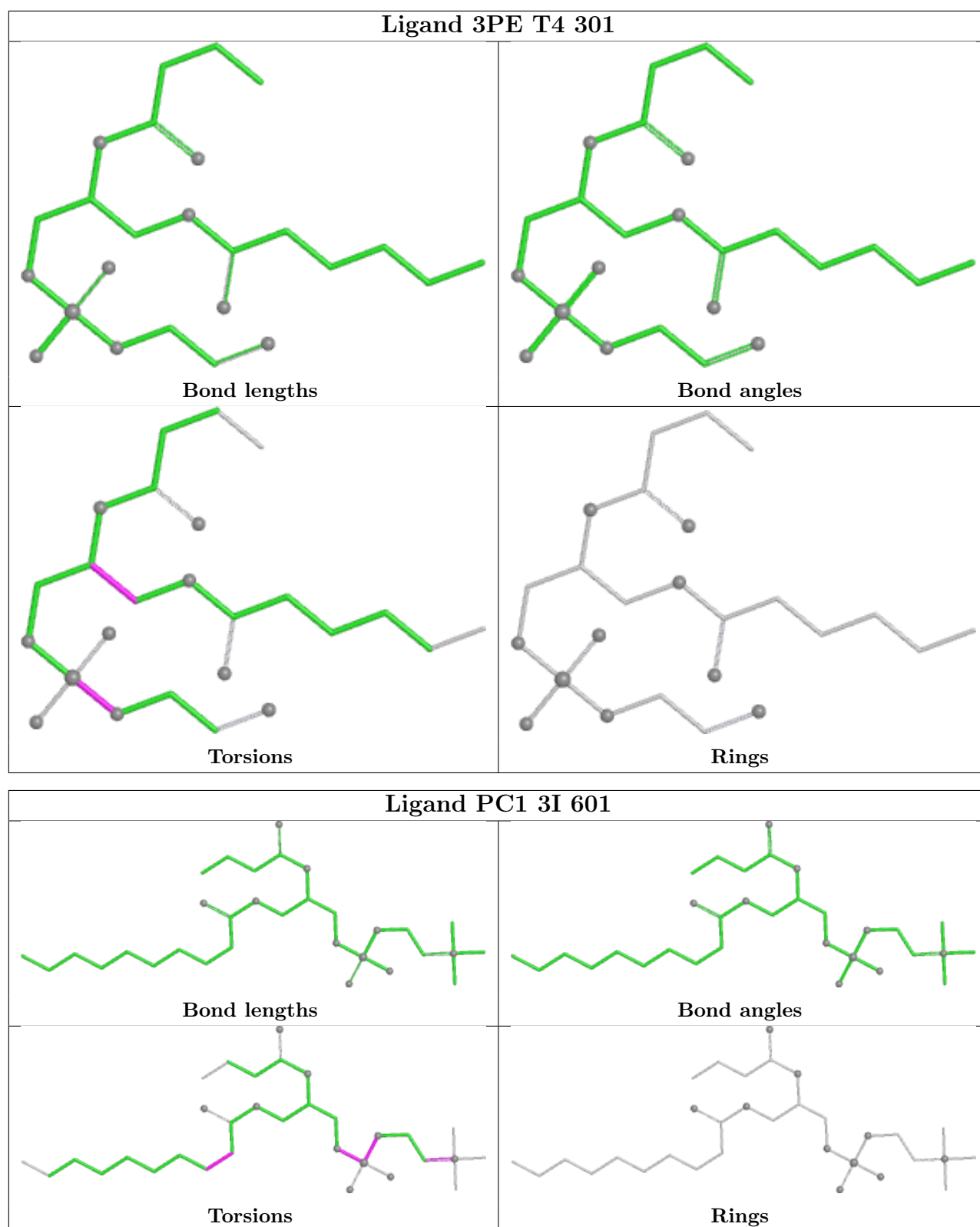
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

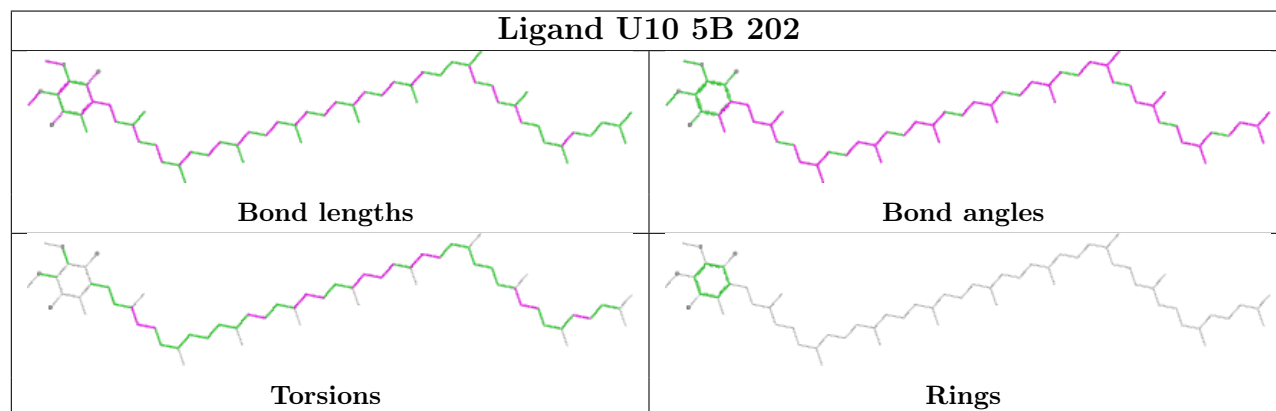
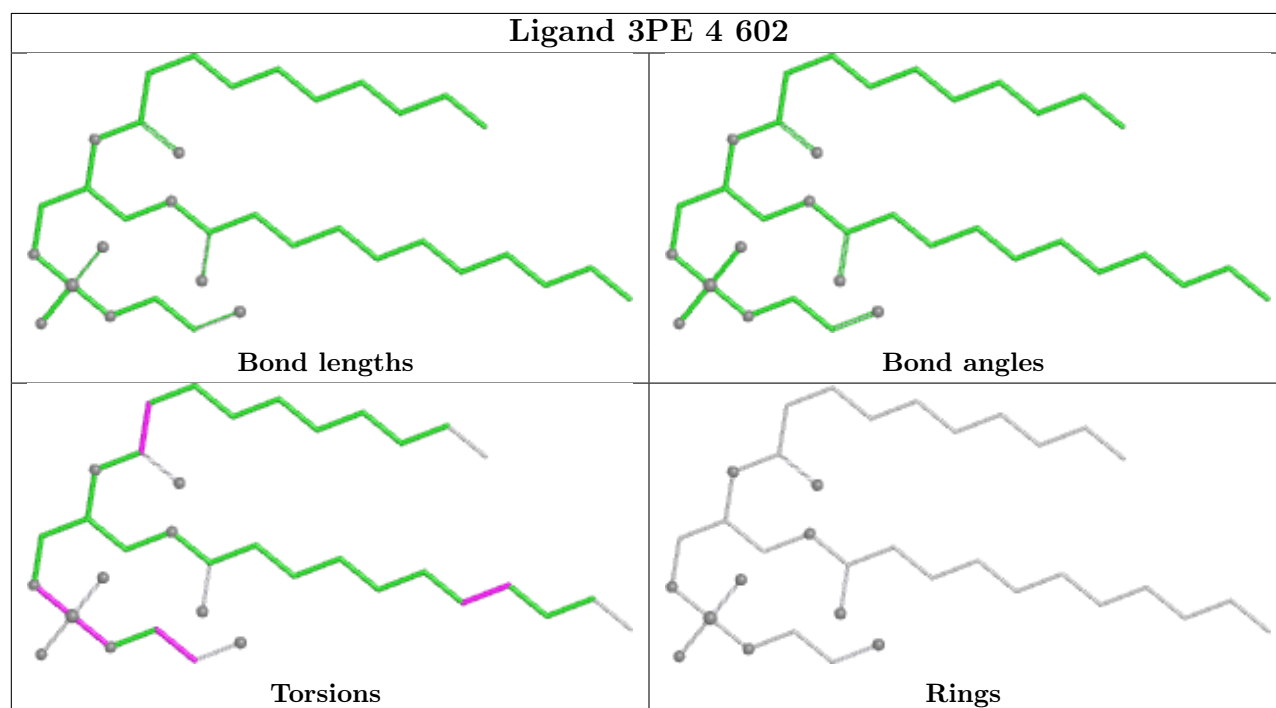
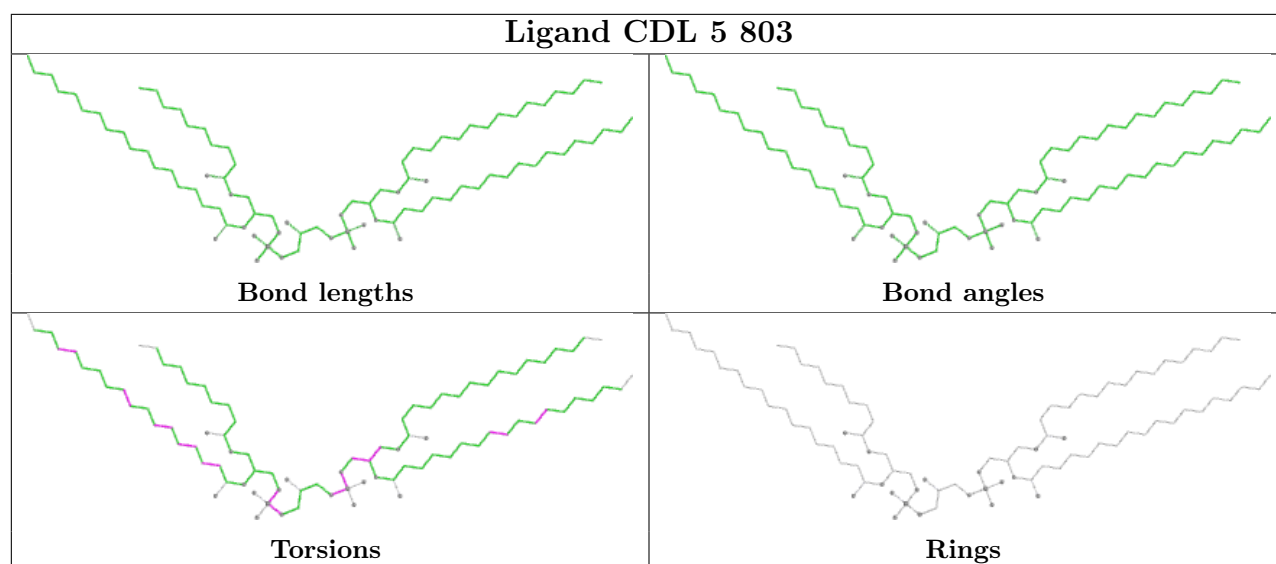
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within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

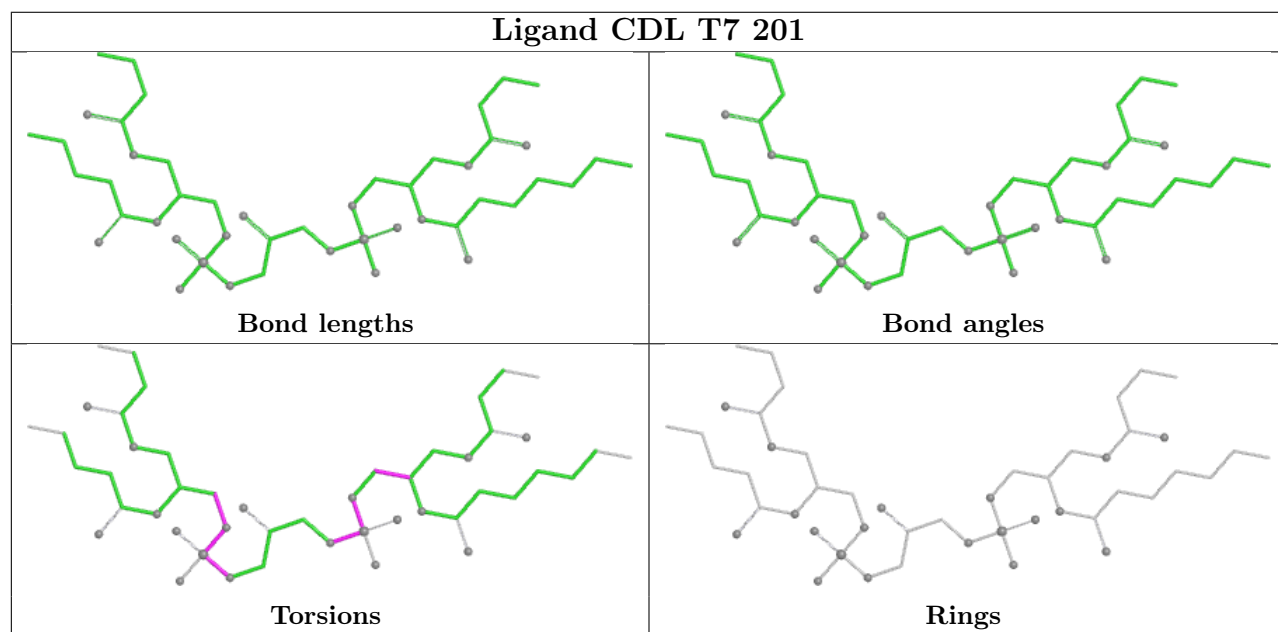
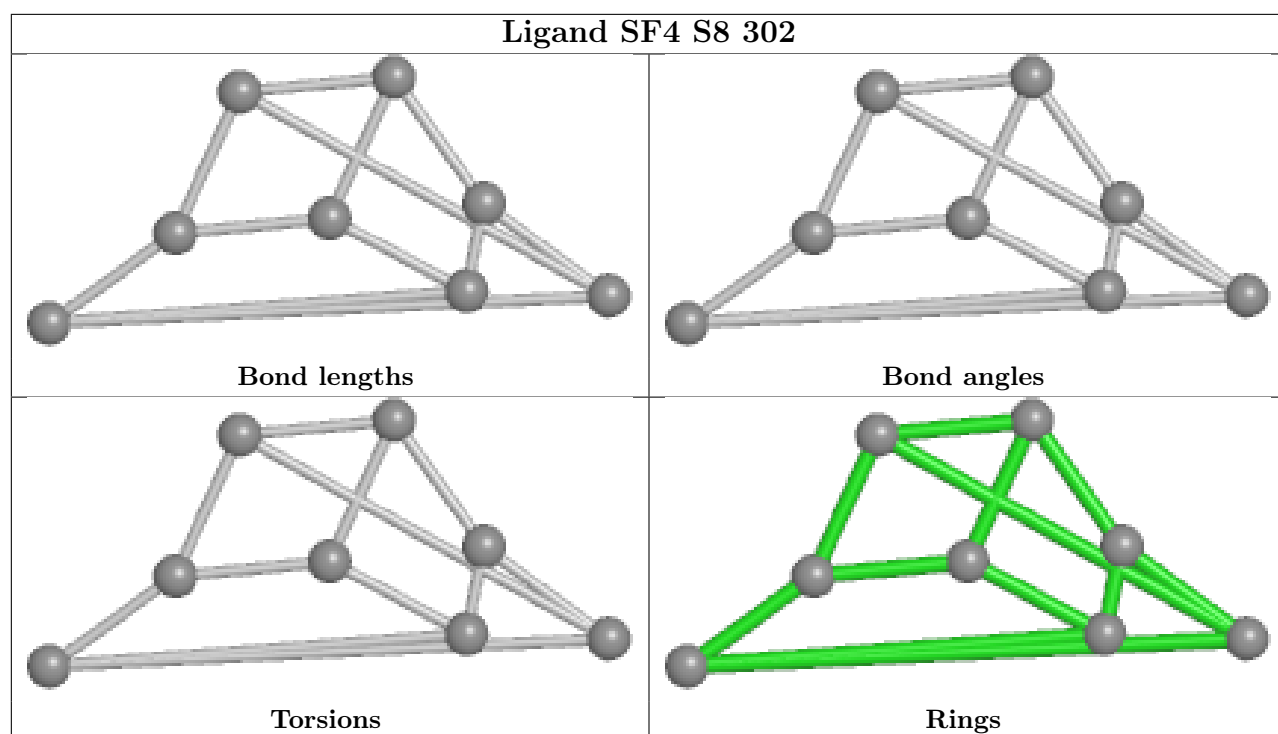


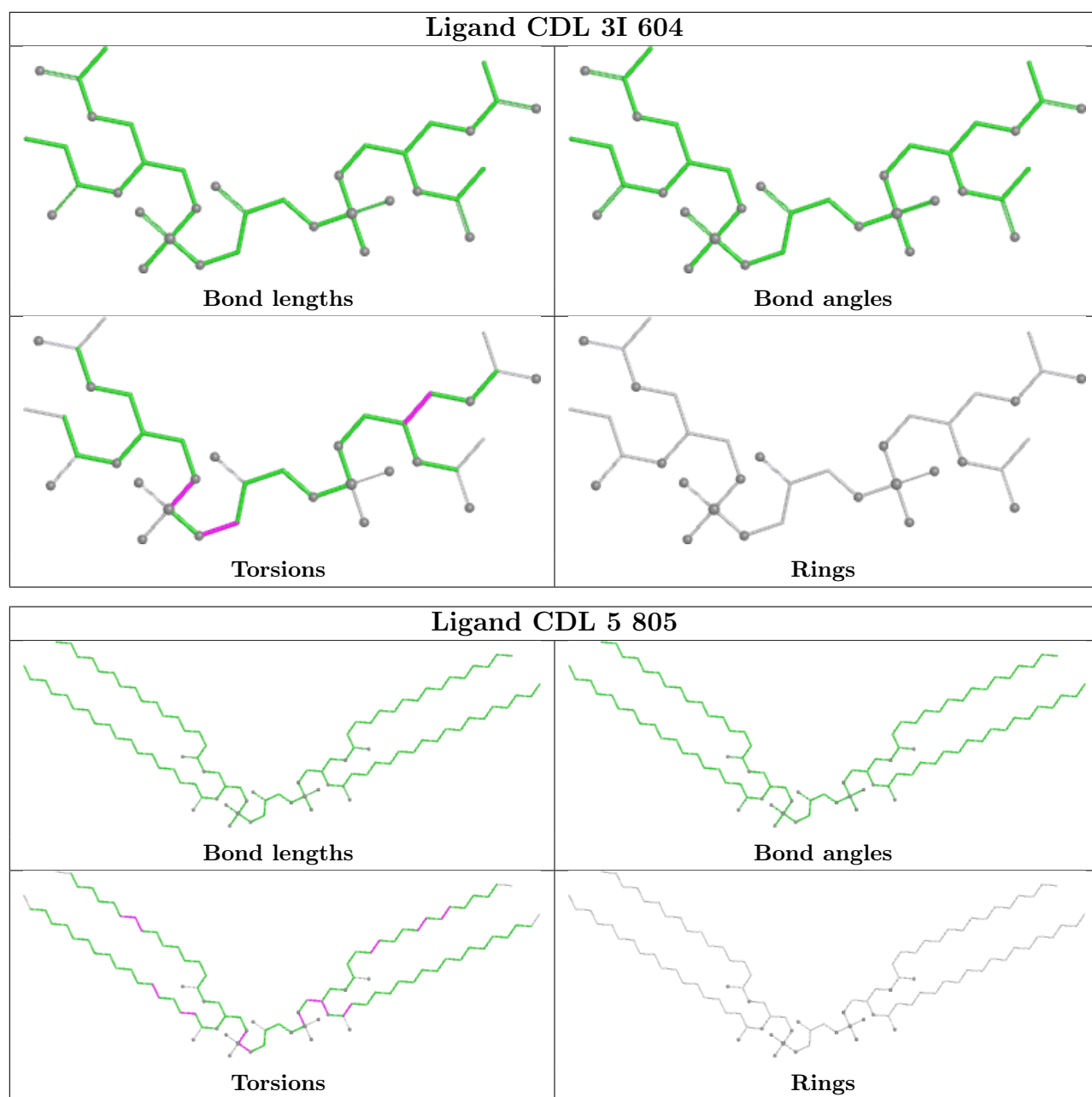


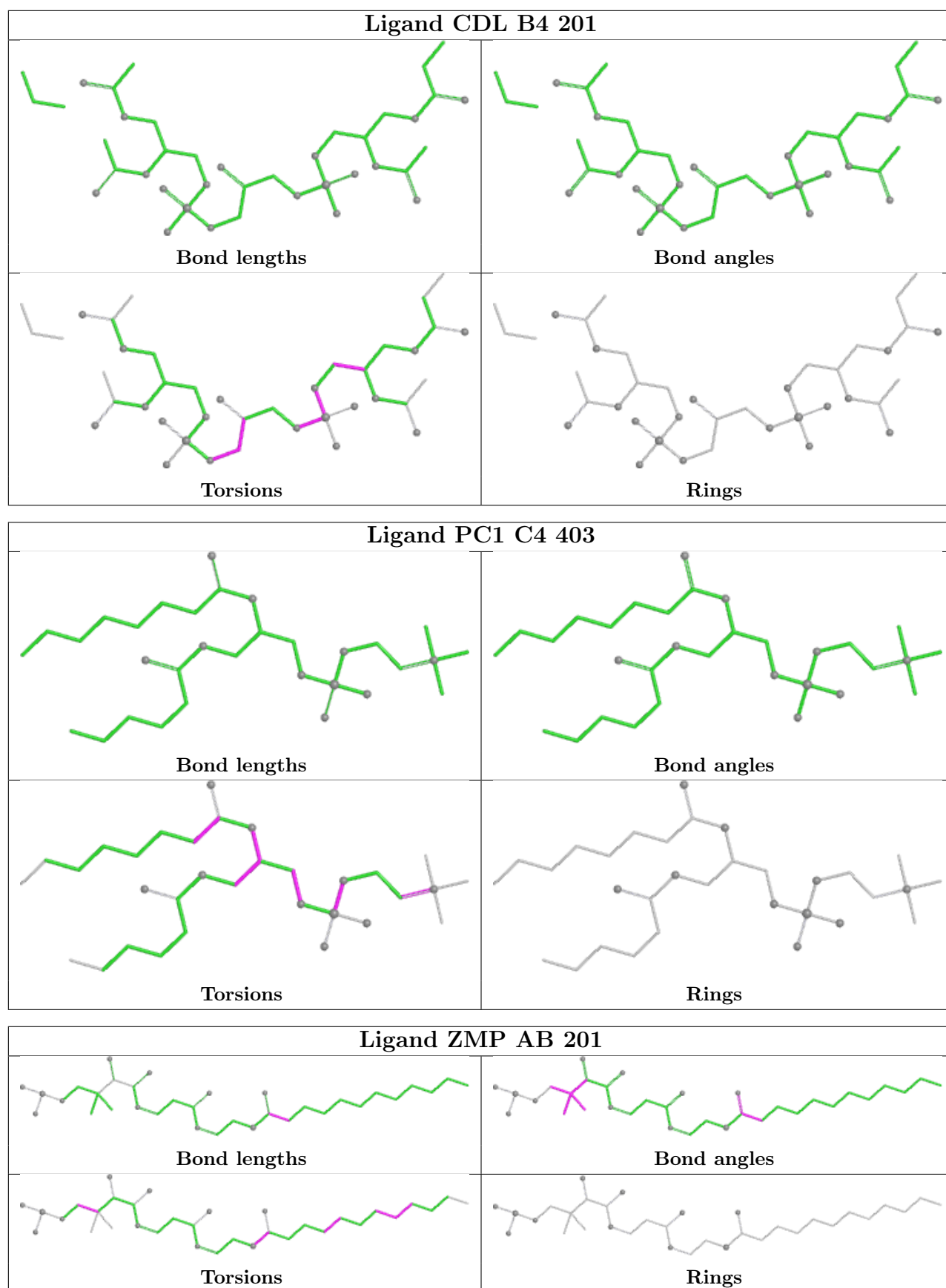


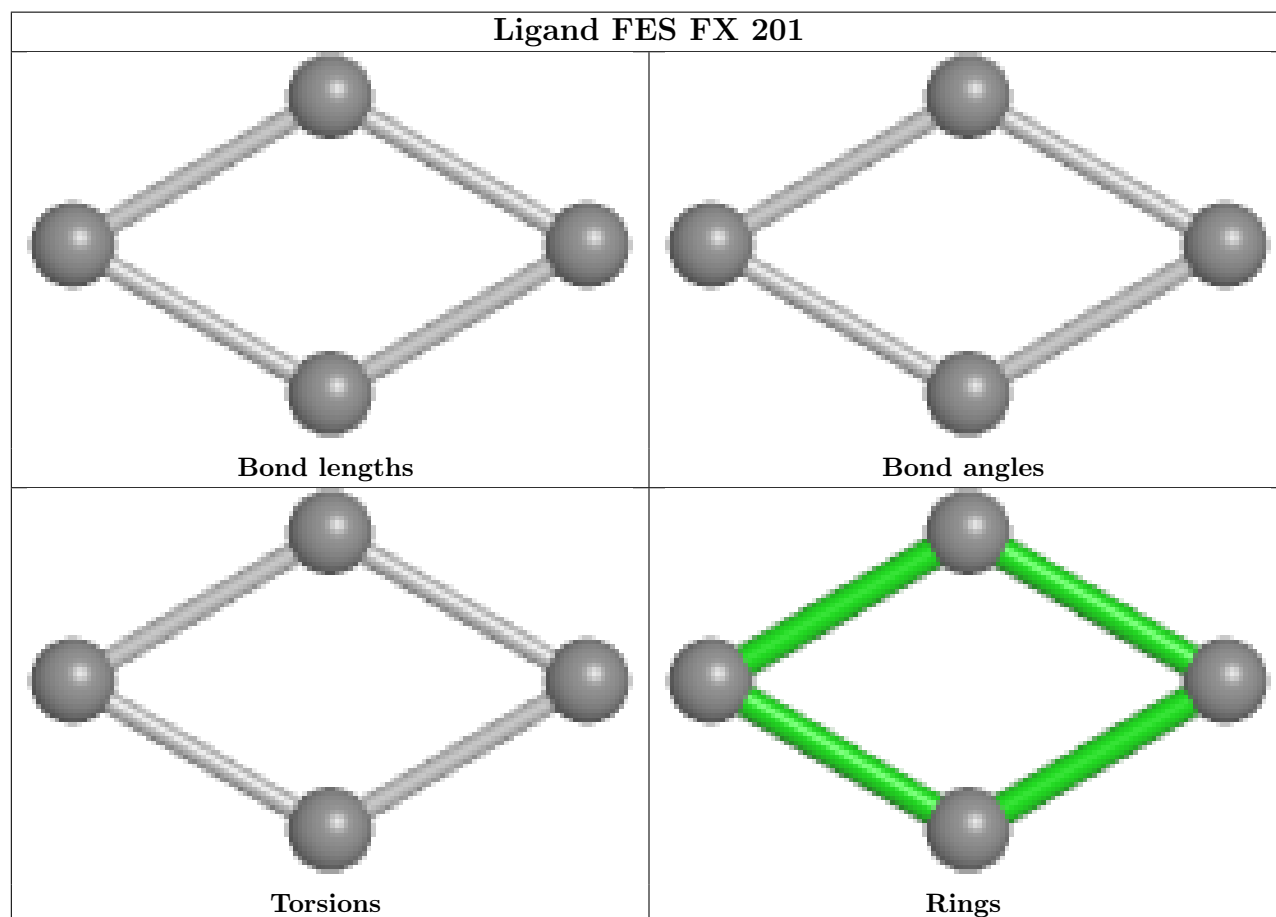
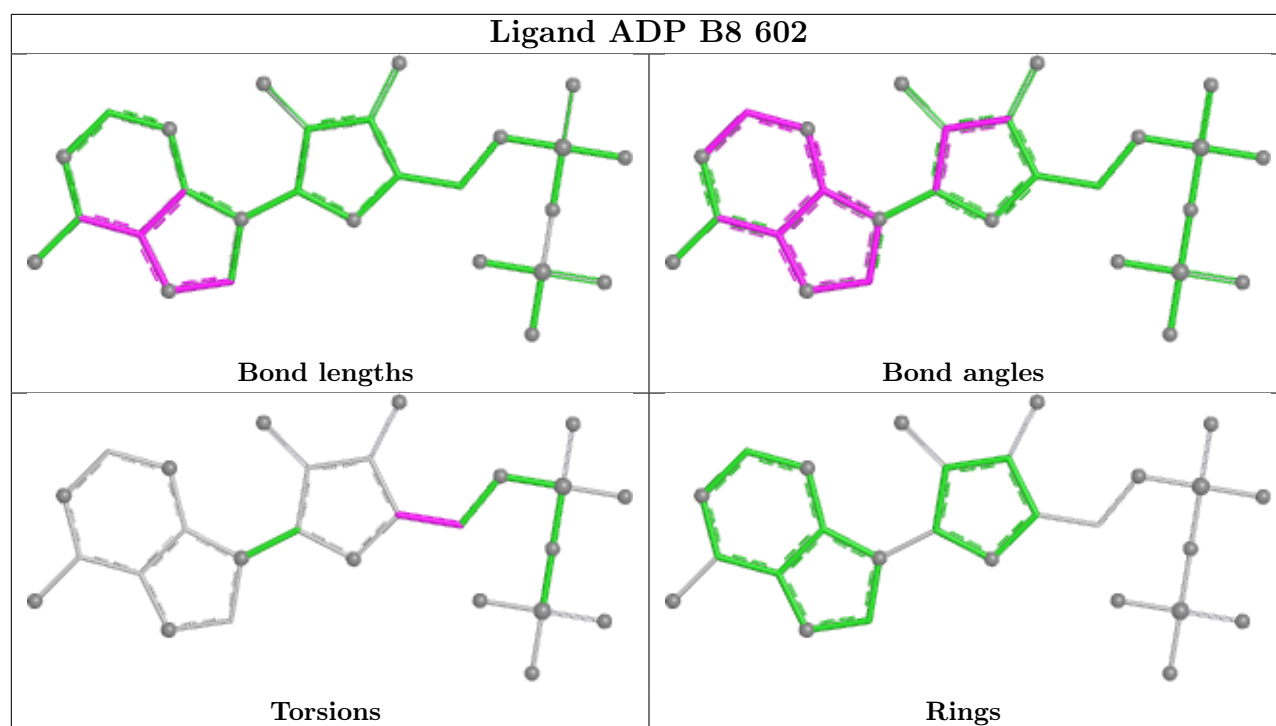


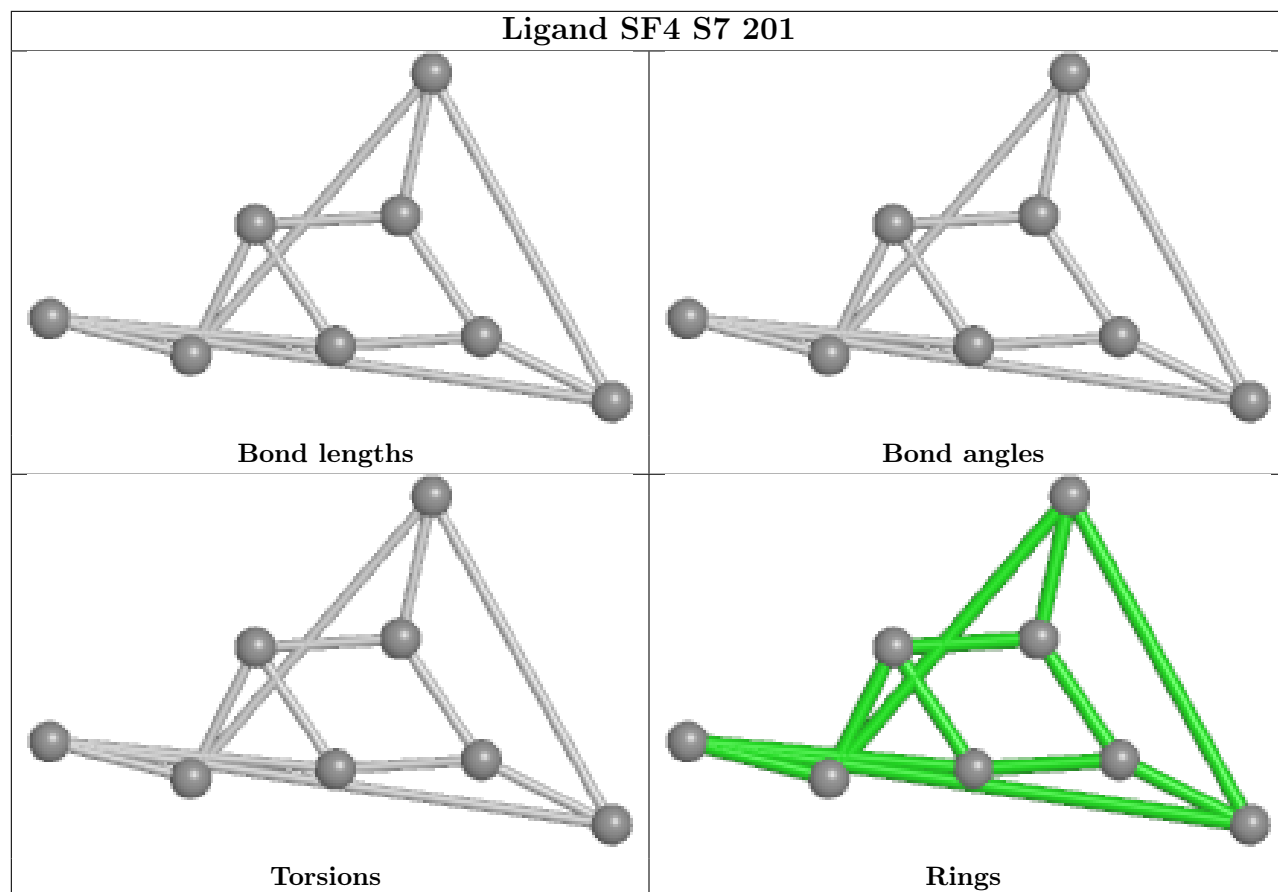


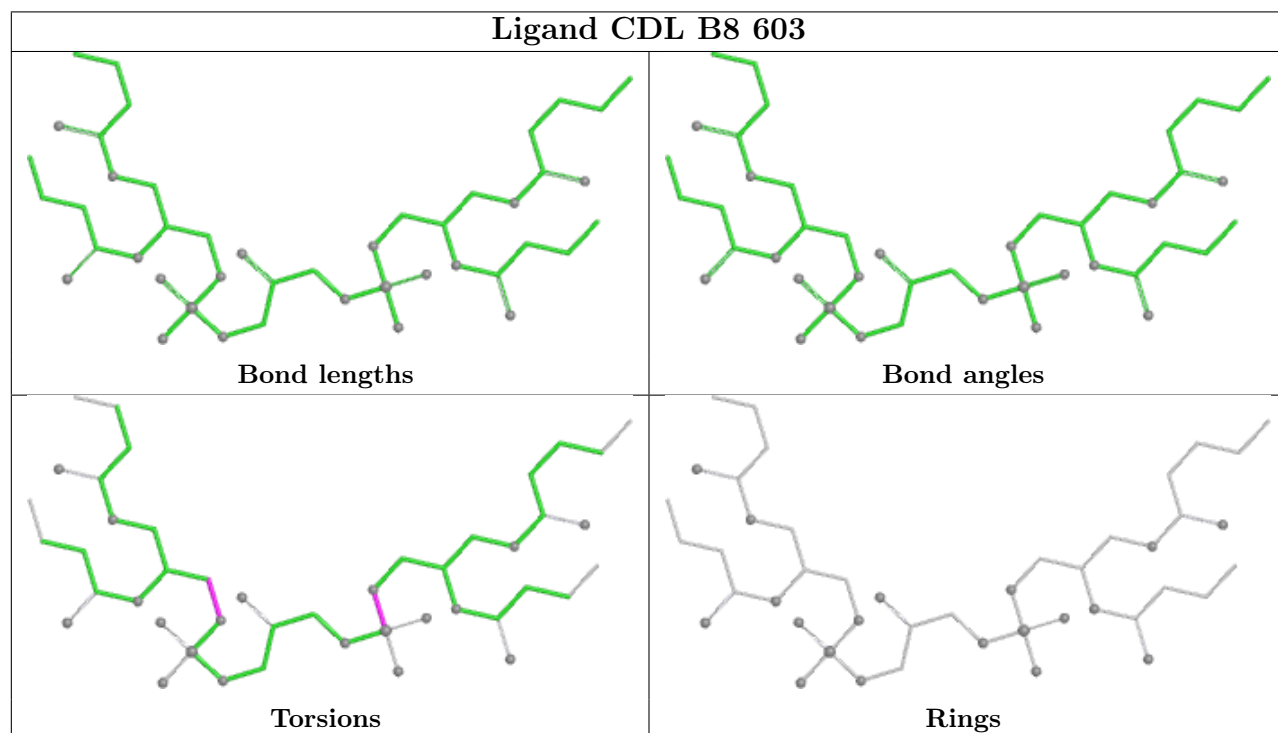
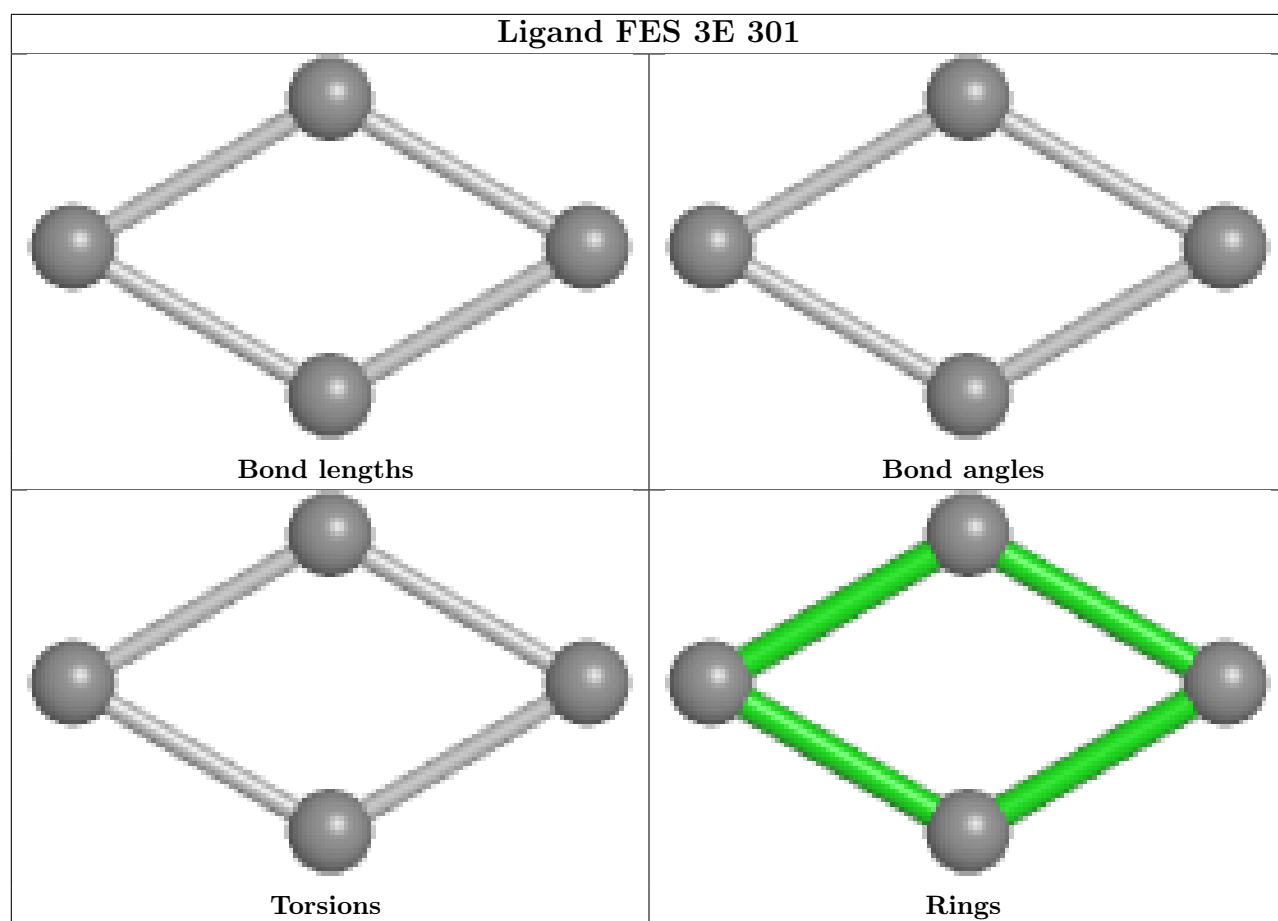




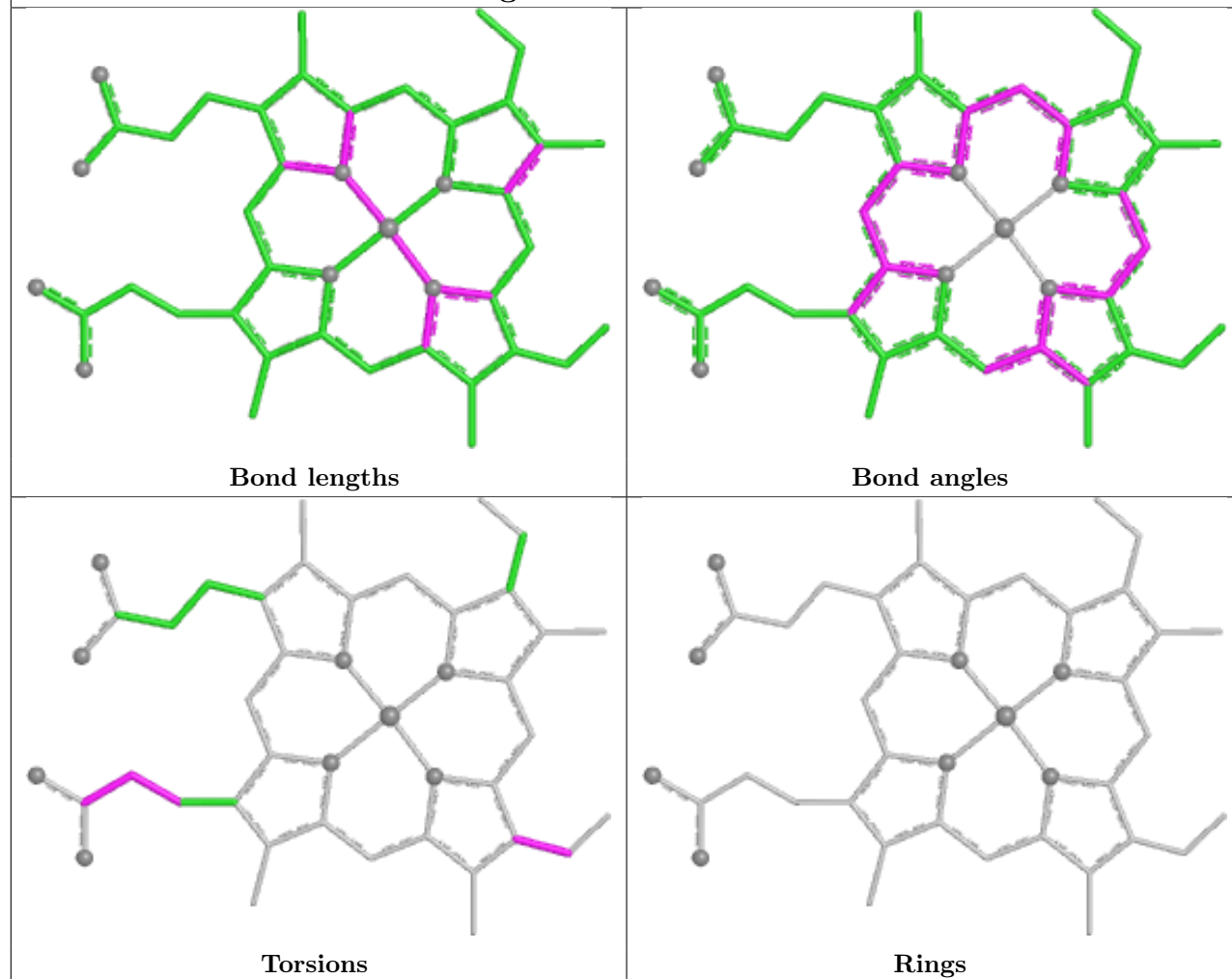




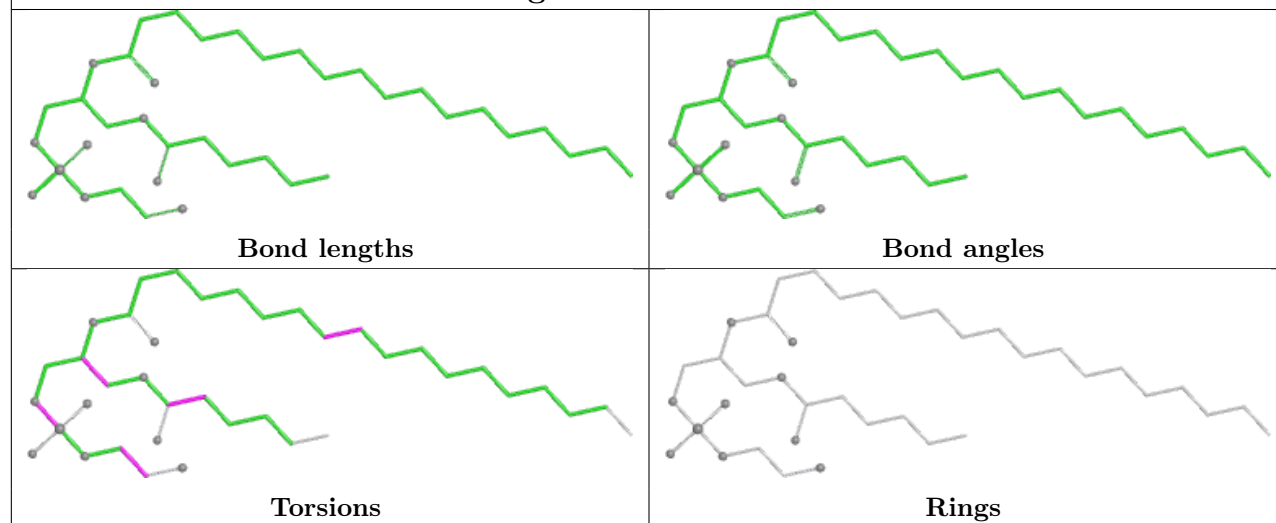


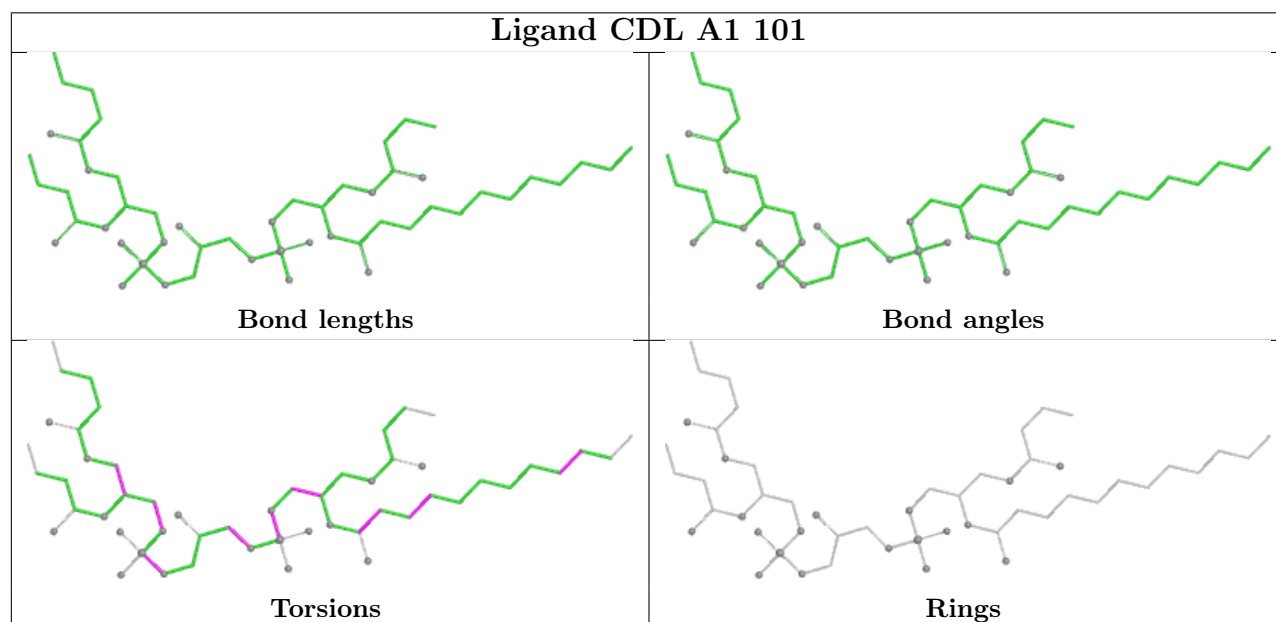
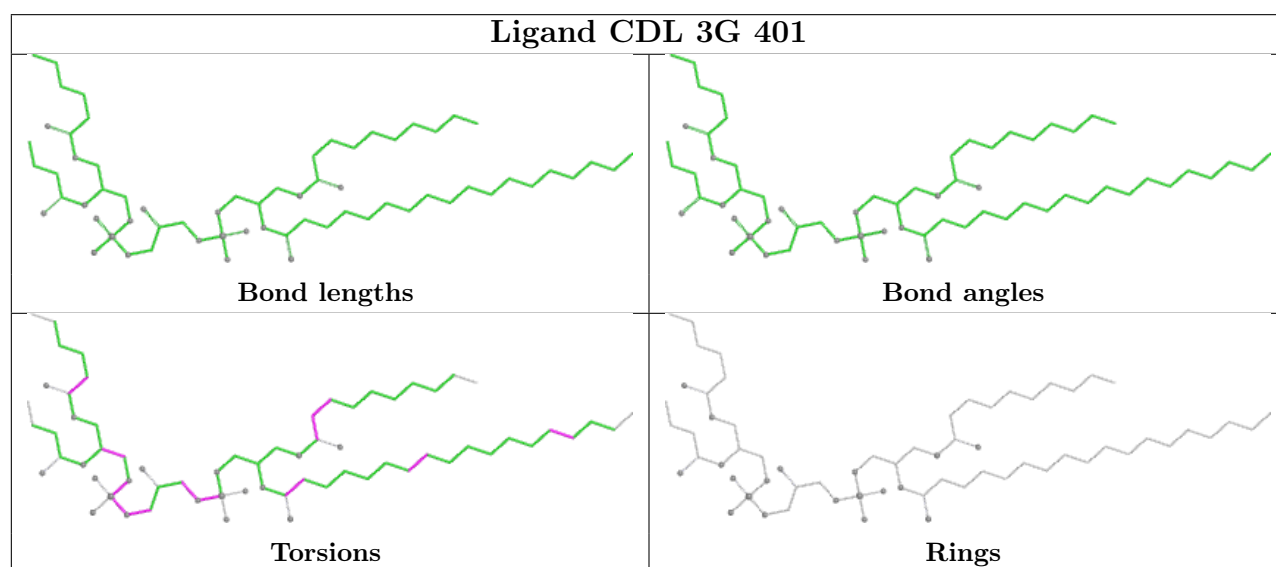
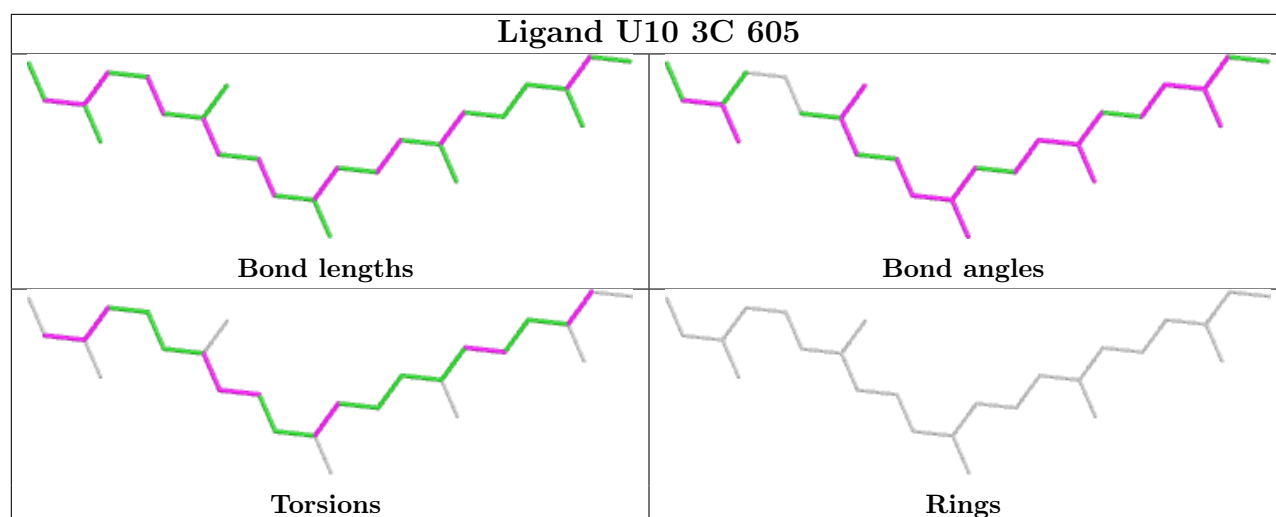


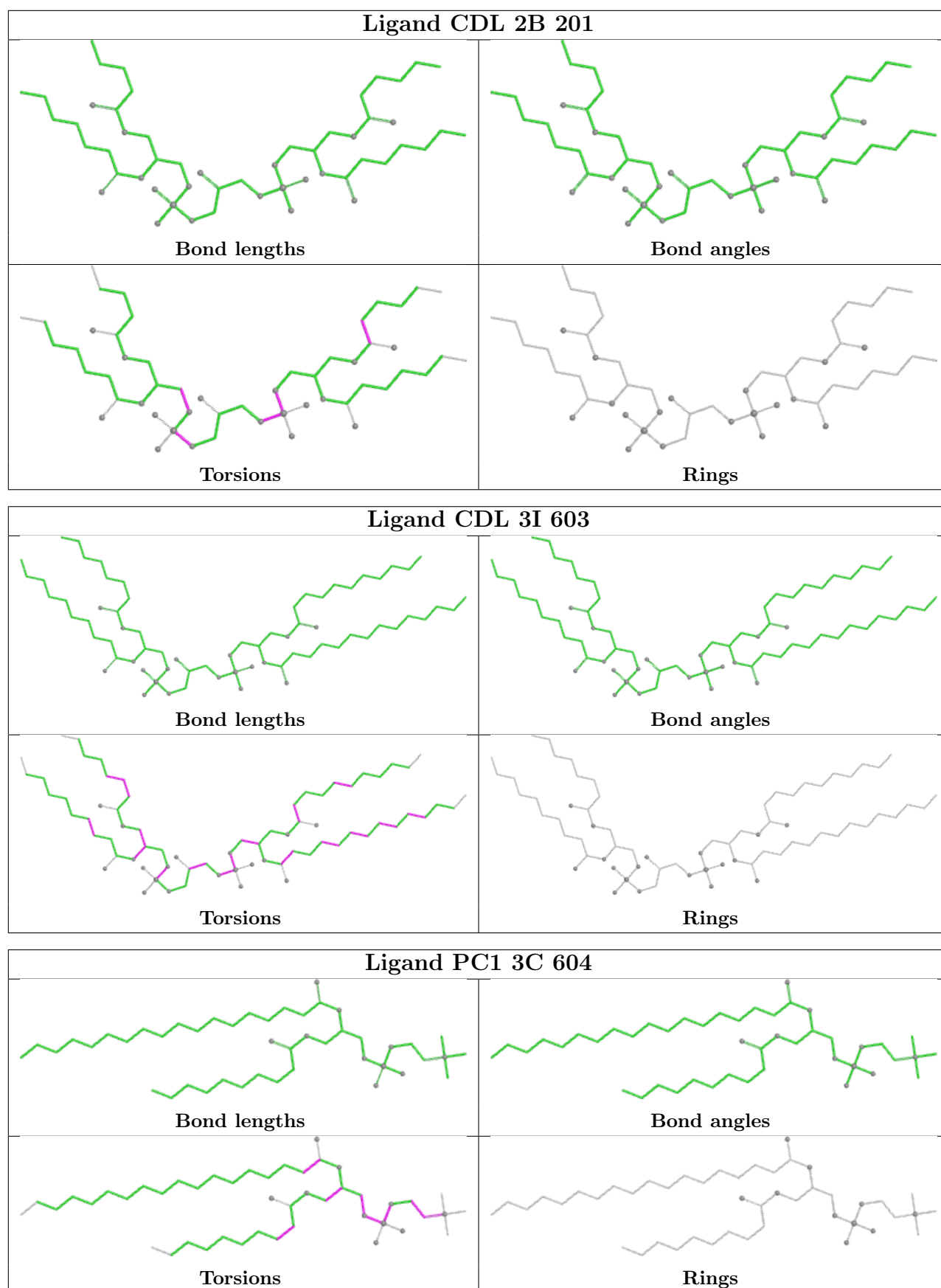
## Ligand HEM 3C 602

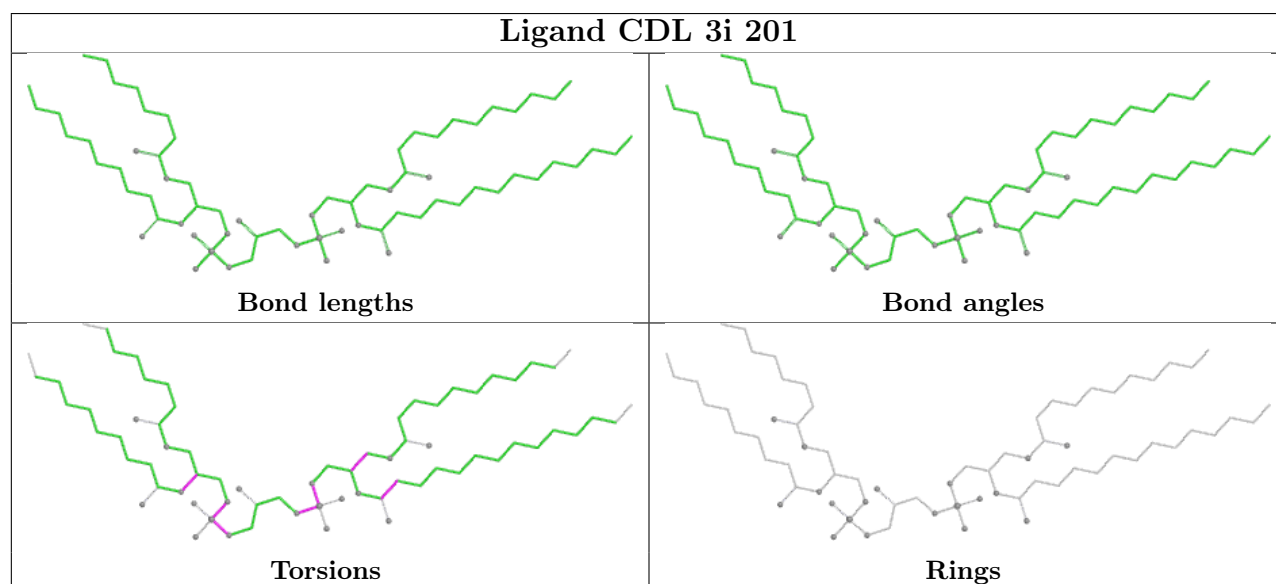
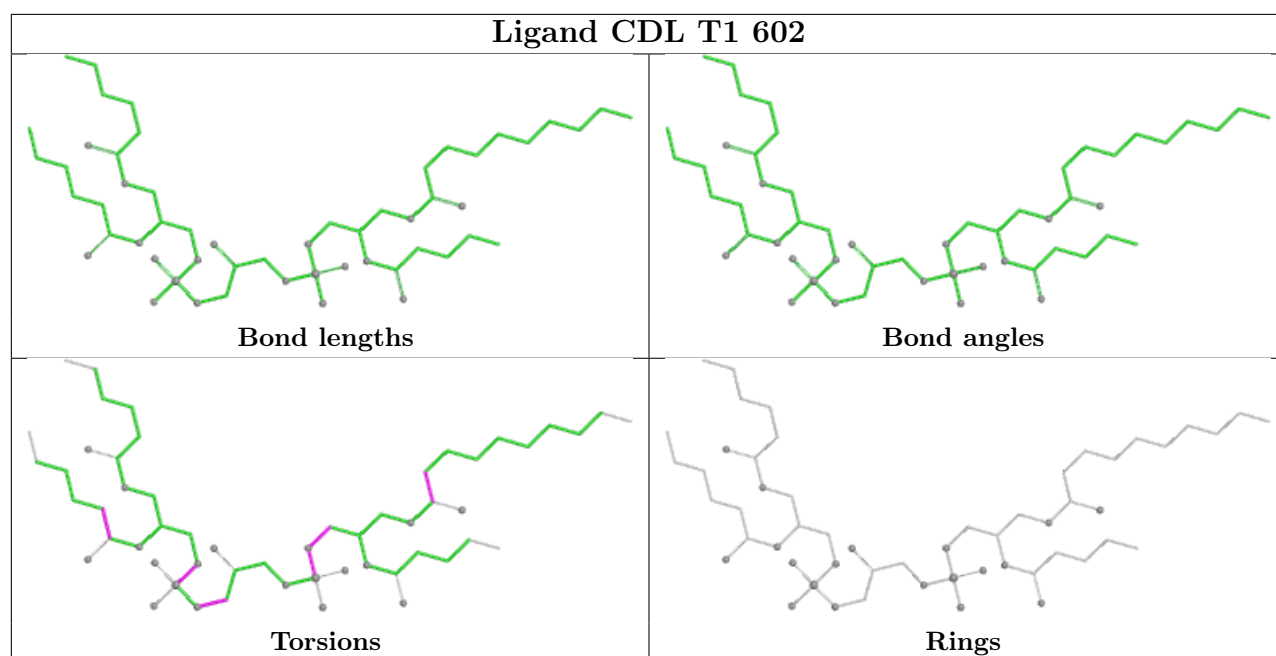


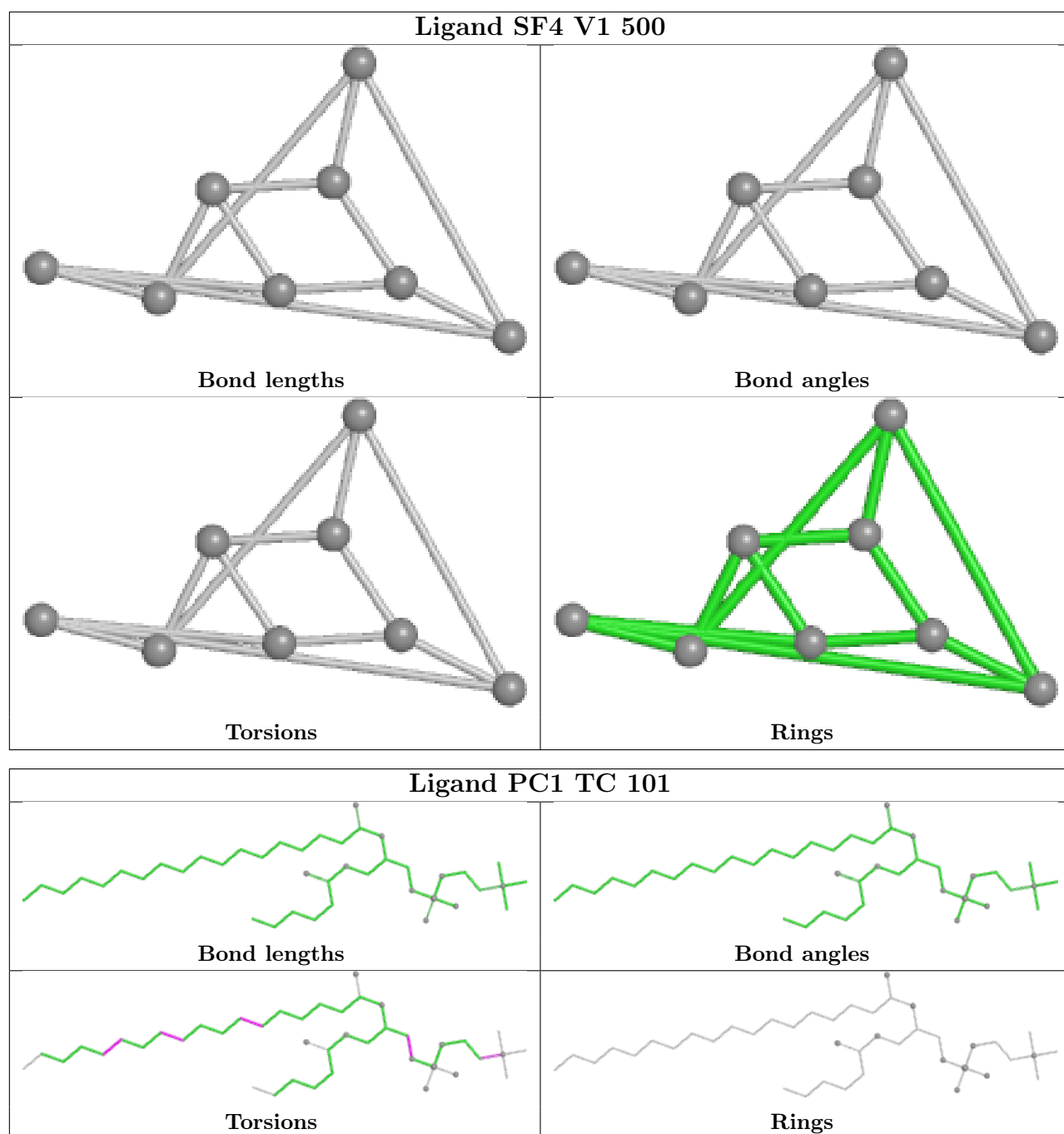
## Ligand 3PE T8 201

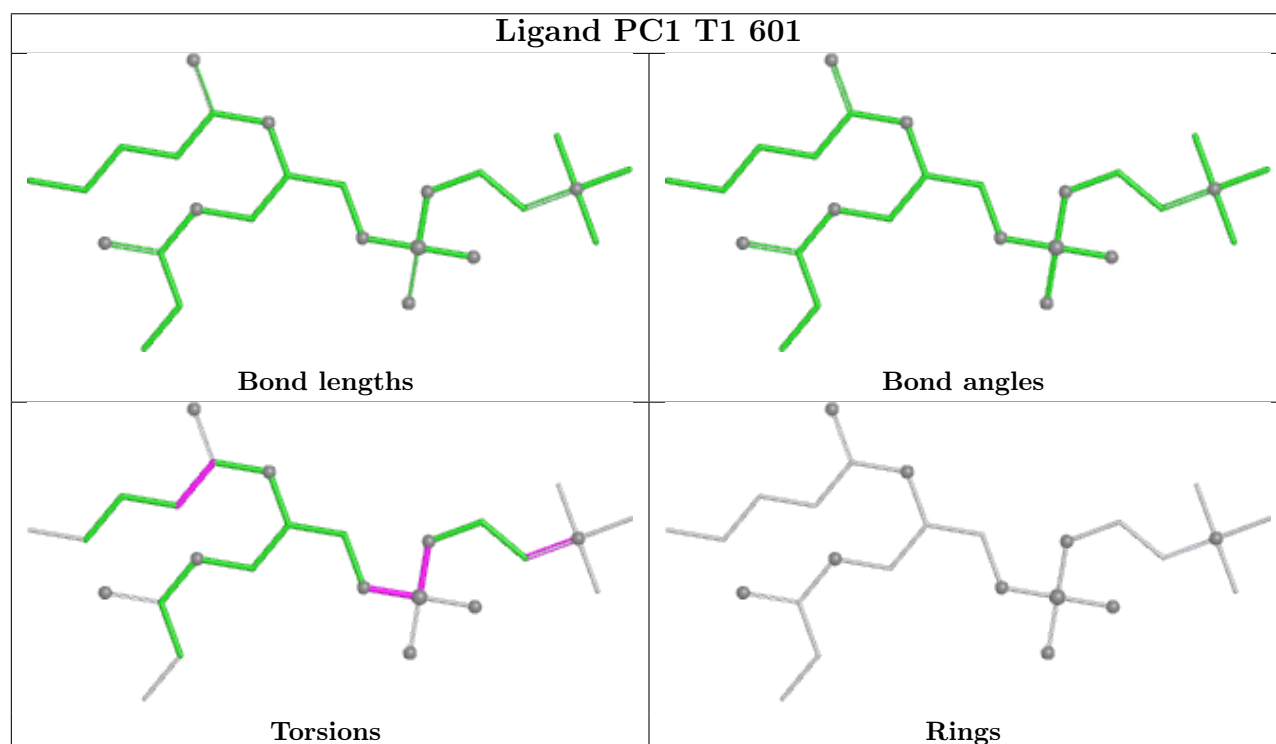
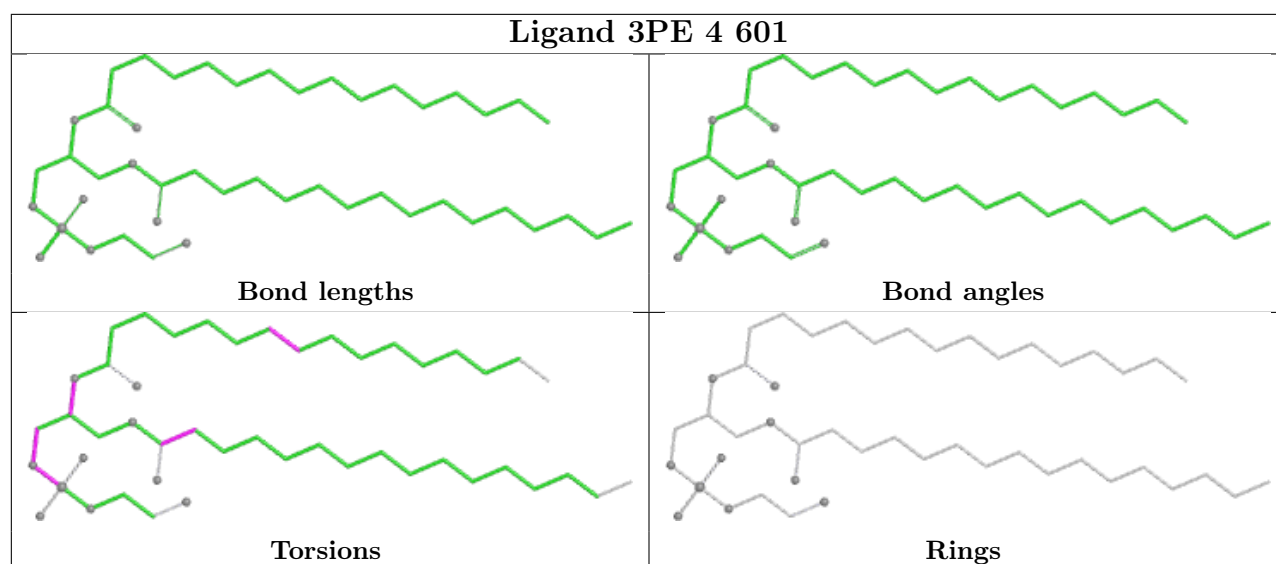


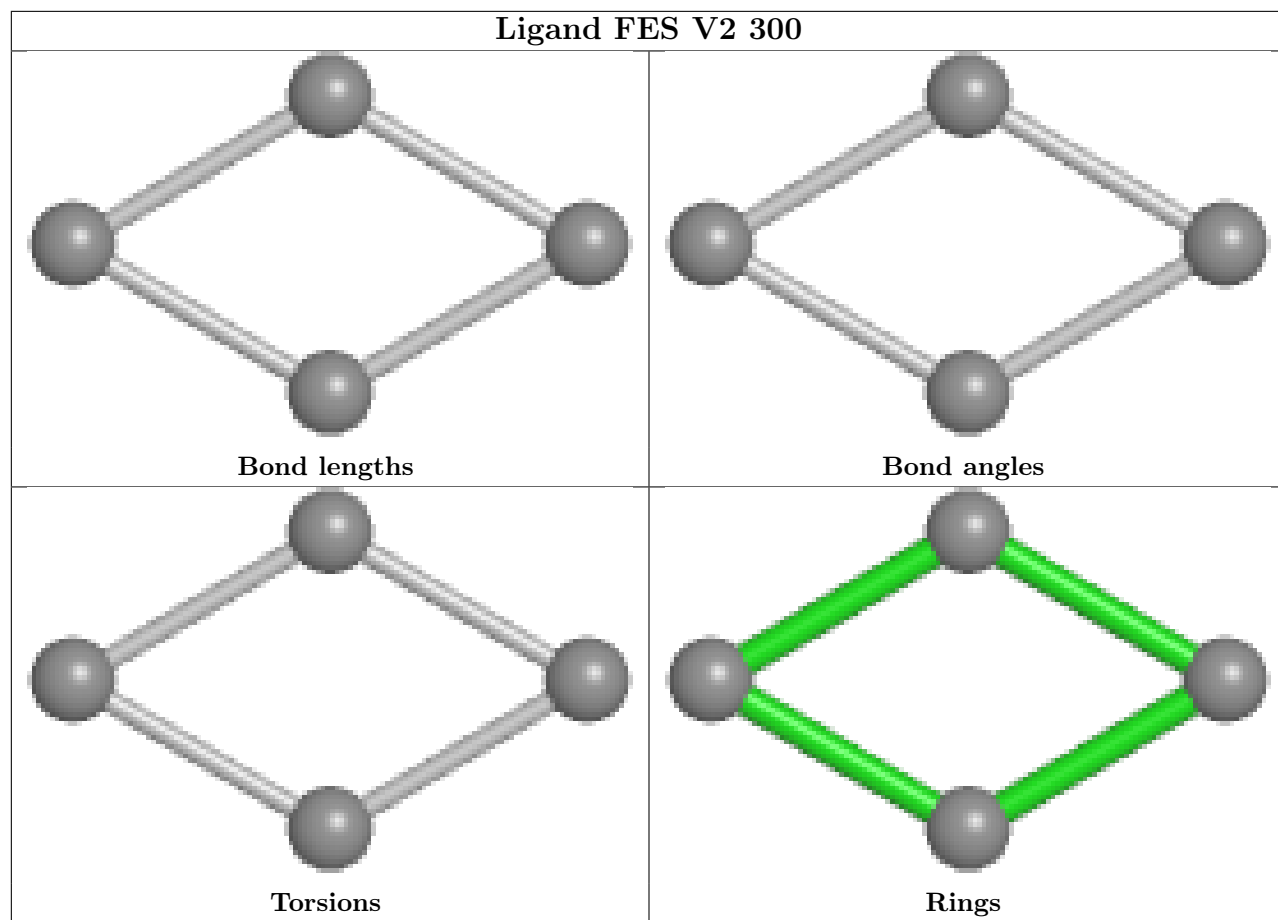


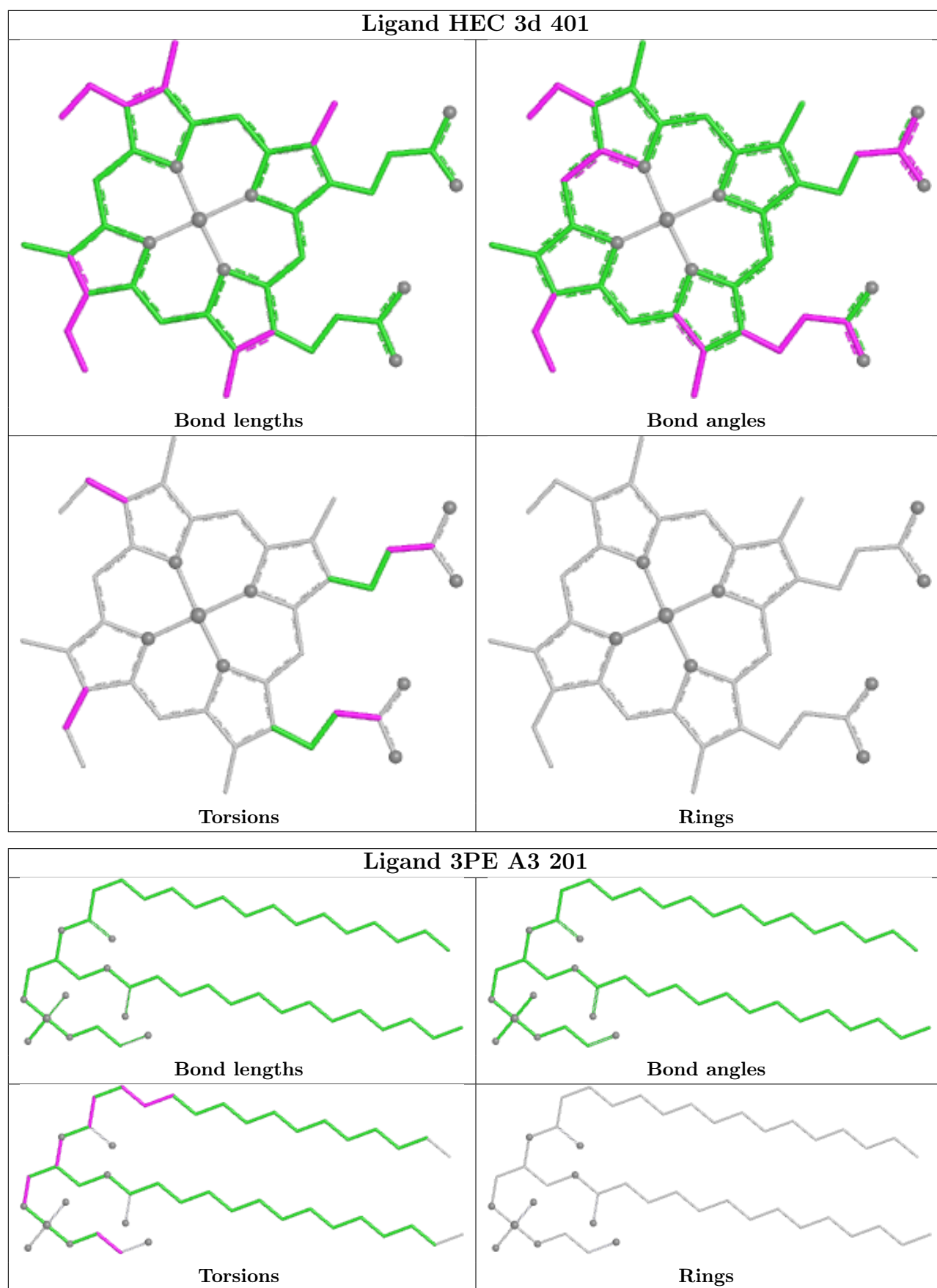


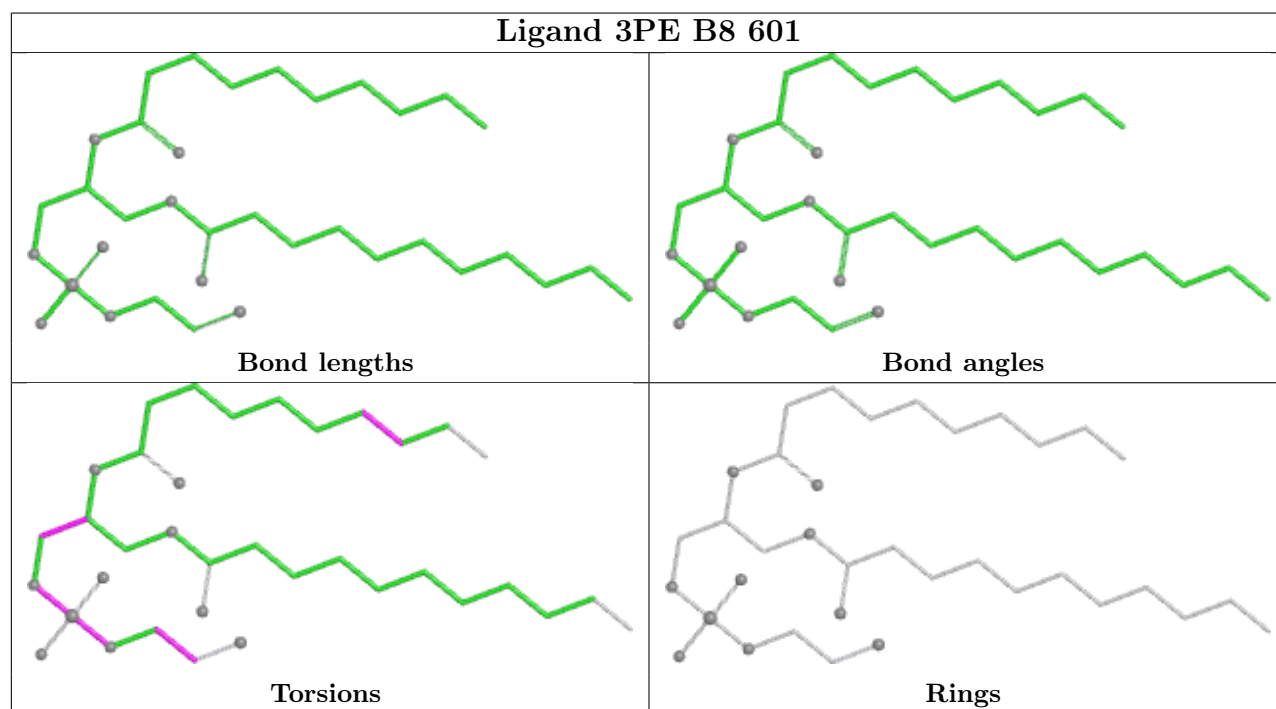
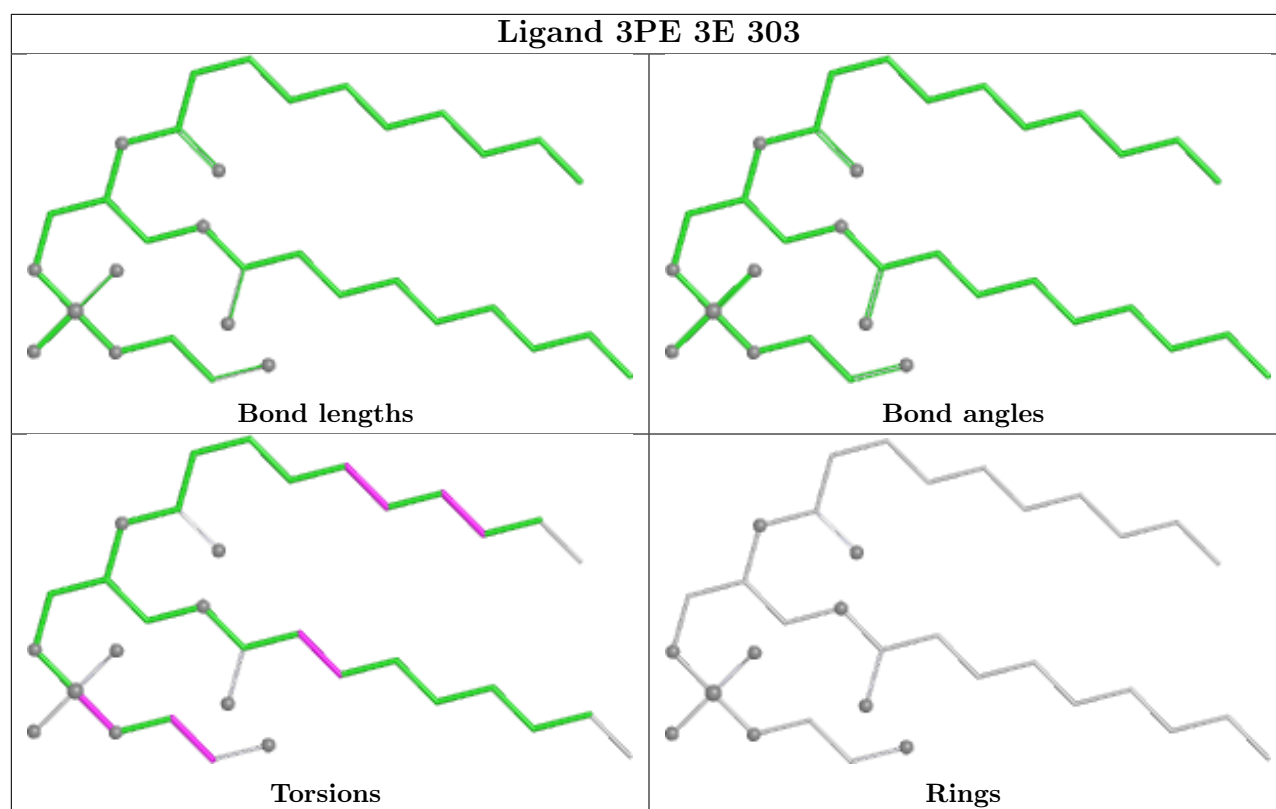


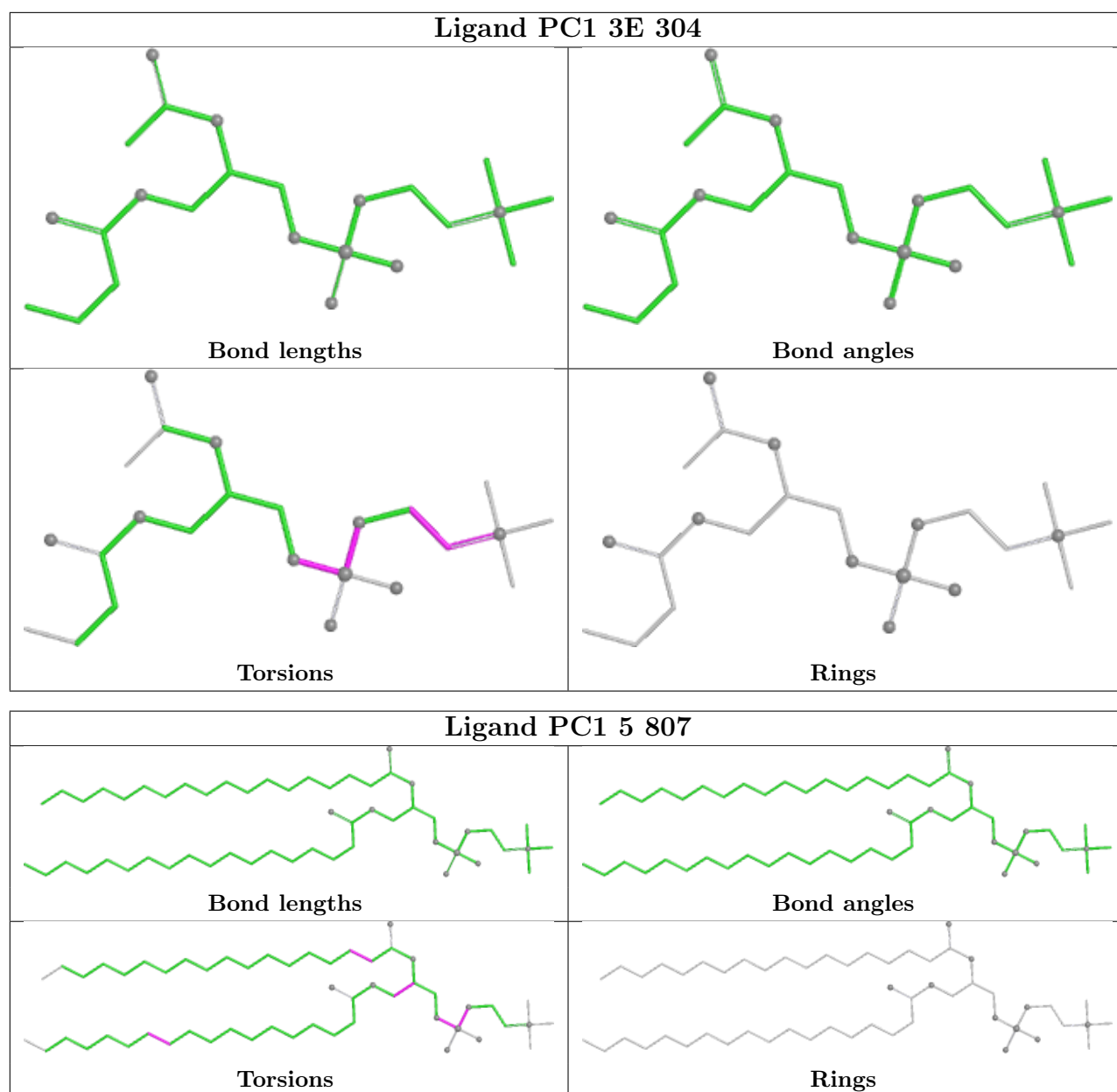


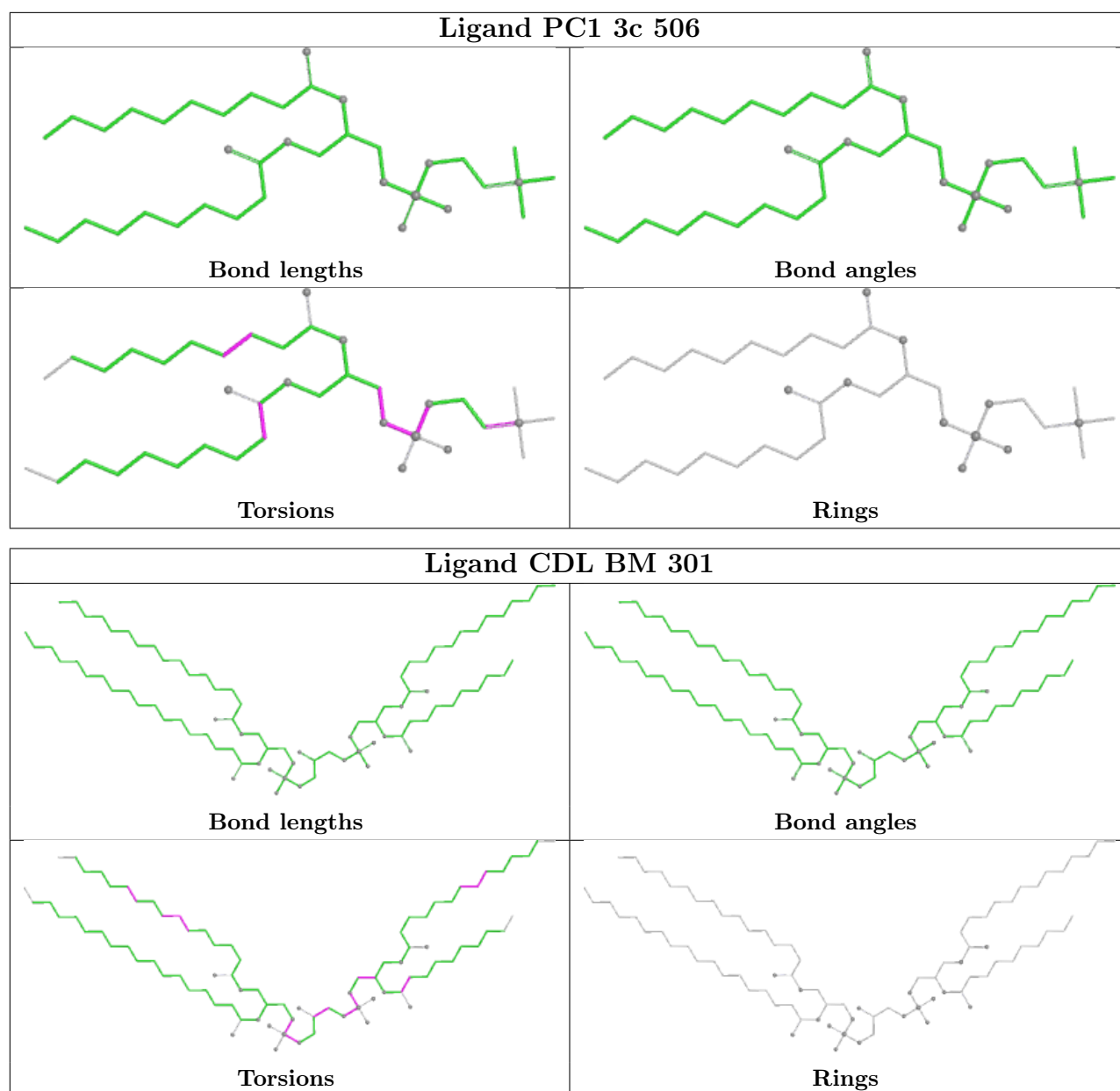


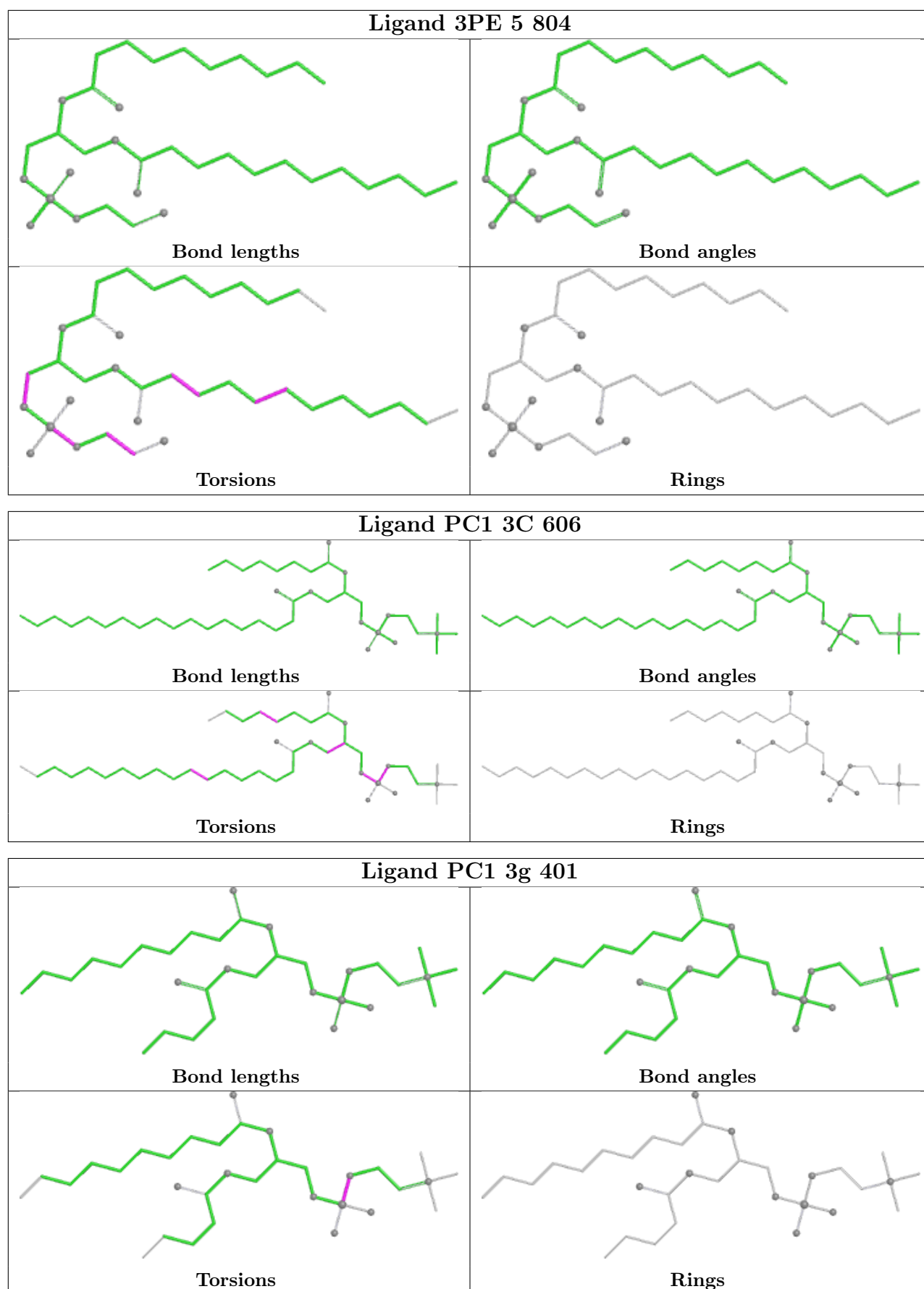


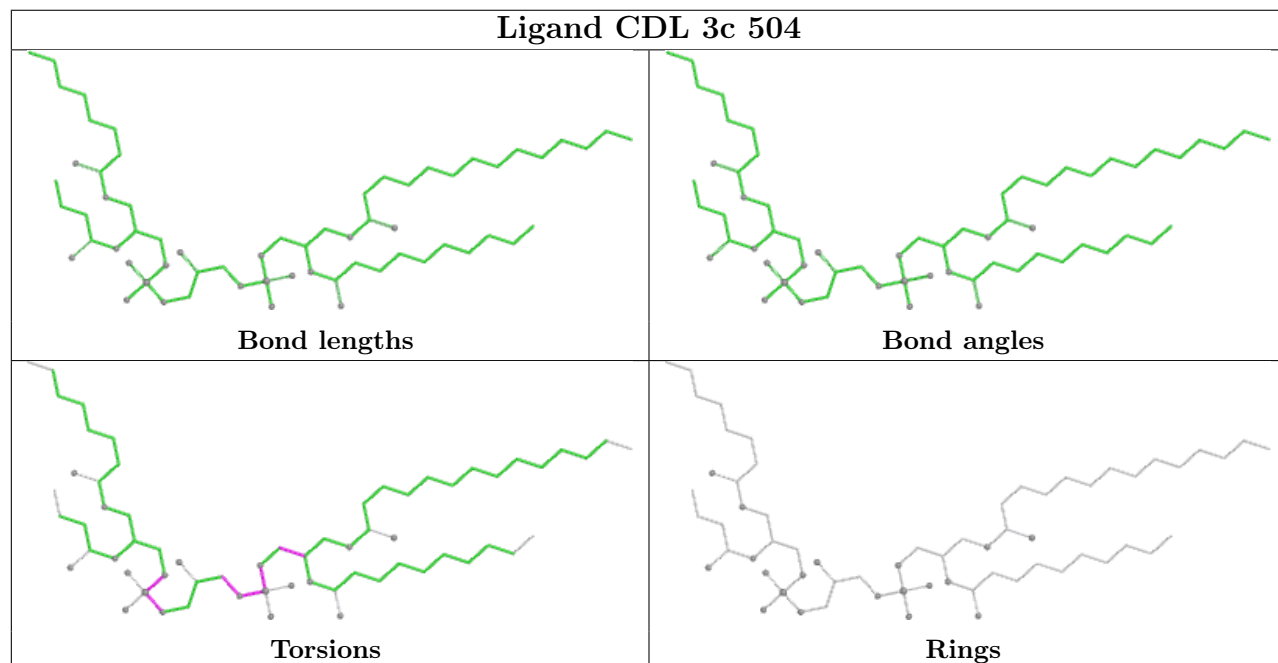
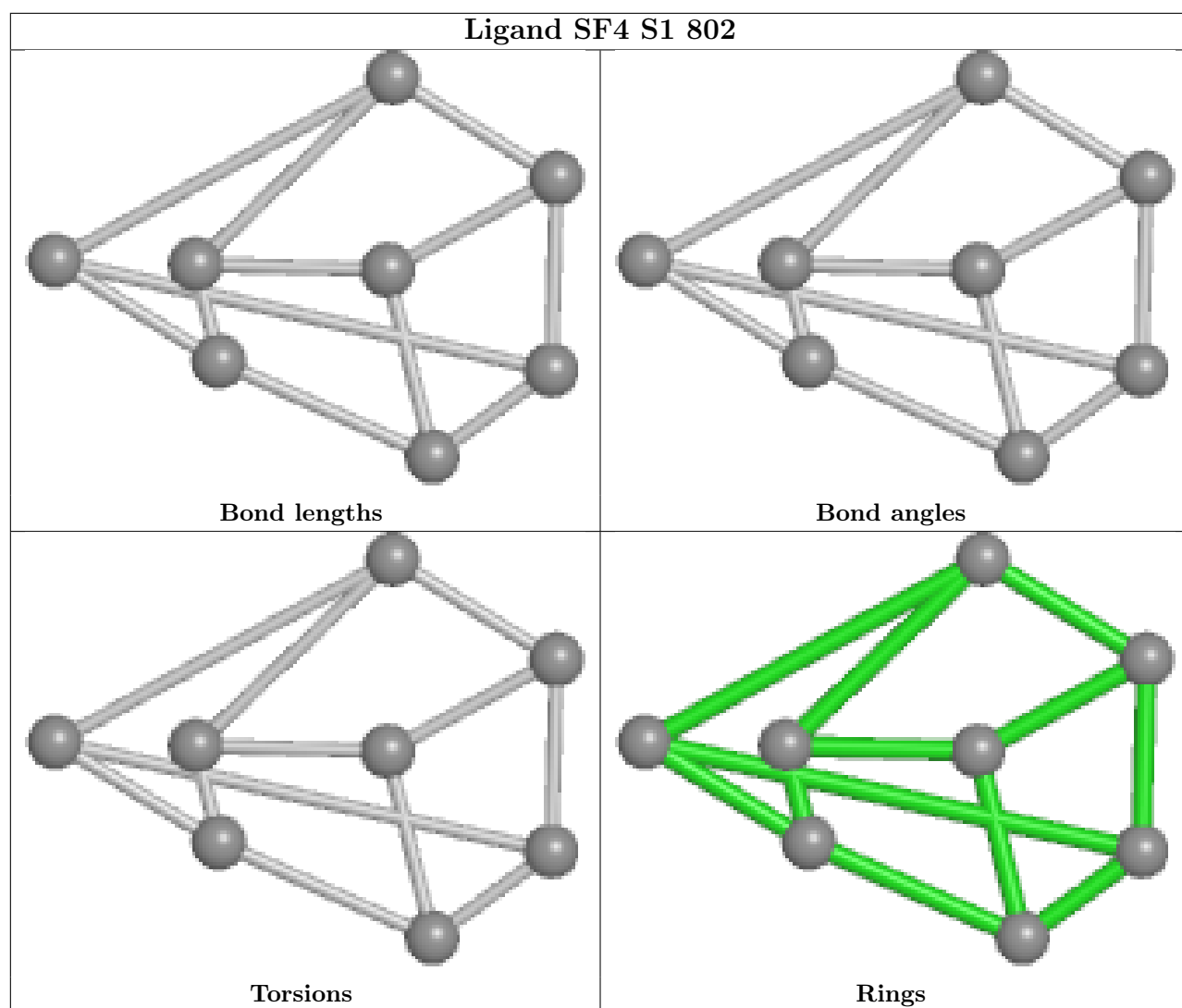


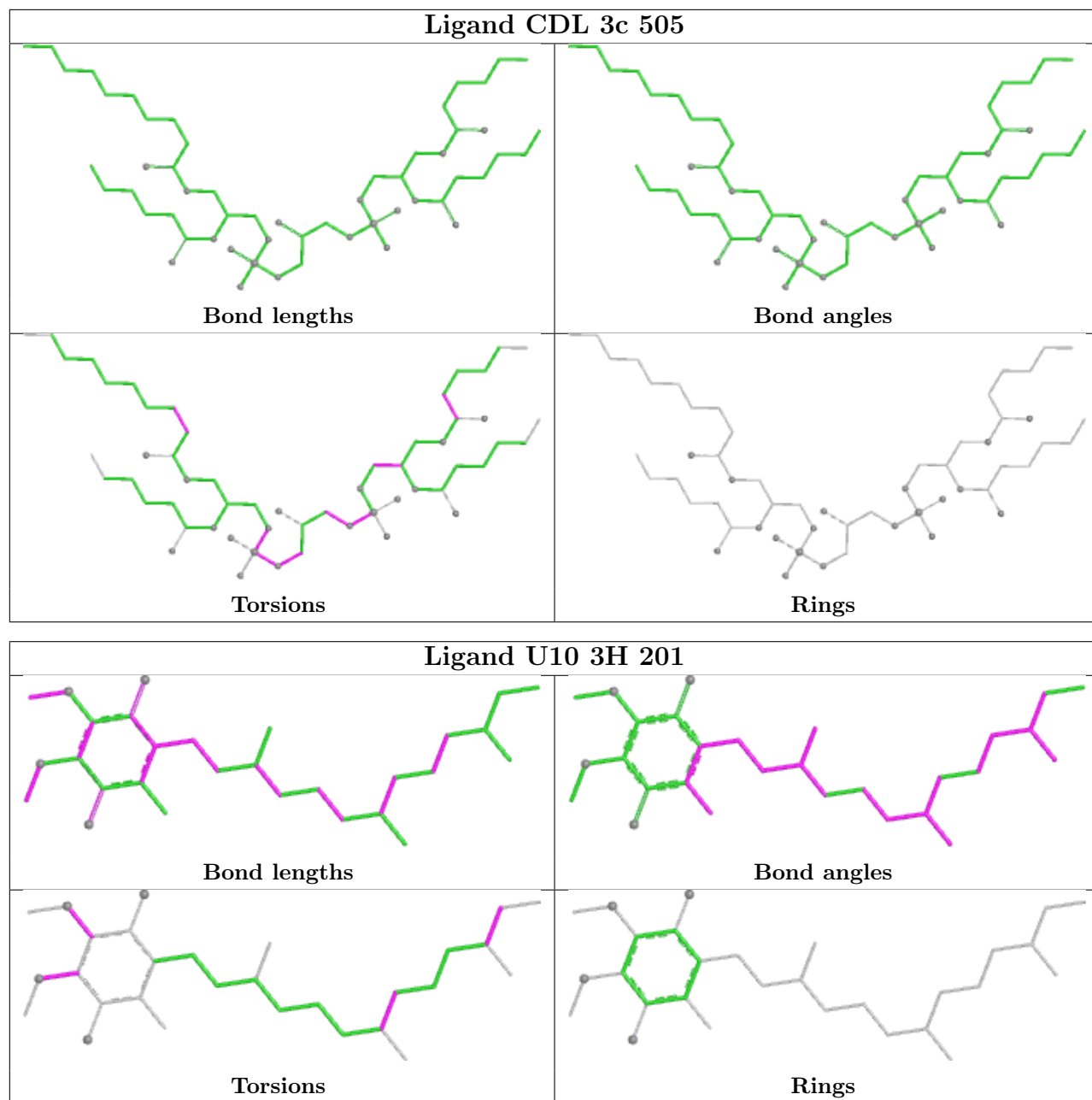


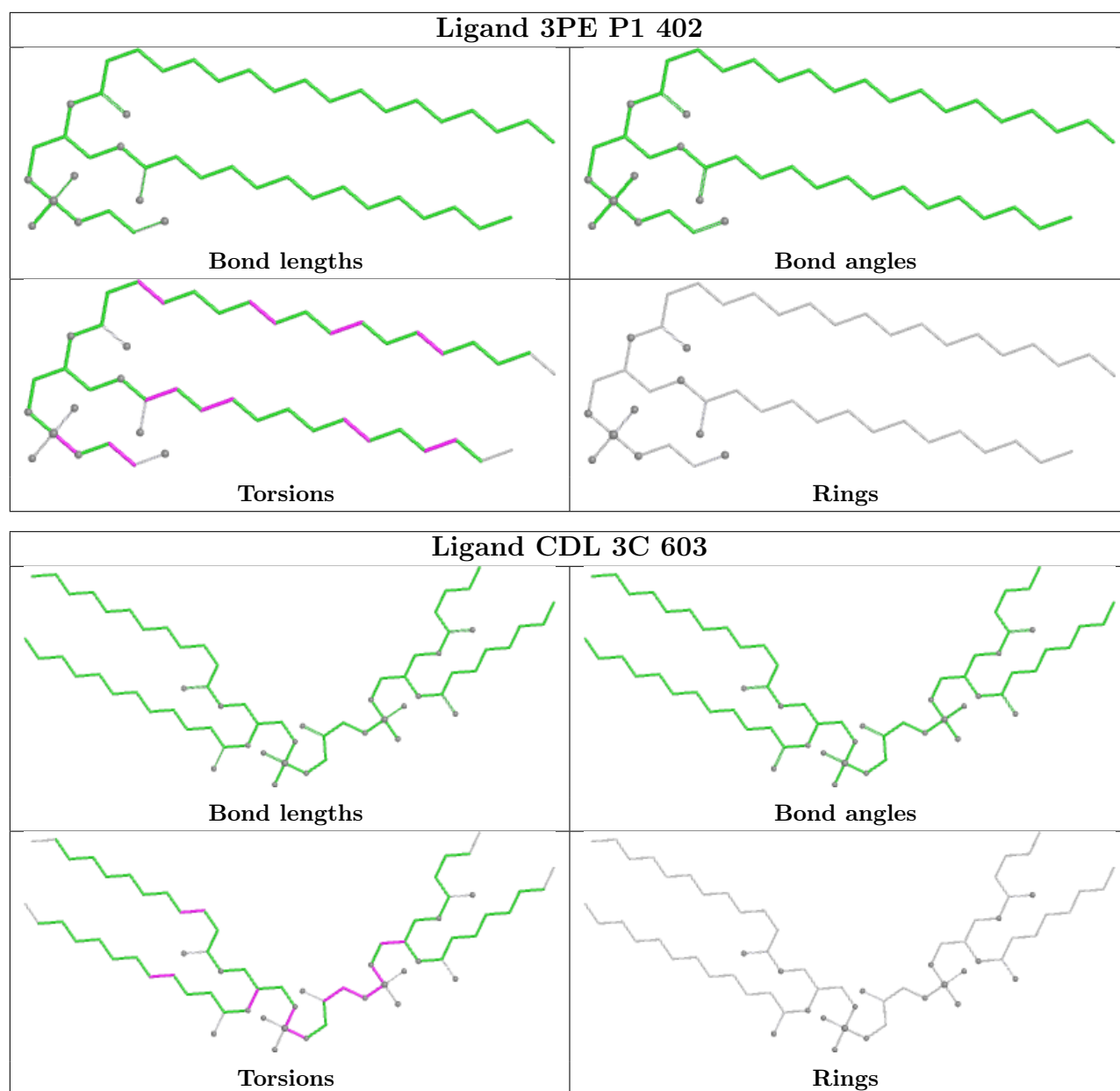




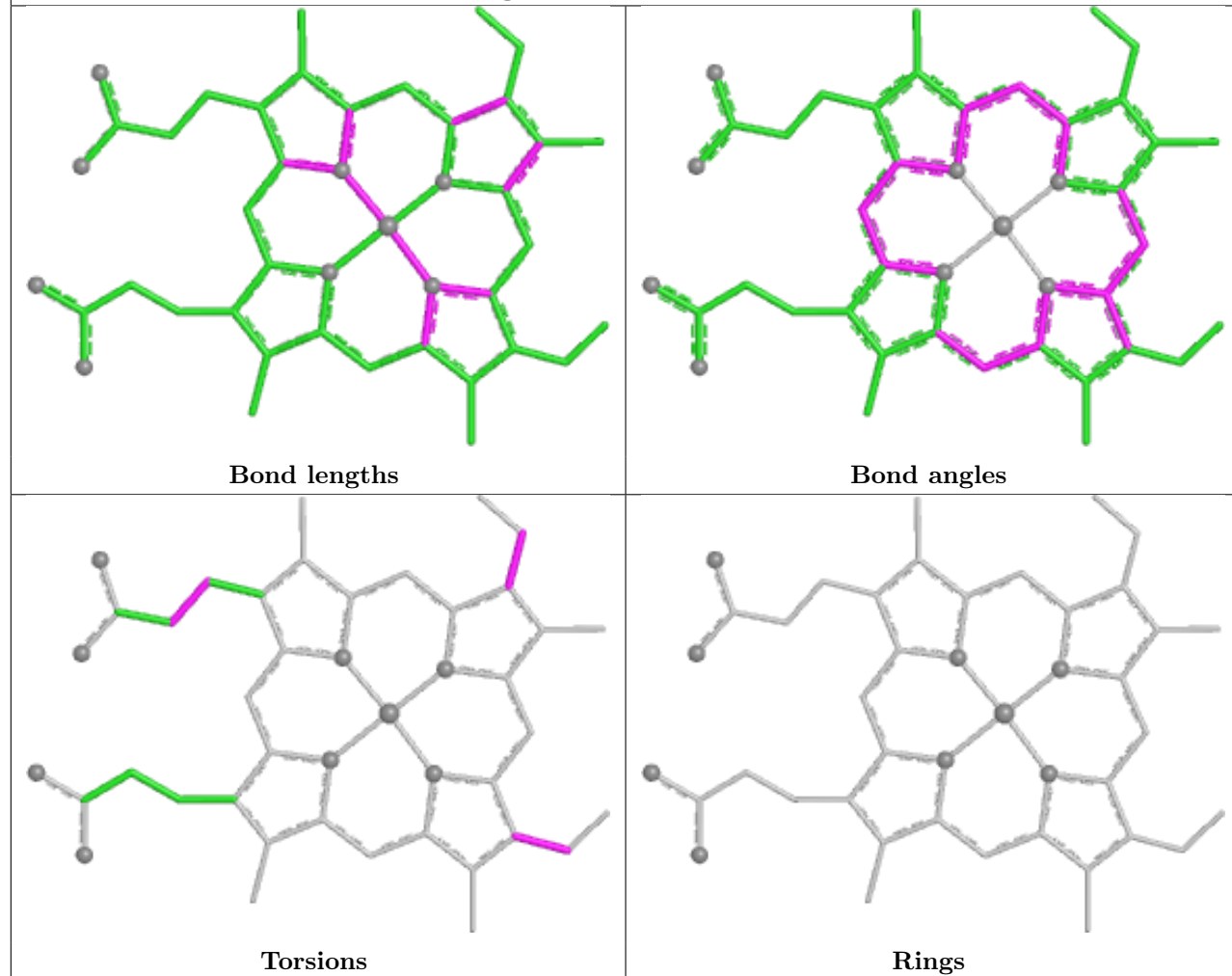


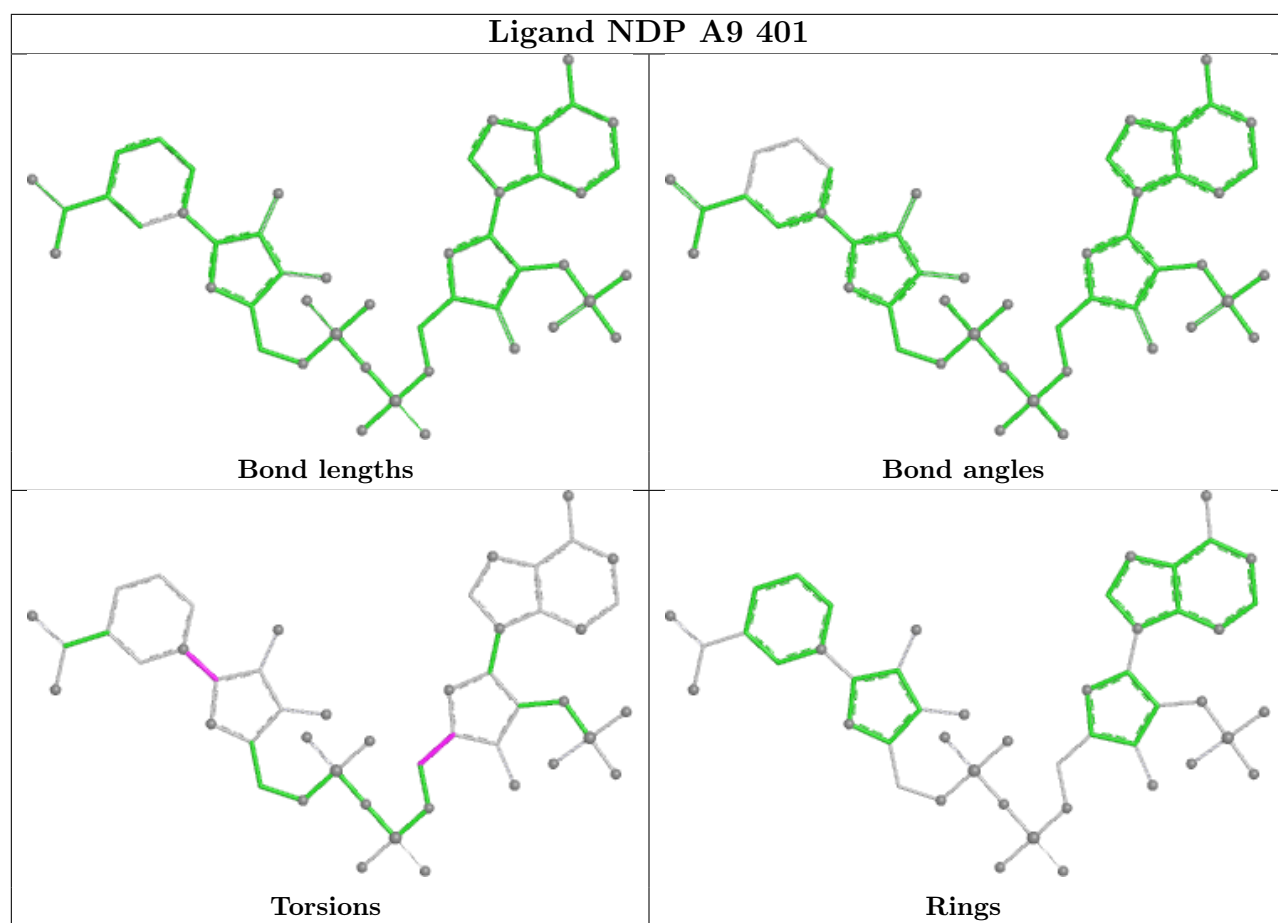


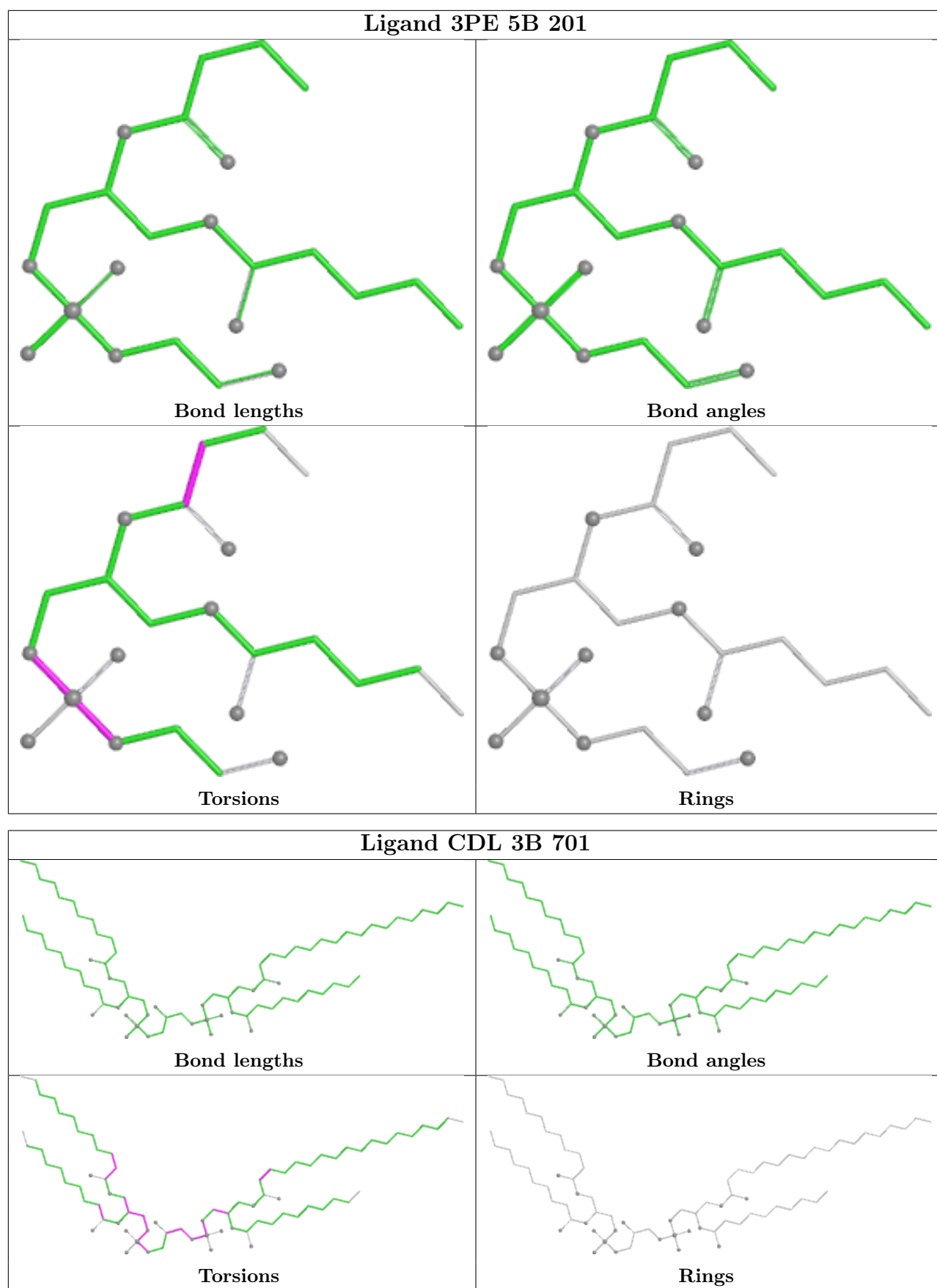




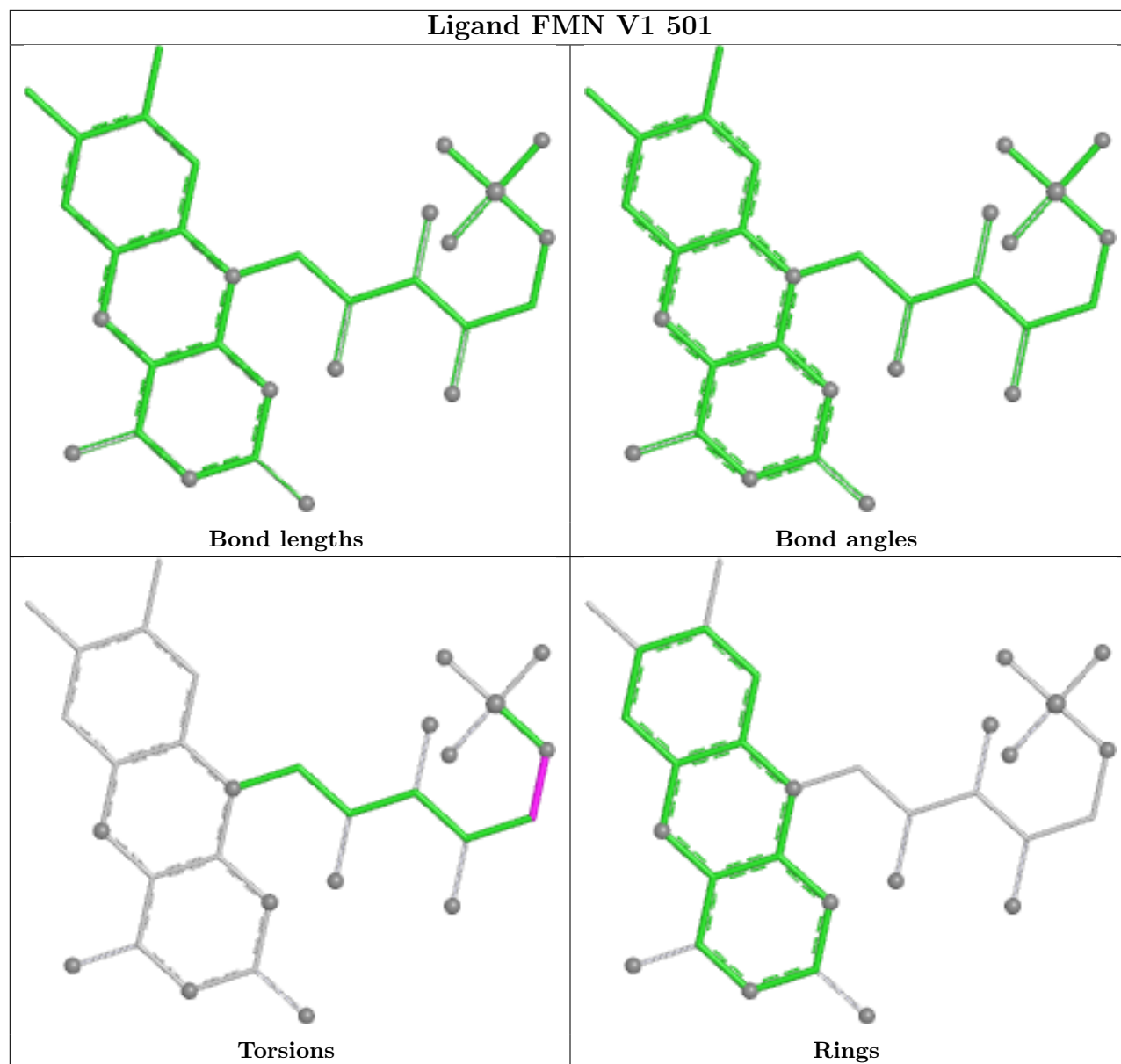
## Ligand HEM 3C 601



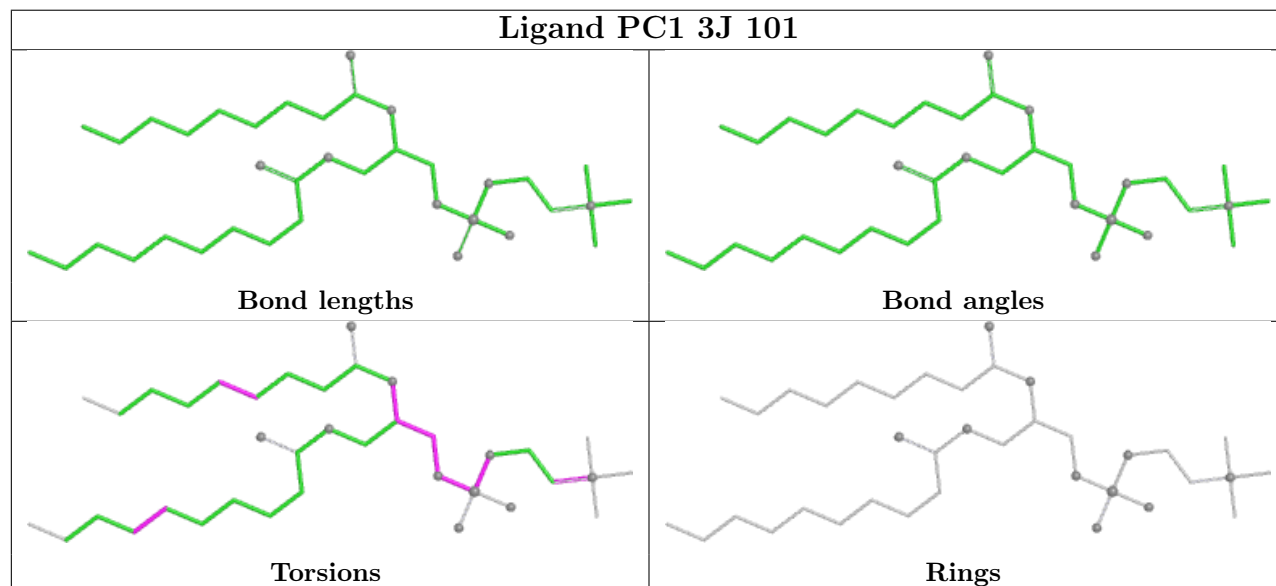


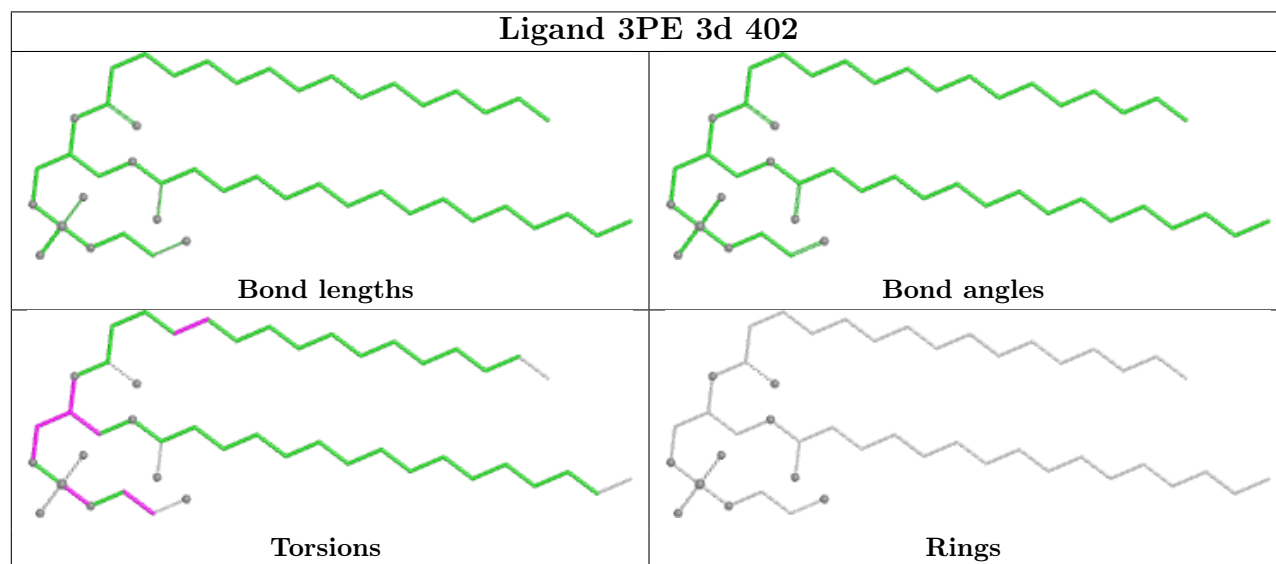
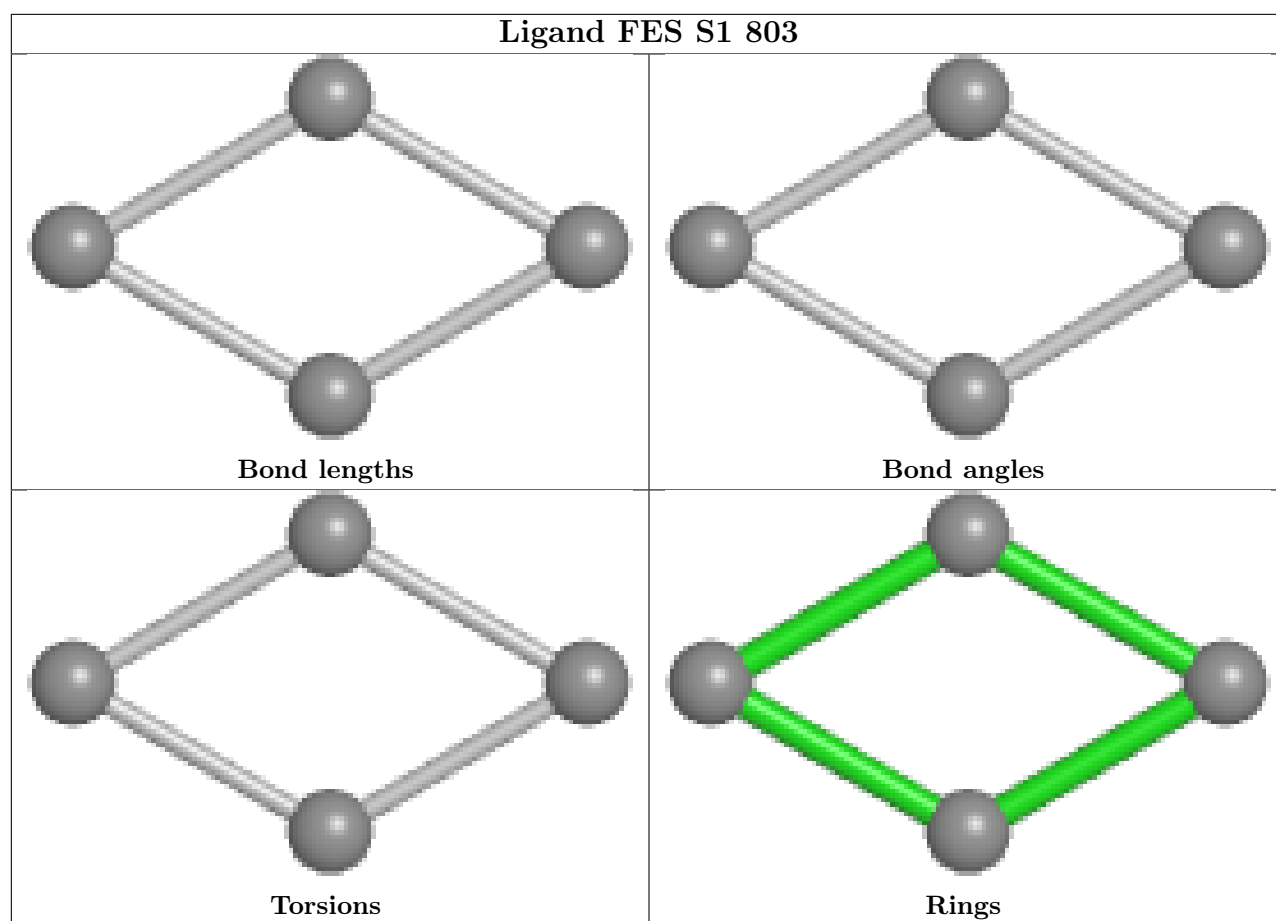


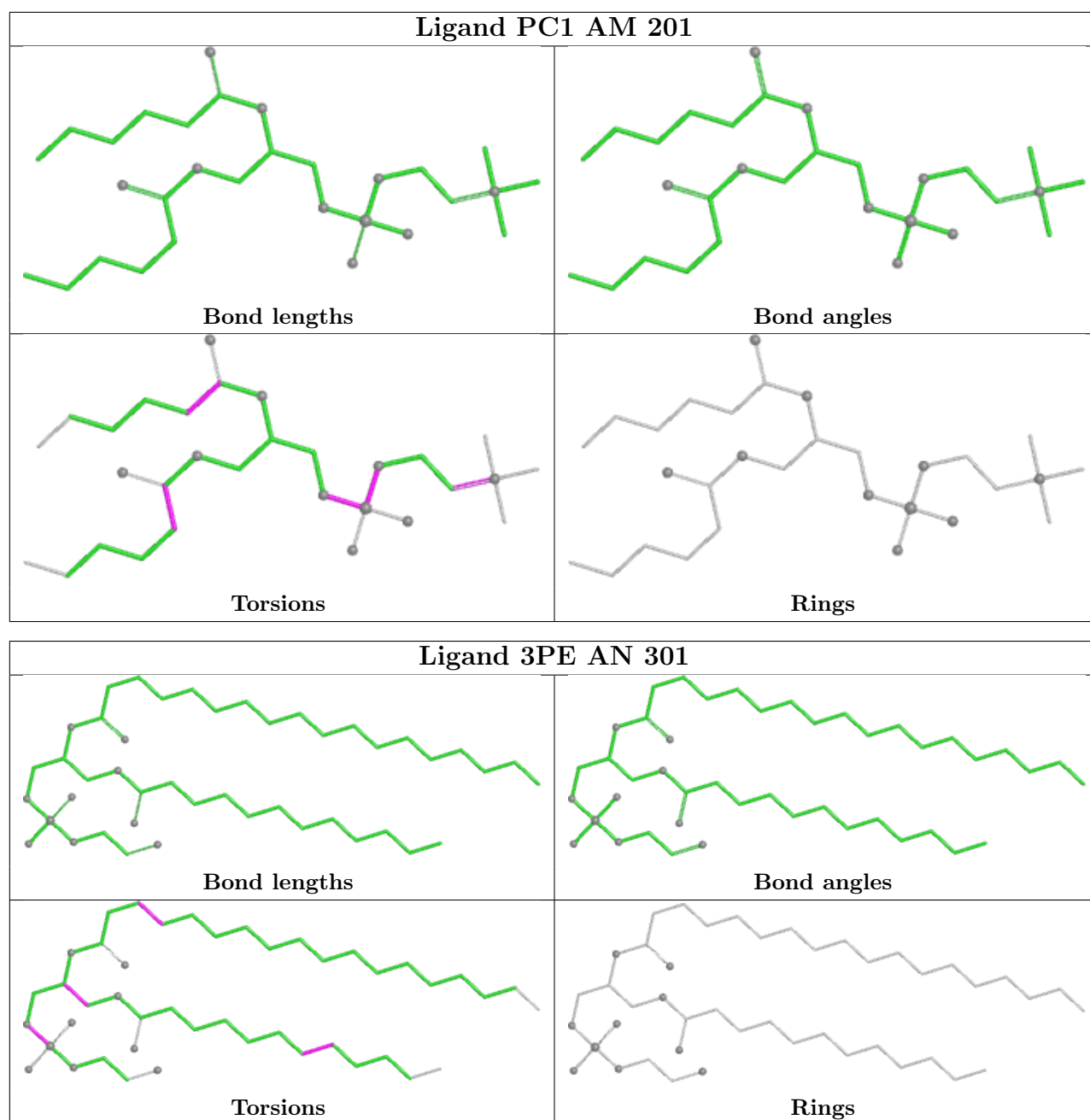
## Ligand FMN V1 501

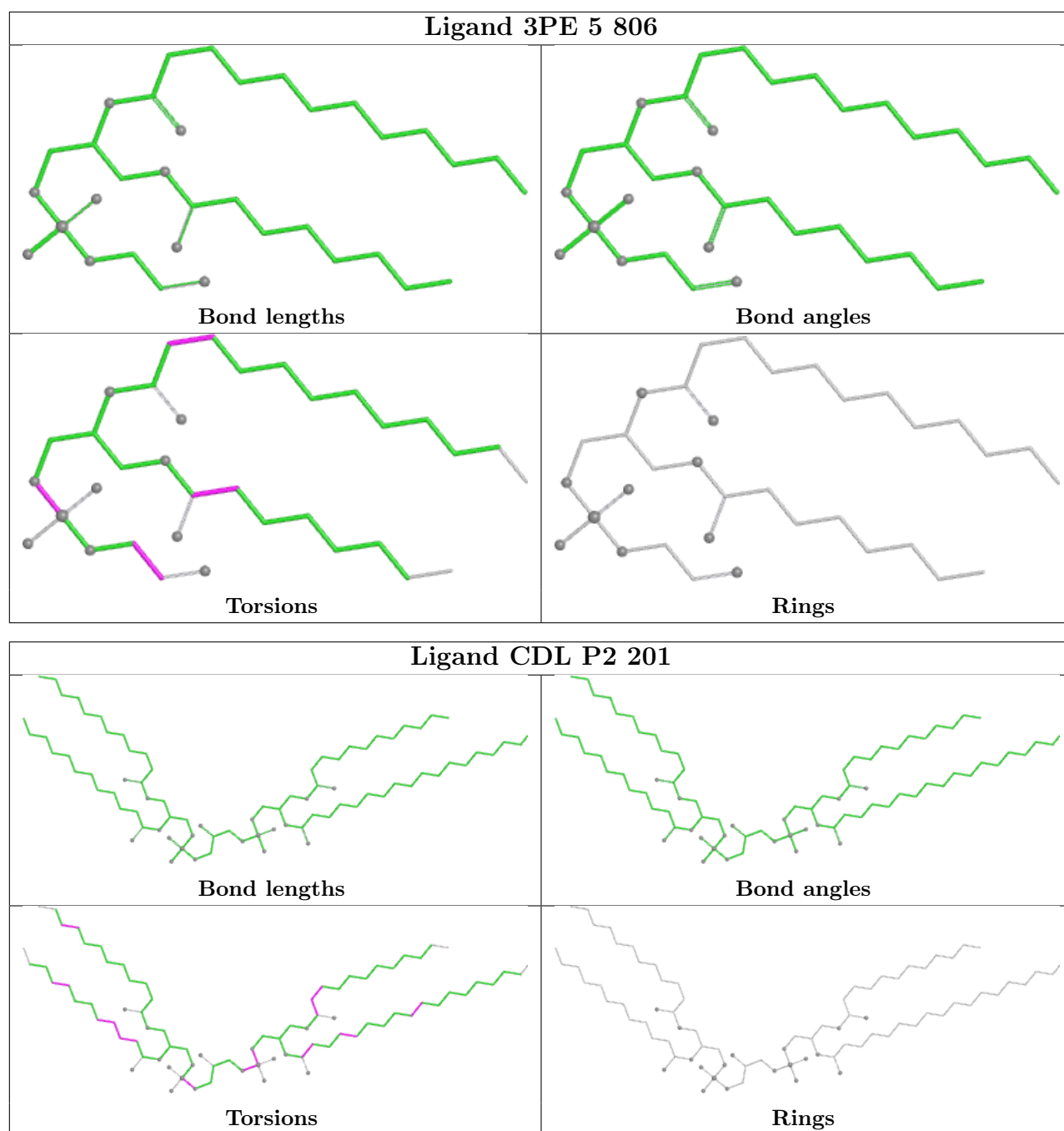


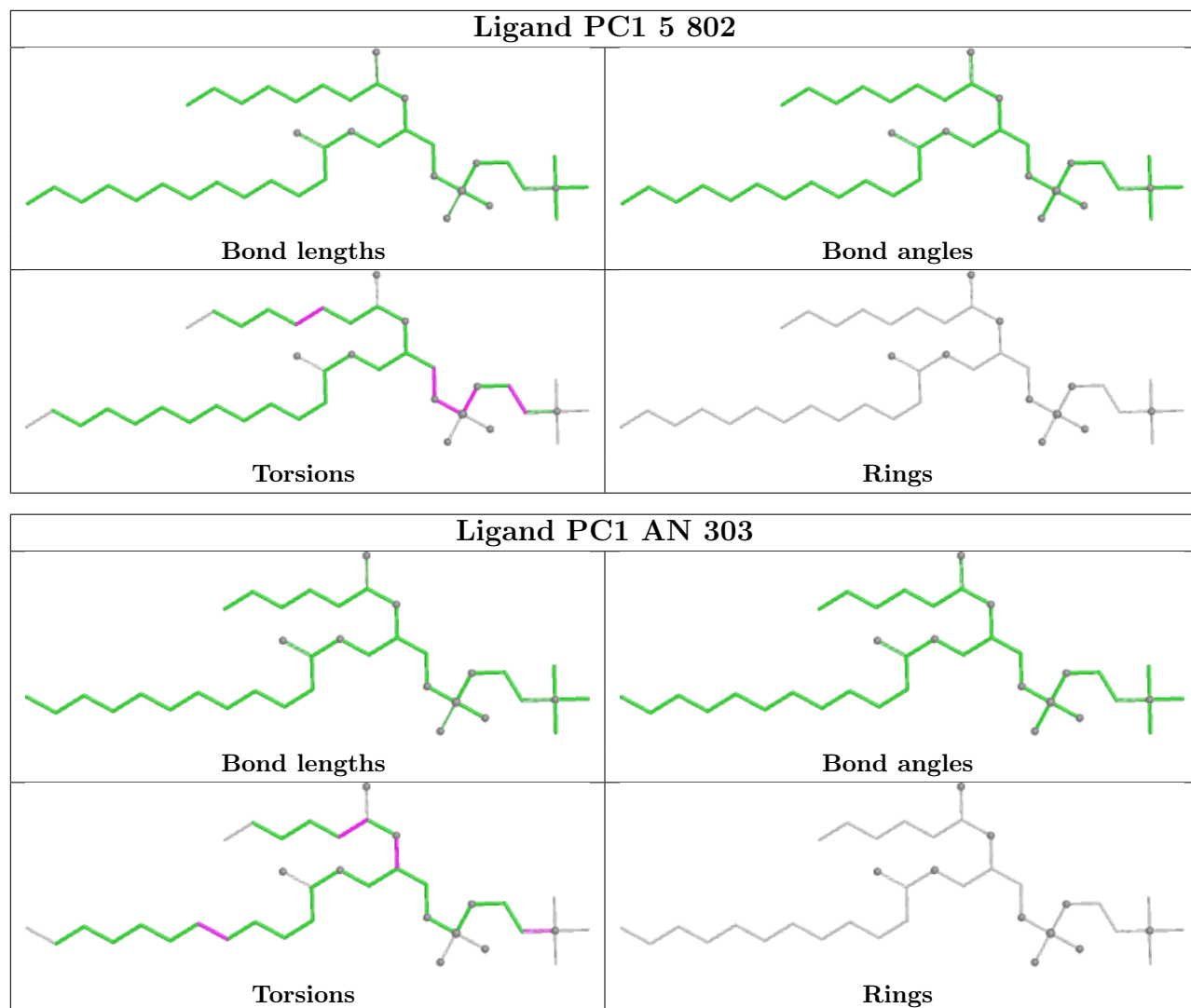
## Ligand PC1 3J 101

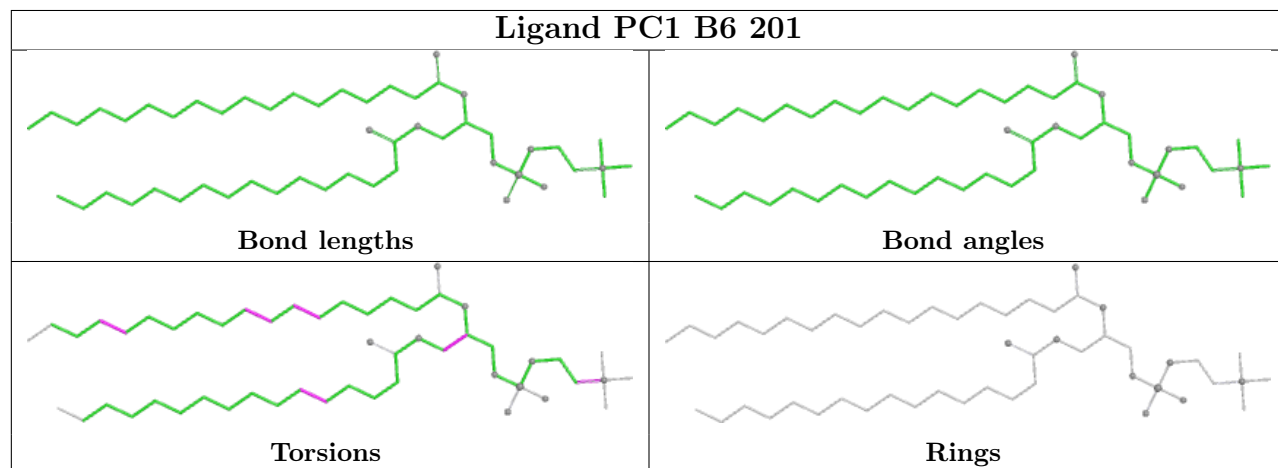
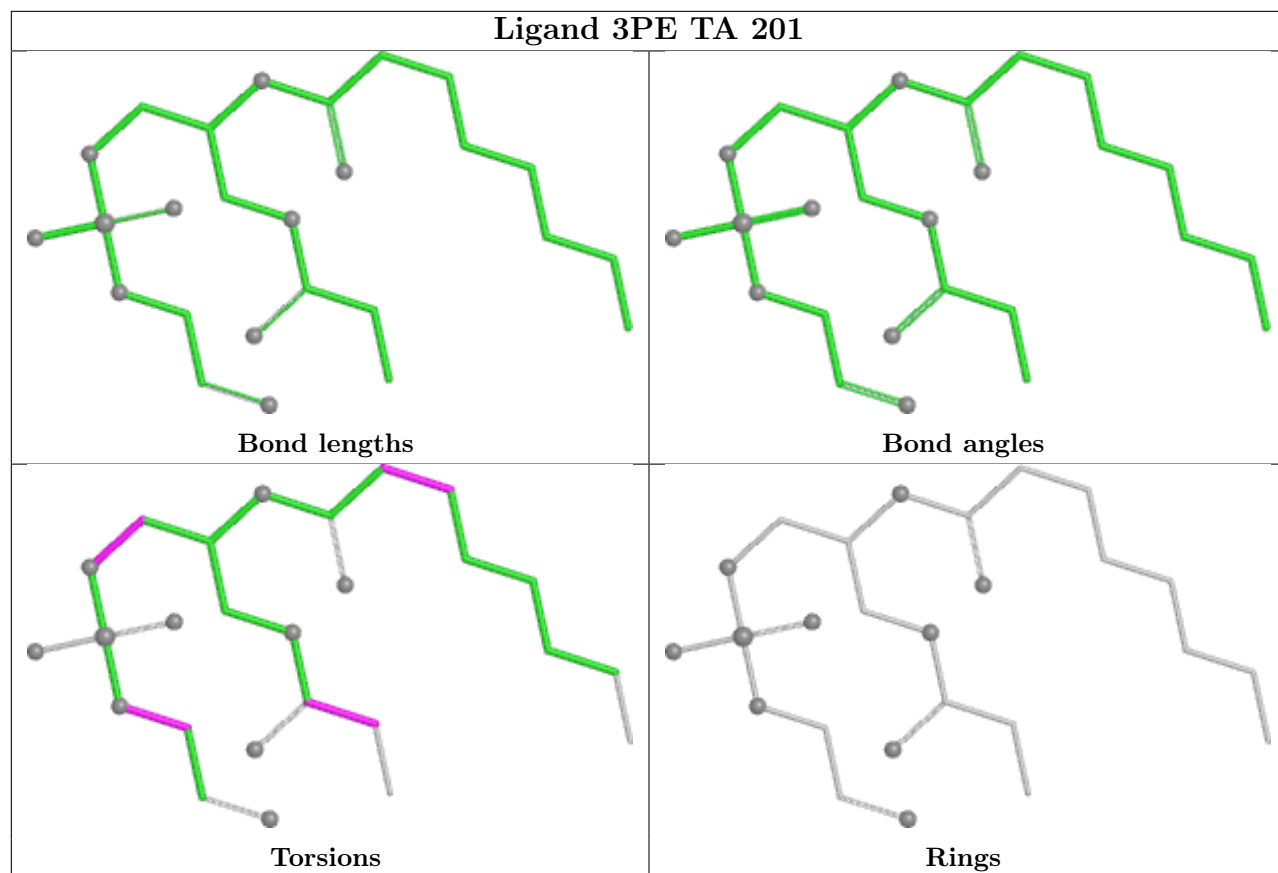


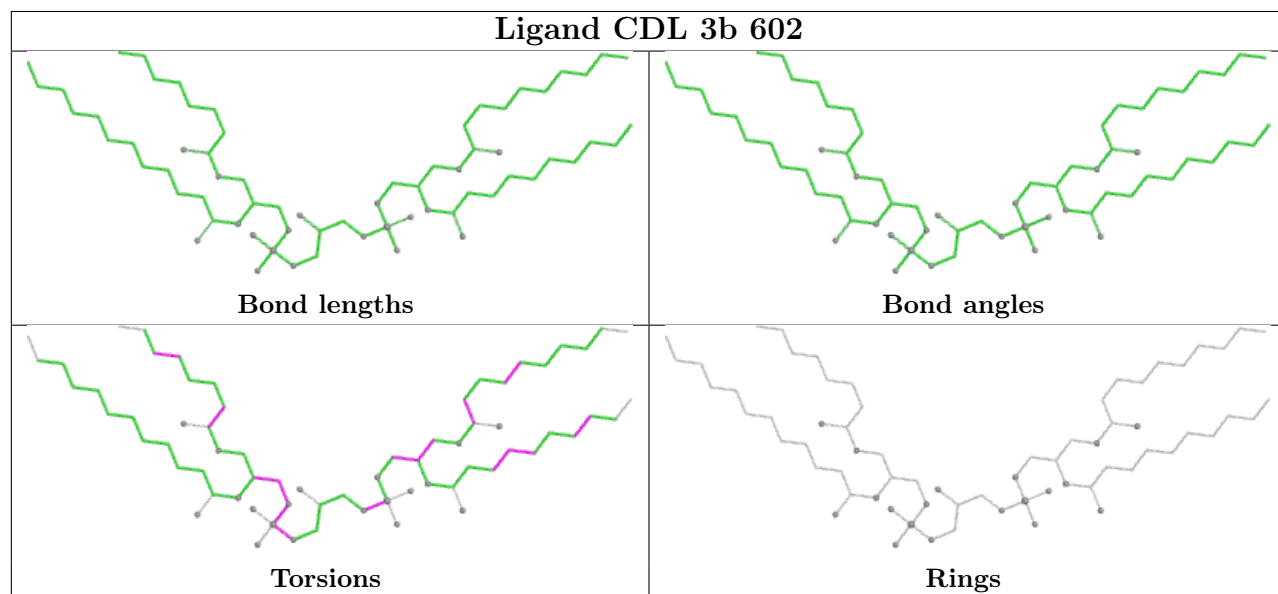
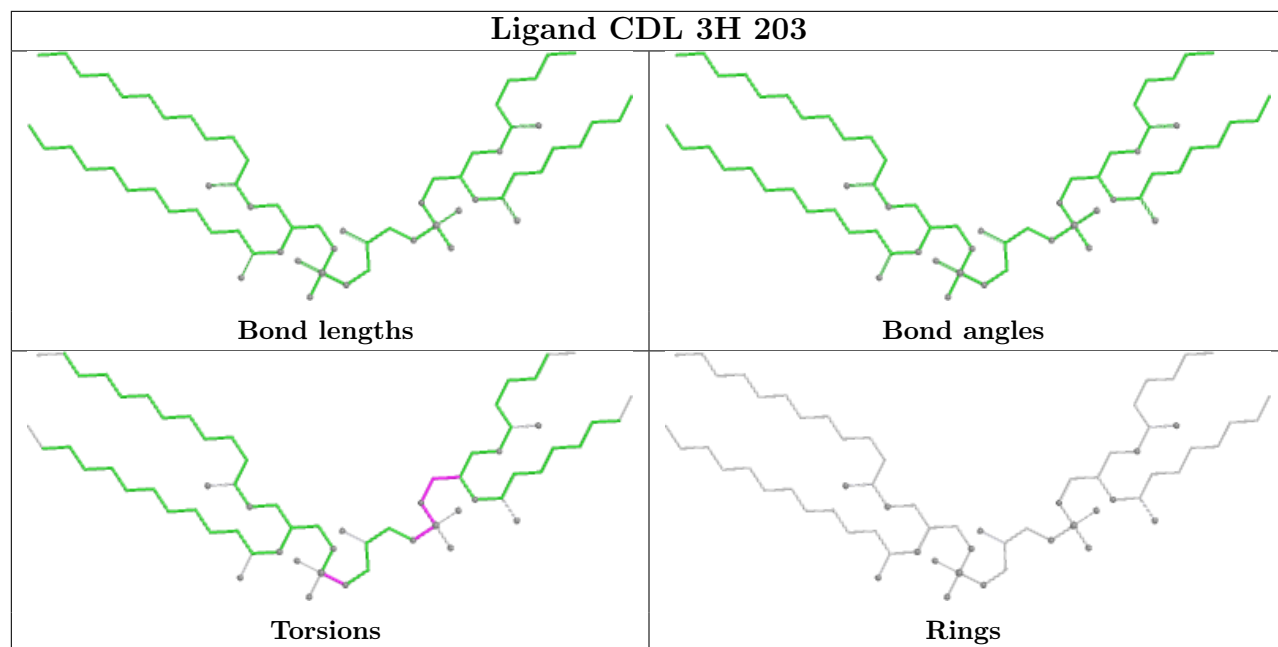




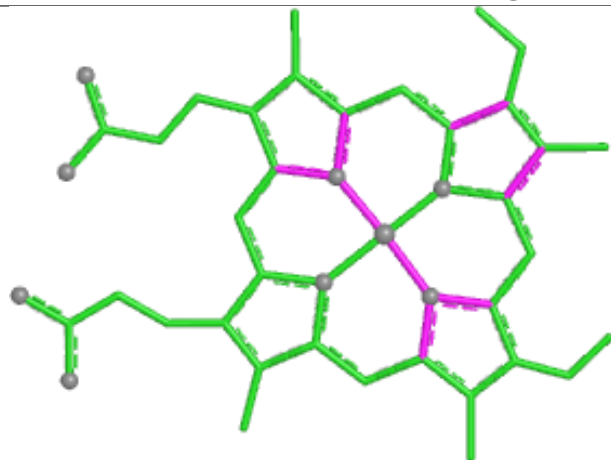




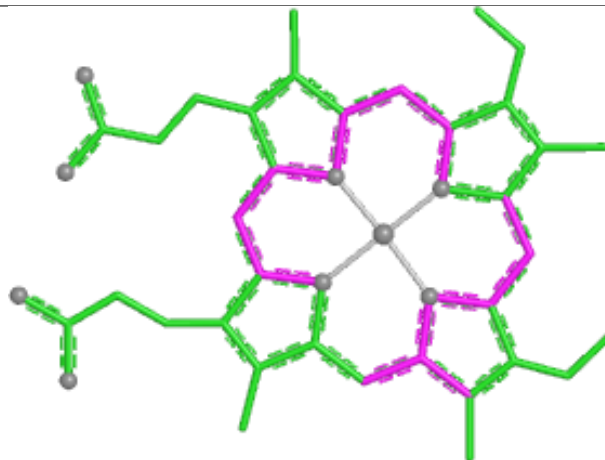




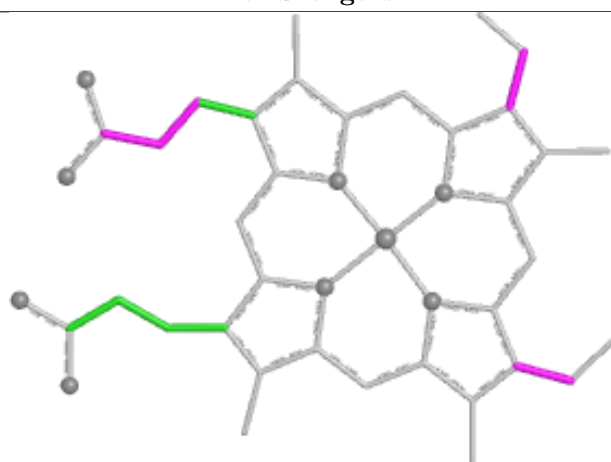
## Ligand HEM 3c 502



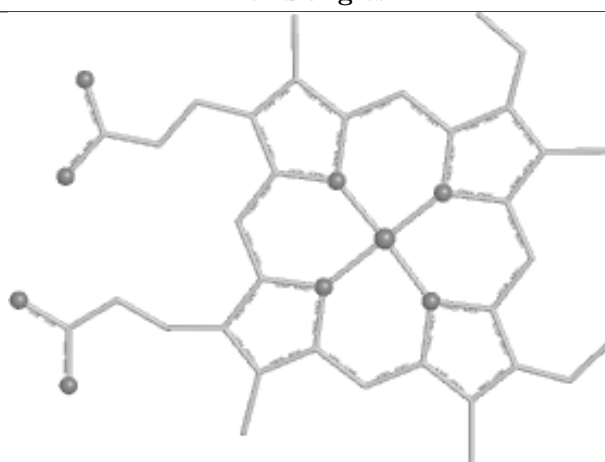
Bond lengths



Bond angles

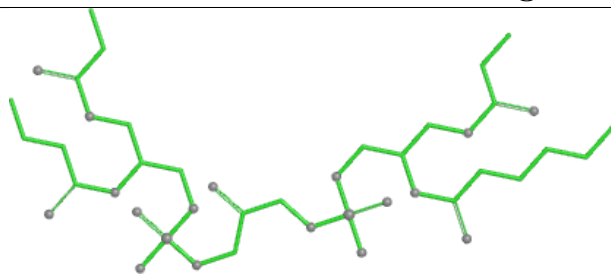


Torsions

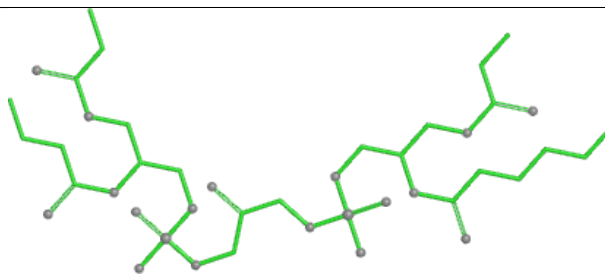


Rings

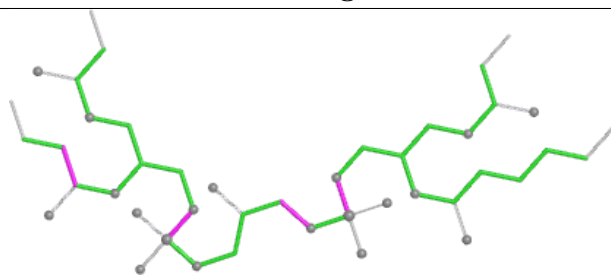
## Ligand CDL 3 202



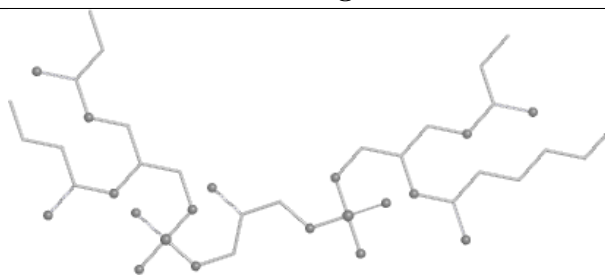
Bond lengths



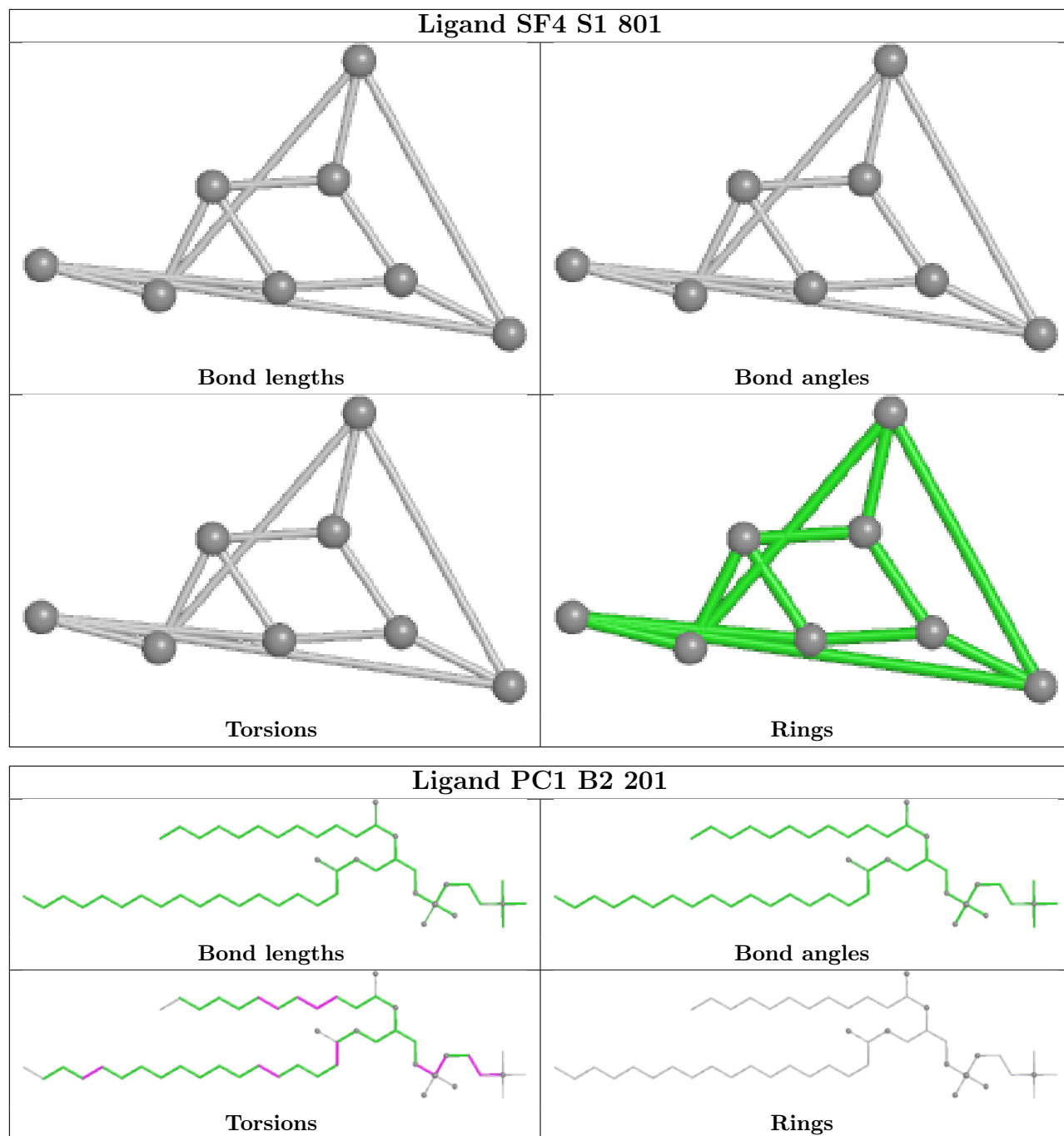
Bond angles

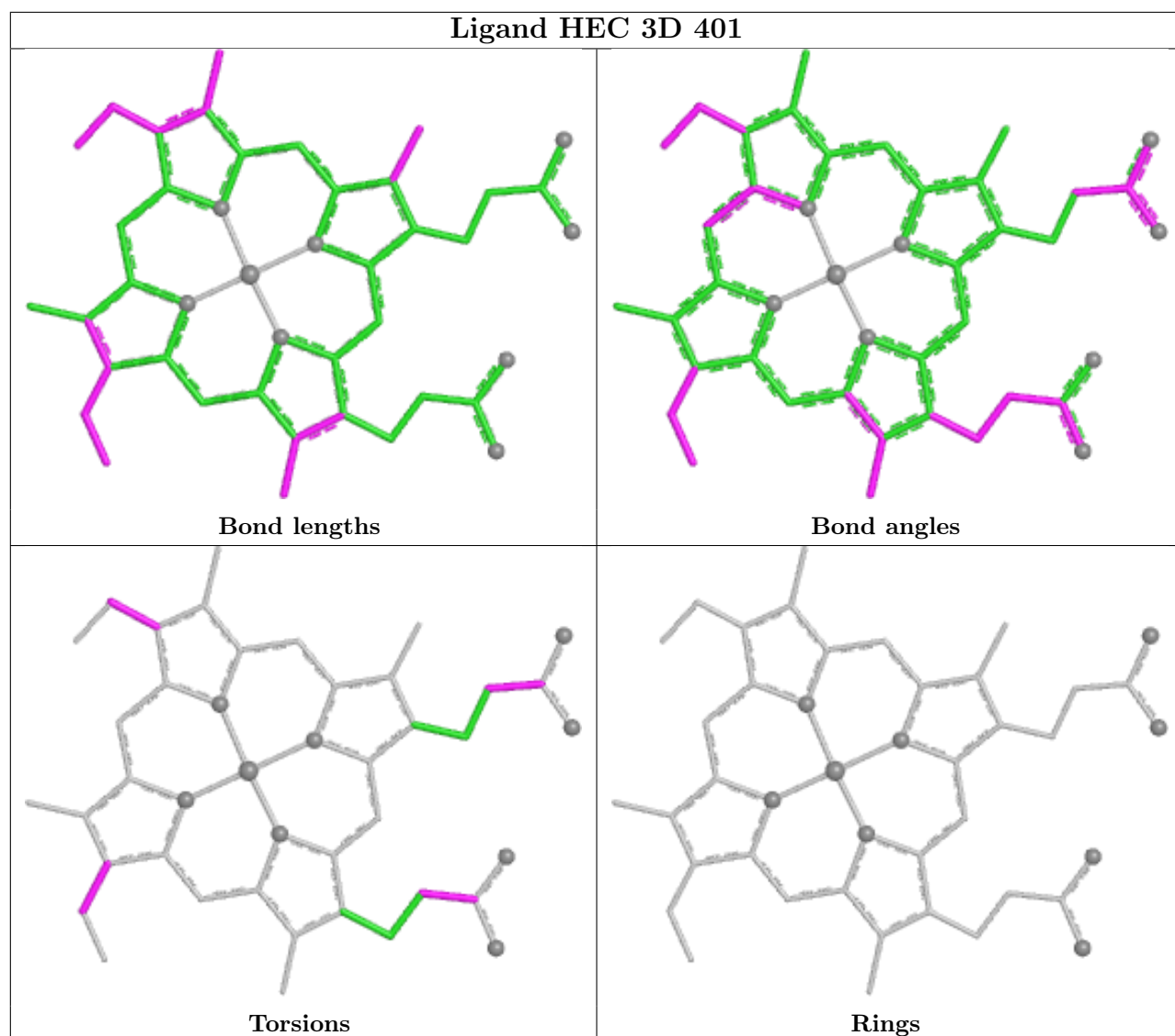
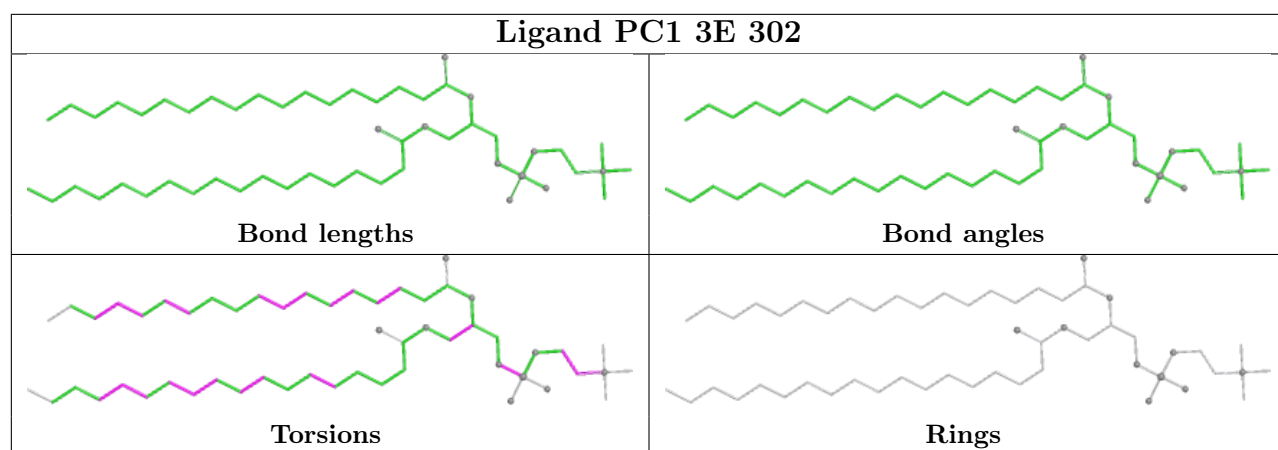


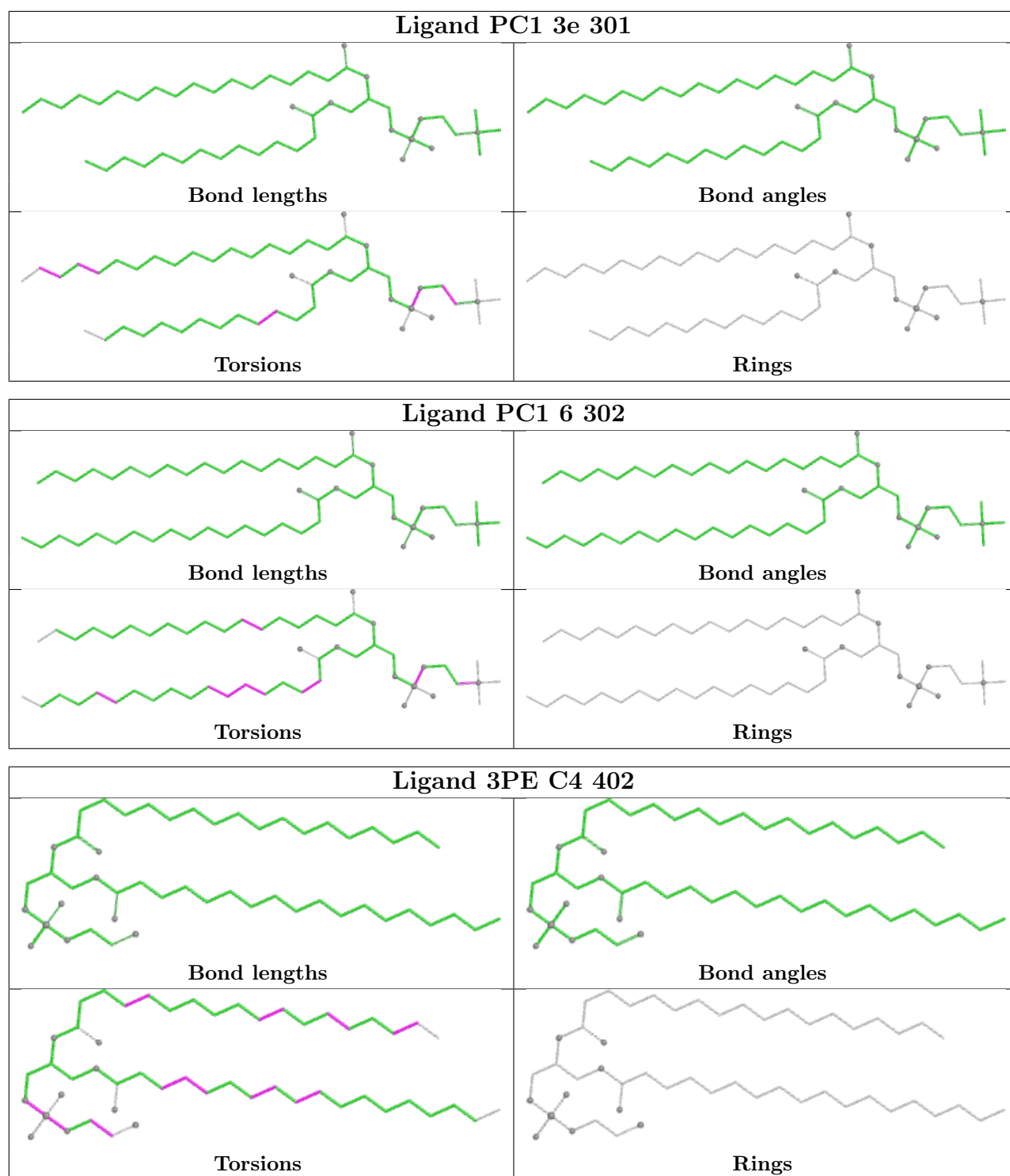
Torsions

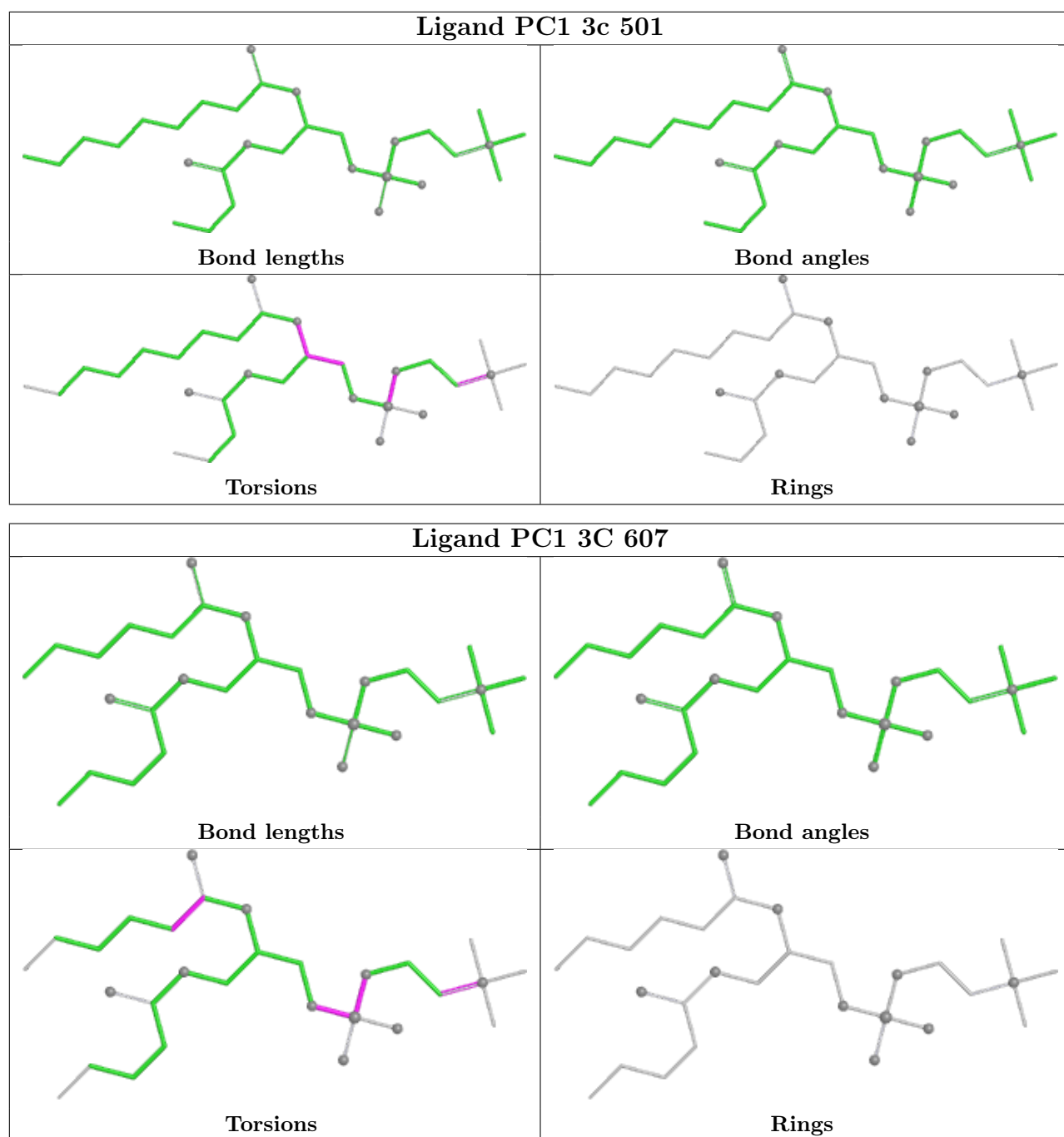


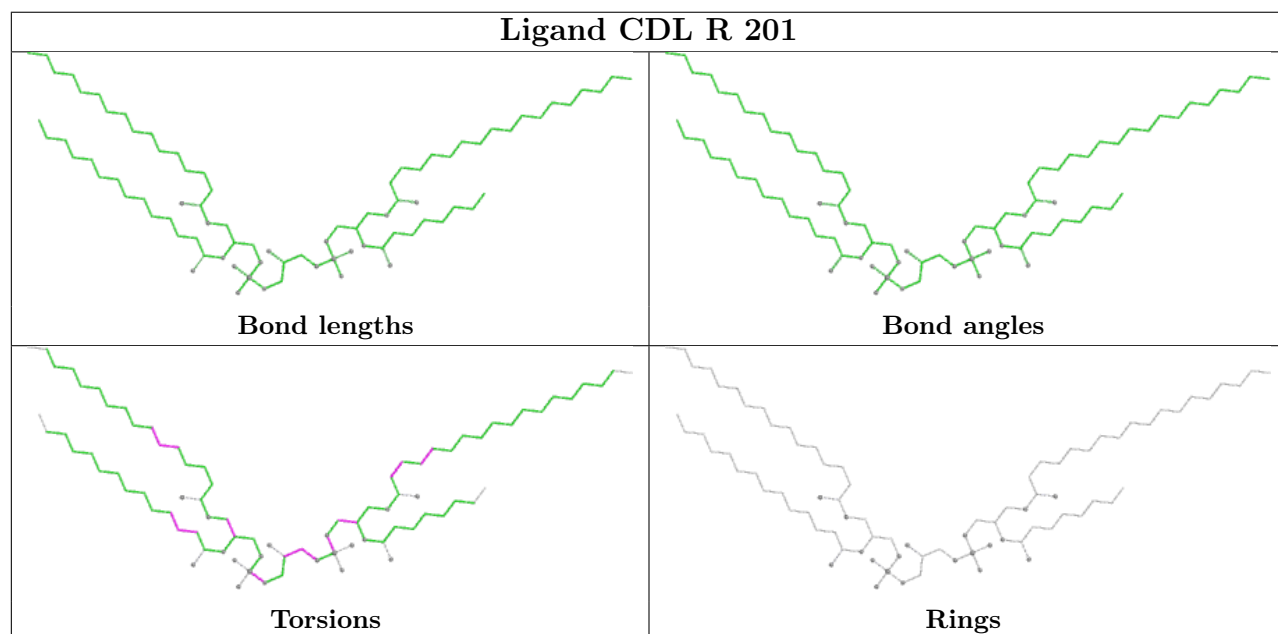
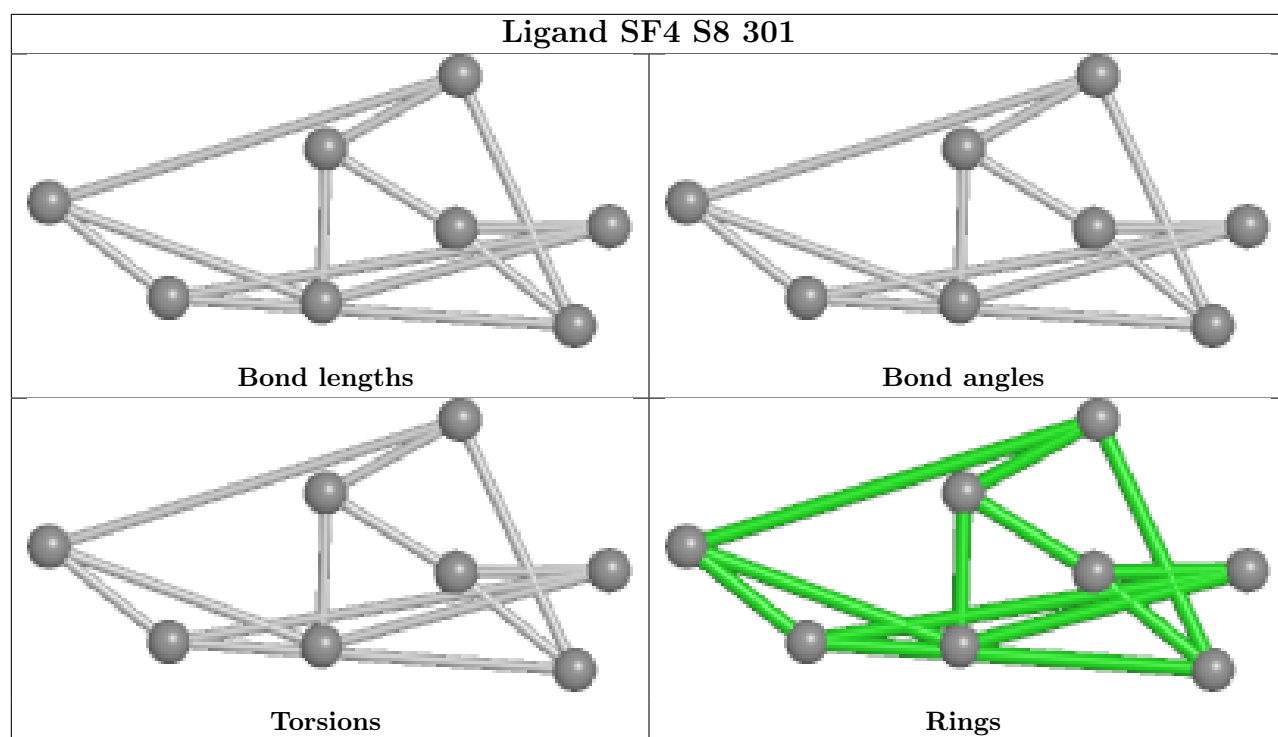
Rings



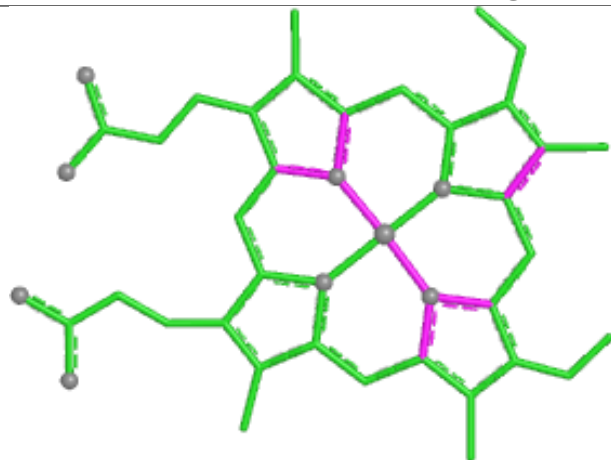




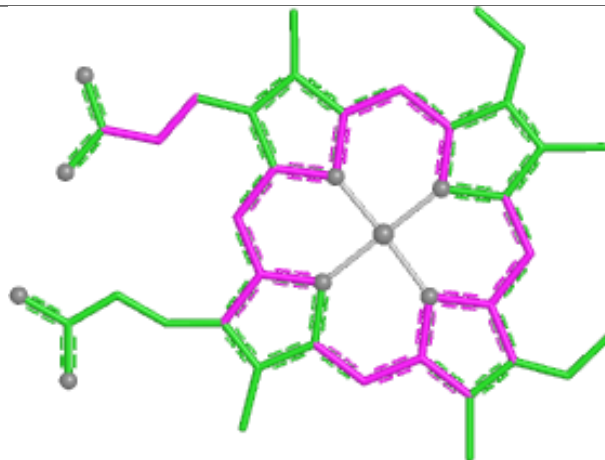




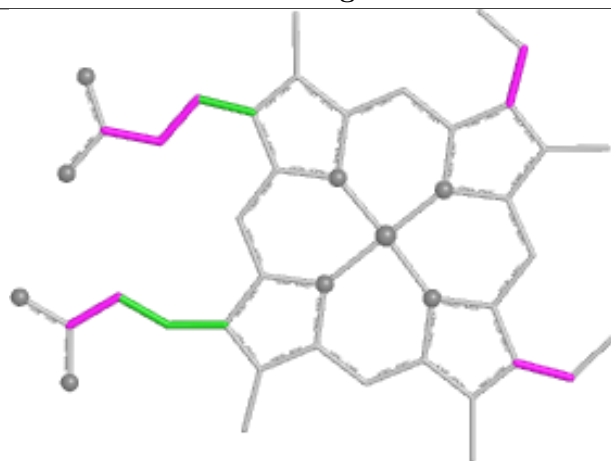
## Ligand HEM 3c 503



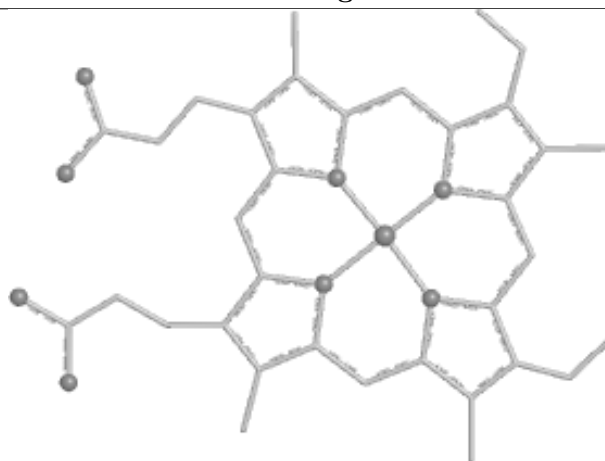
Bond lengths



Bond angles

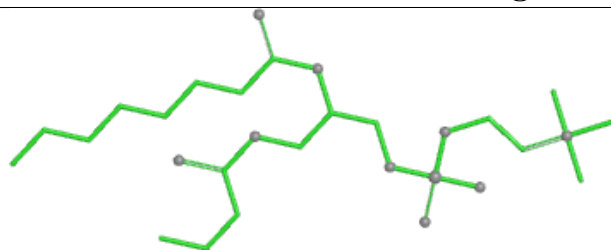


Torsions

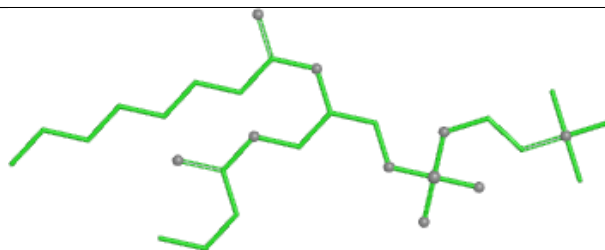


Rings

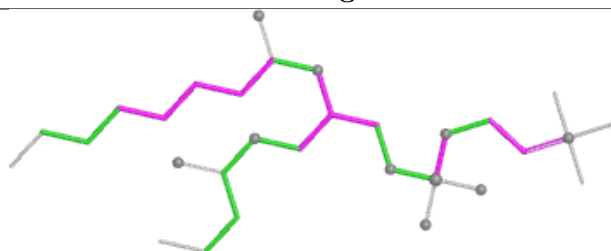
## Ligand PC1 3b 601



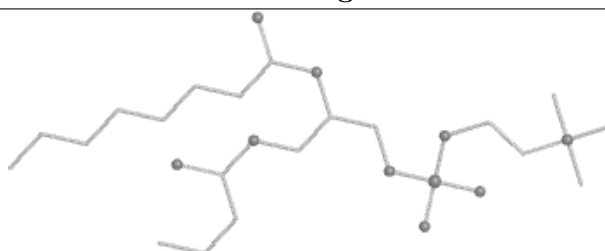
Bond lengths



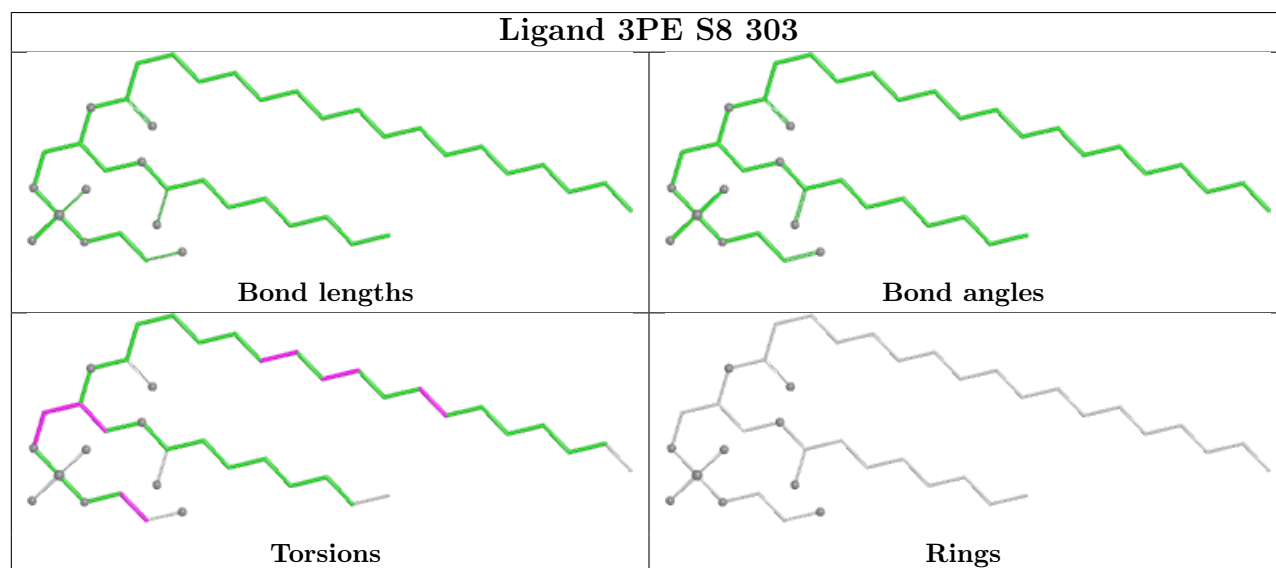
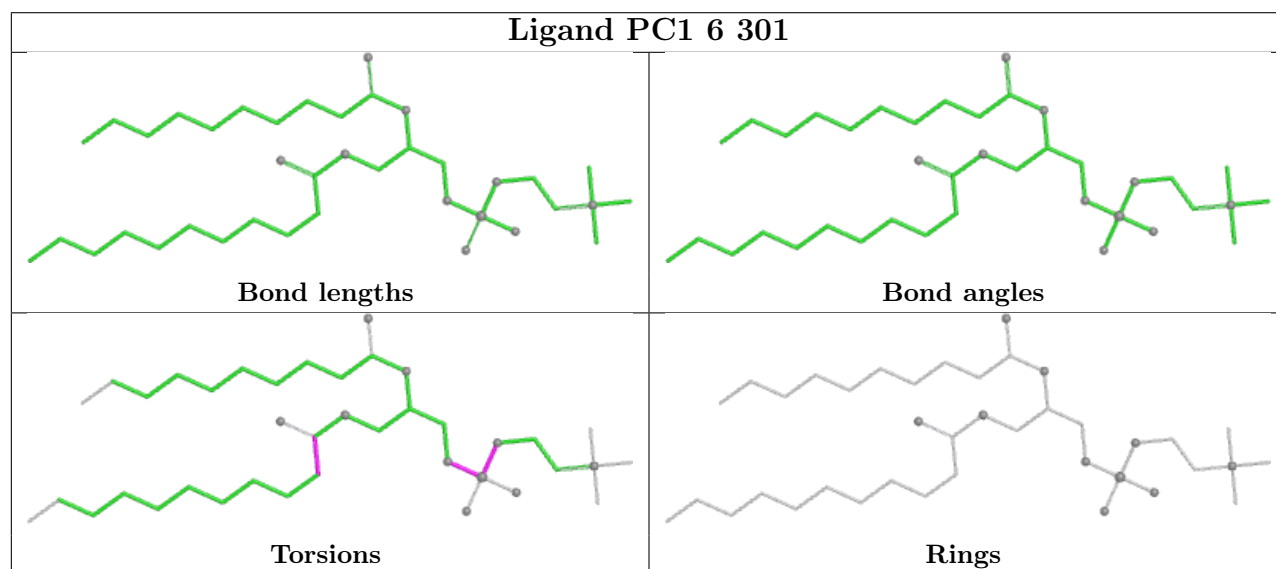
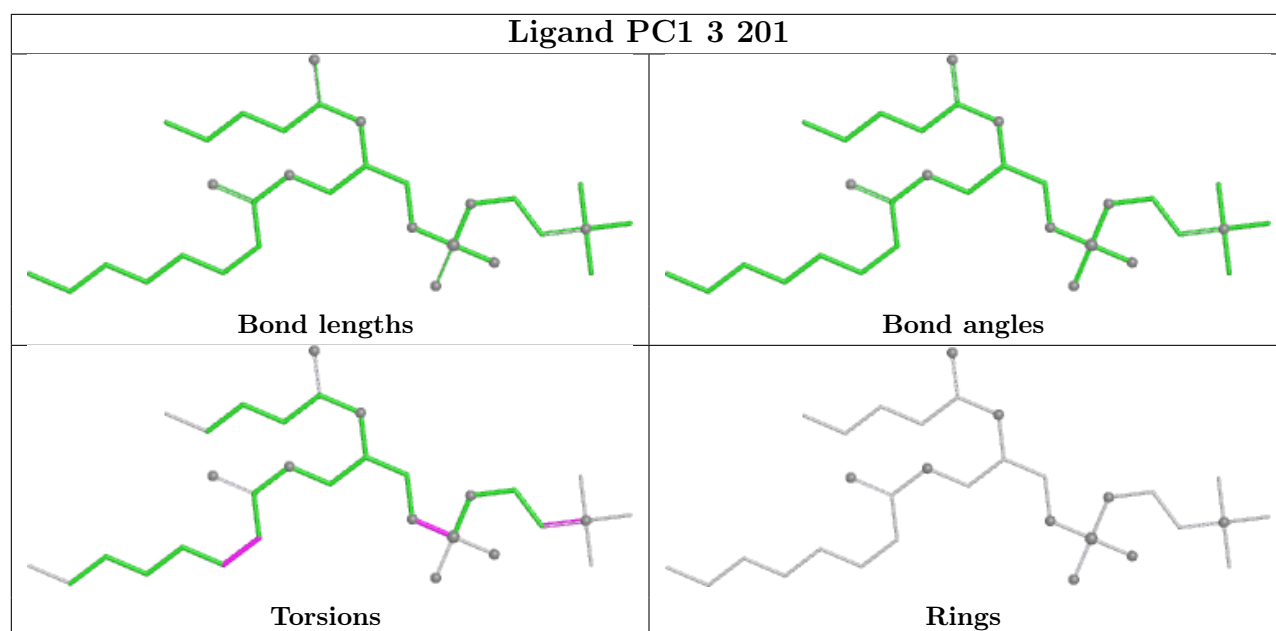
Bond angles

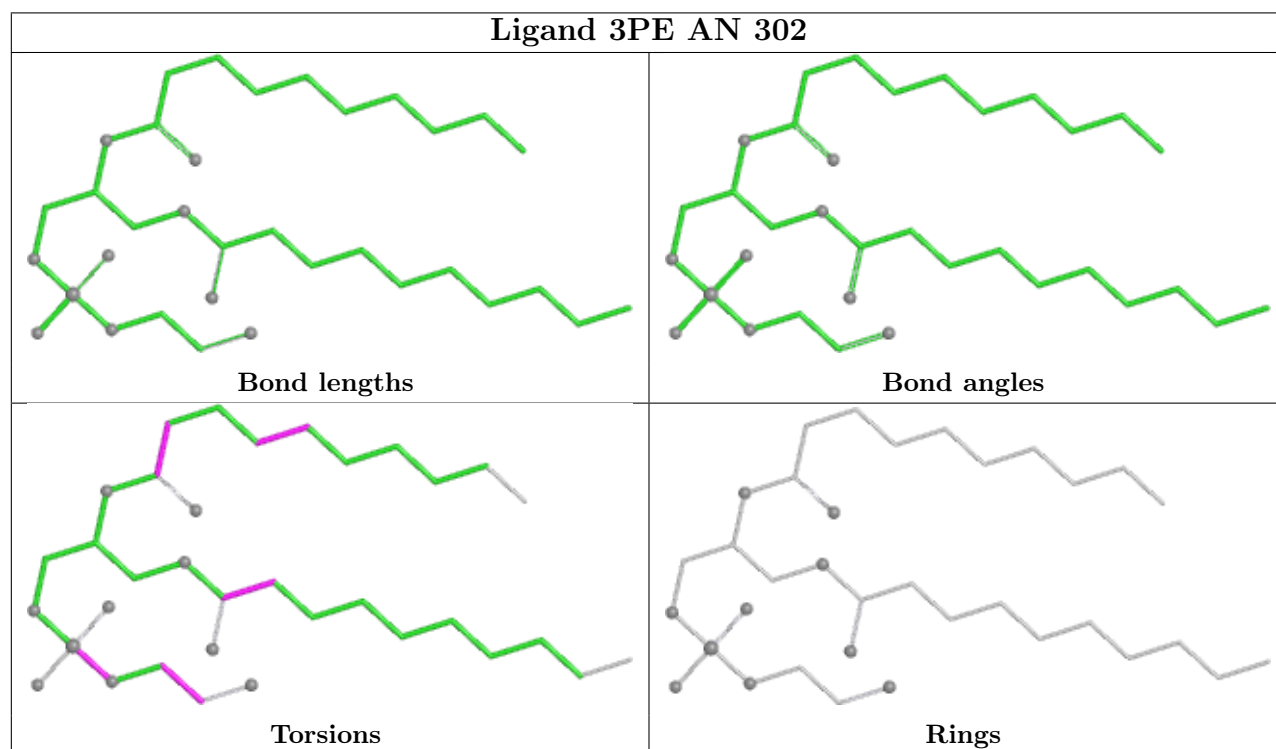
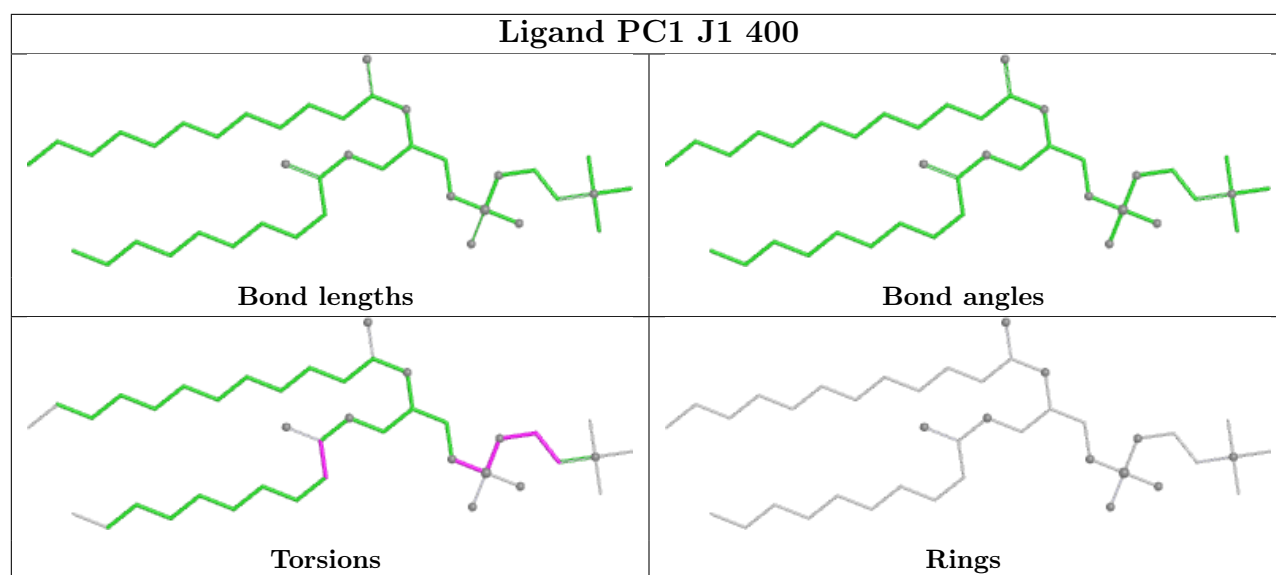


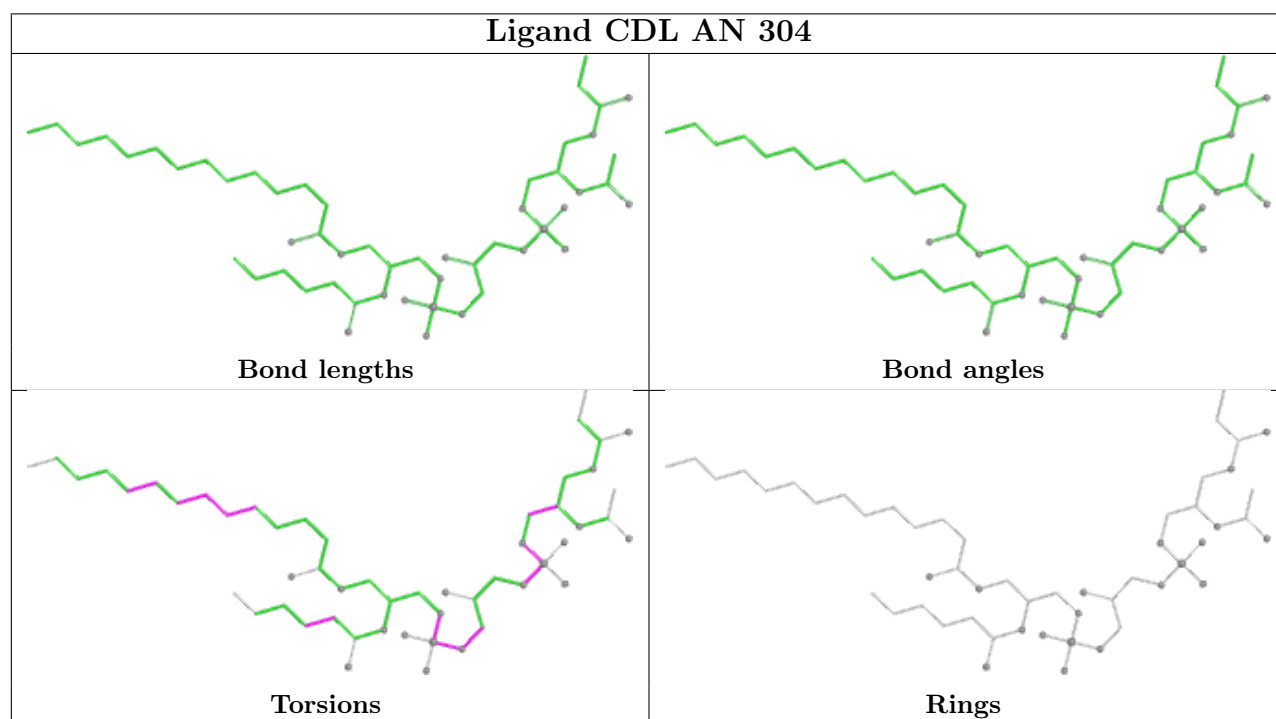
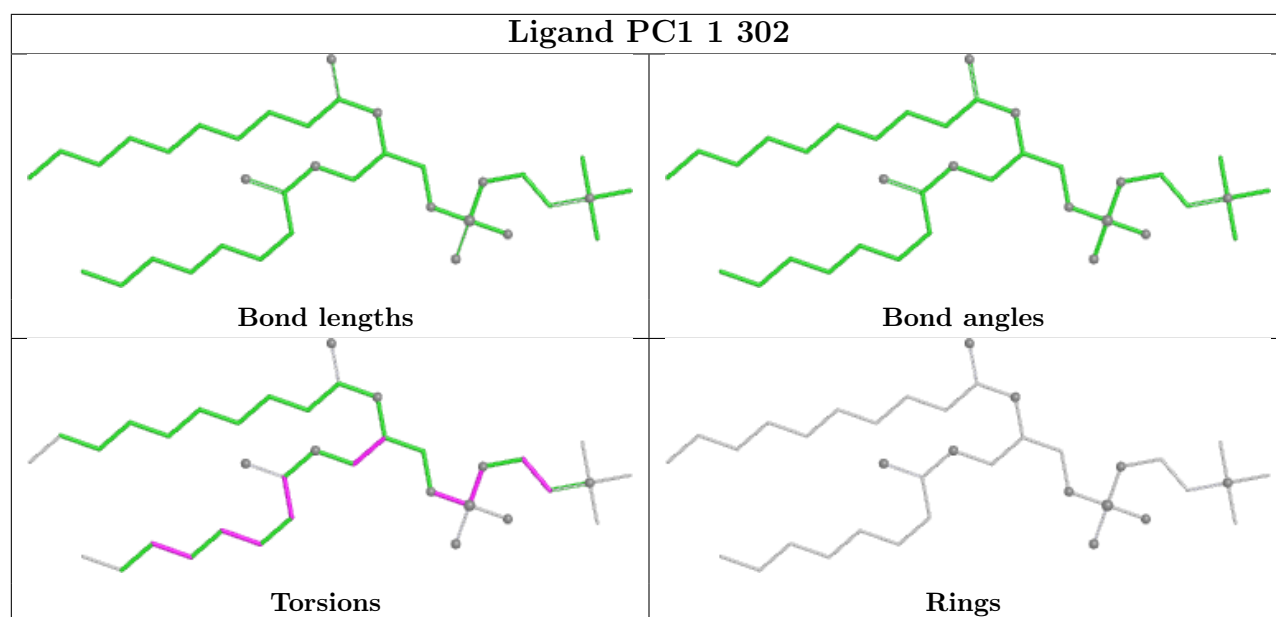
Torsions

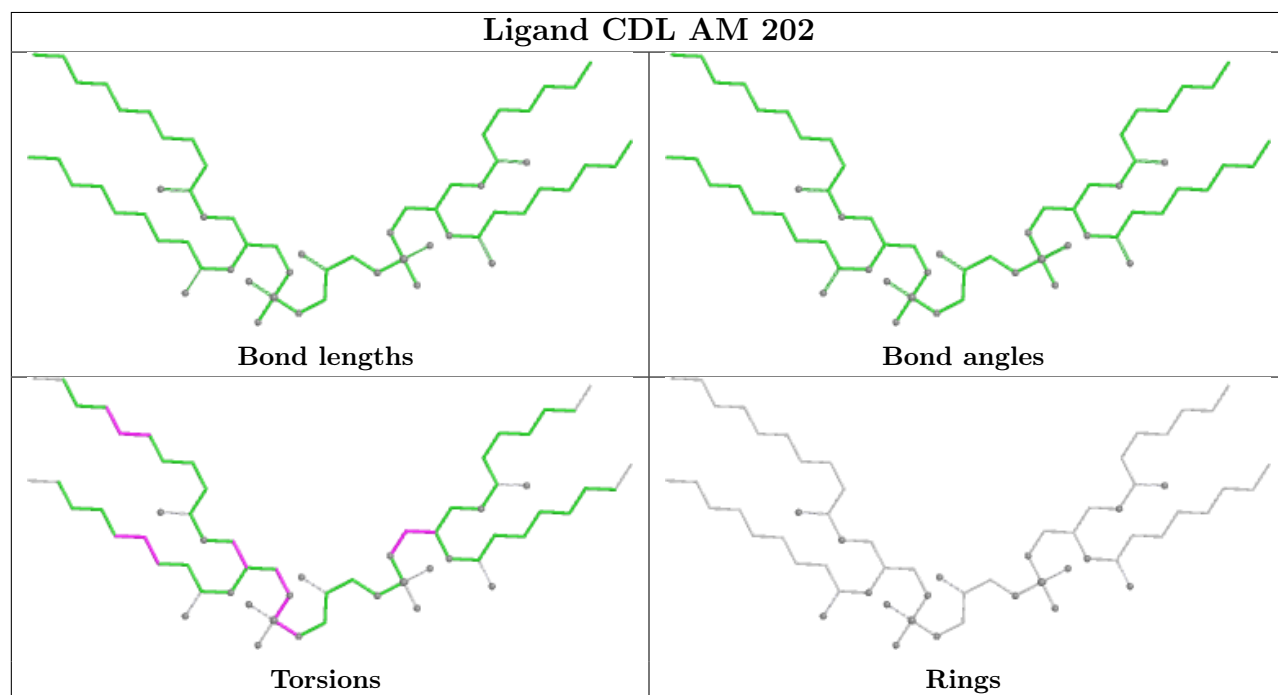
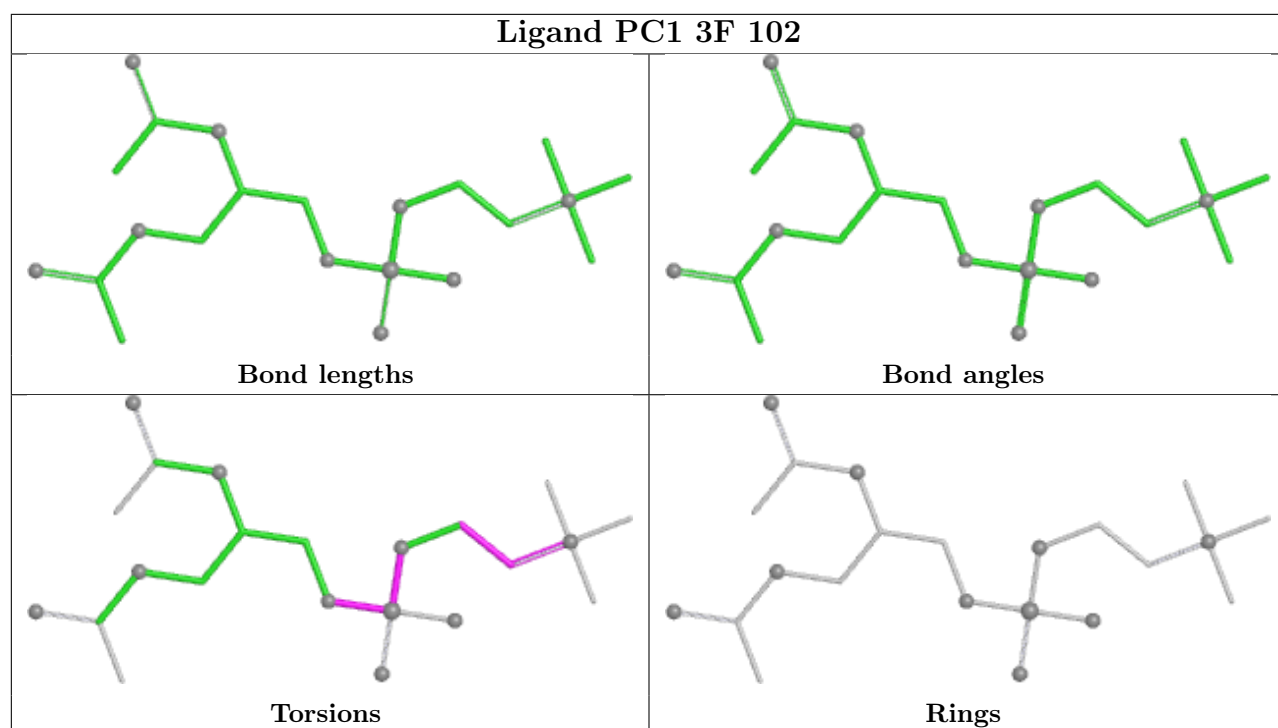


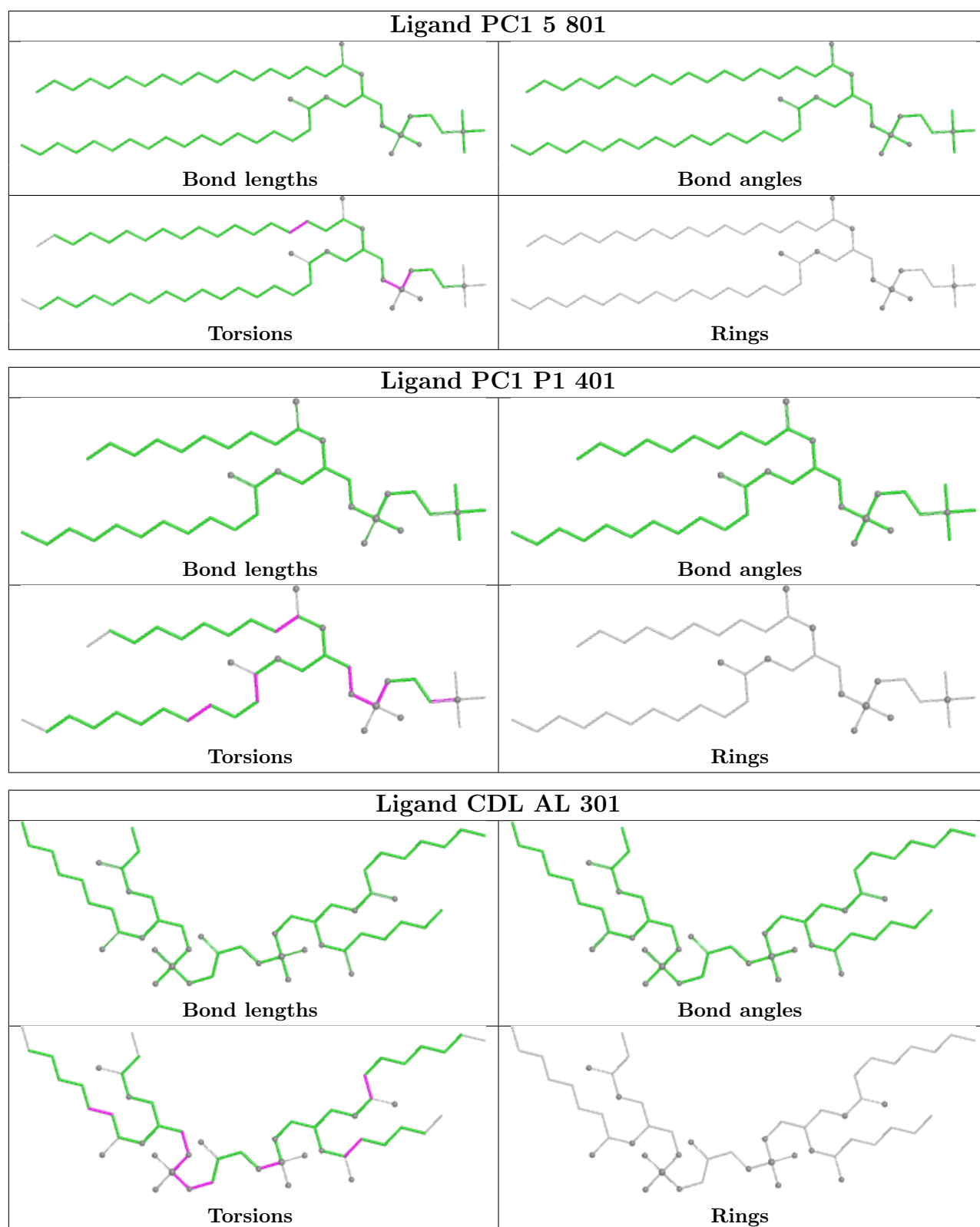
Rings











## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

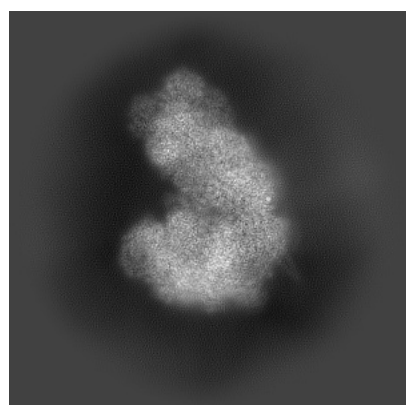
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25882. These allow visual inspection of the internal detail of the map and identification of artifacts.

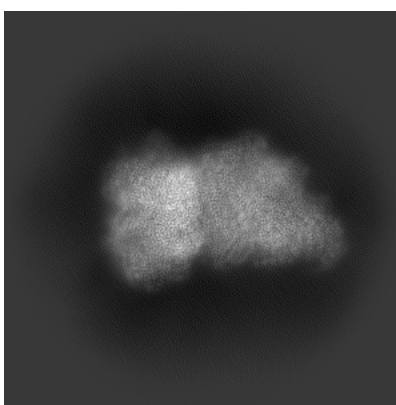
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

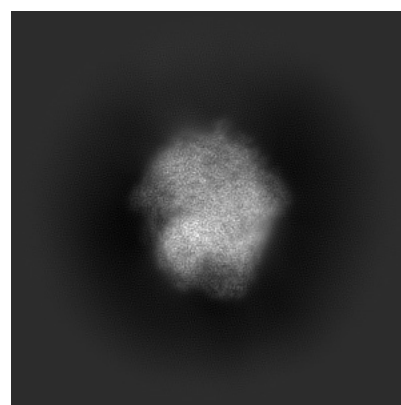
#### 6.1.1 Primary map



X



Y

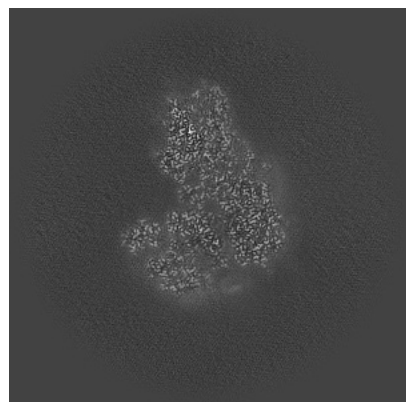


Z

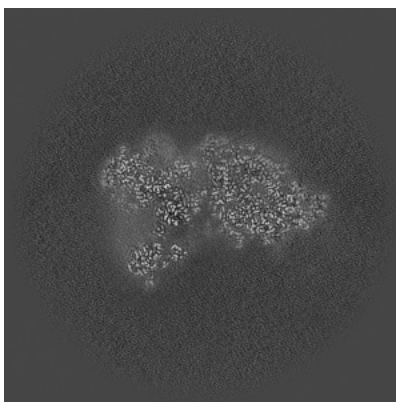
The images above show the map projected in three orthogonal directions.

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

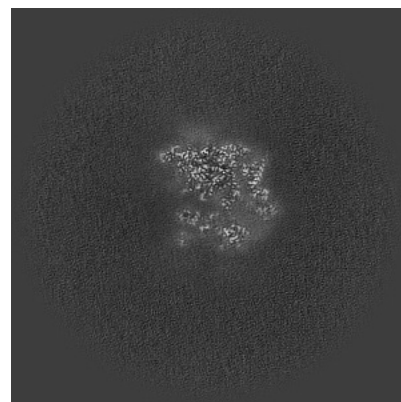
#### 6.2.1 Primary map



X Index: 300



Y Index: 300

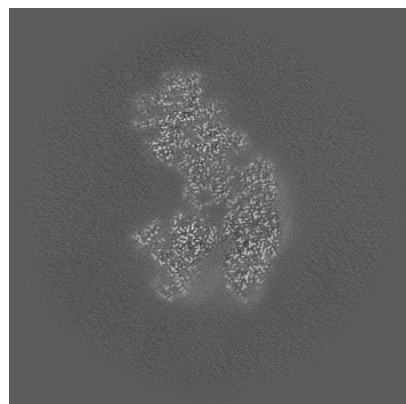


Z Index: 300

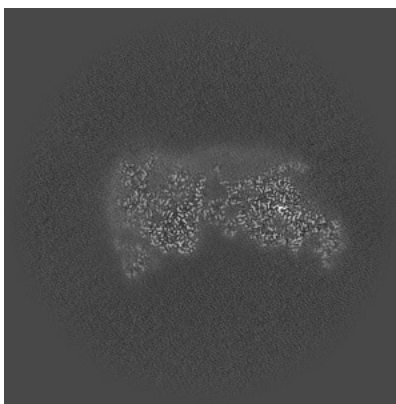
The images above show central slices of the map in three orthogonal directions.

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

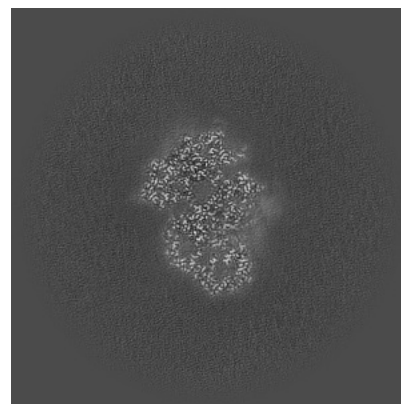
### 6.3.1 Primary map



X Index: 276



Y Index: 271

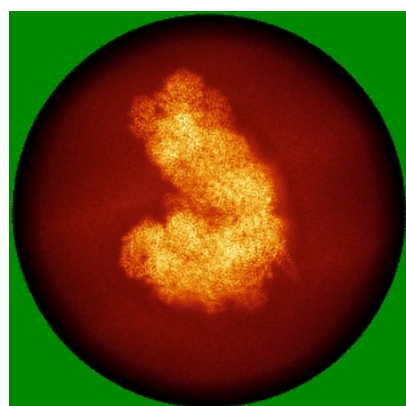


Z Index: 248

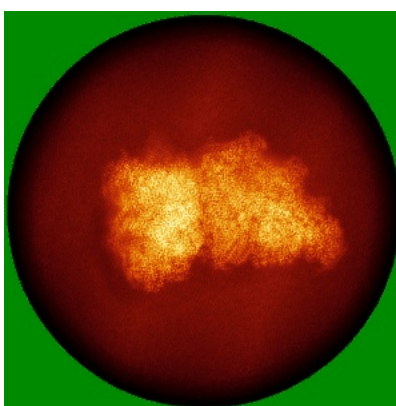
The images above show the largest variance slices of the map in three orthogonal directions.

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

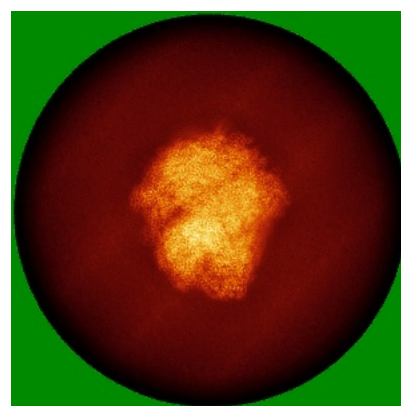
### 6.4.1 Primary map



X



Y



Z

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

## 6.5 Orthogonal surface views

This section was not generated.

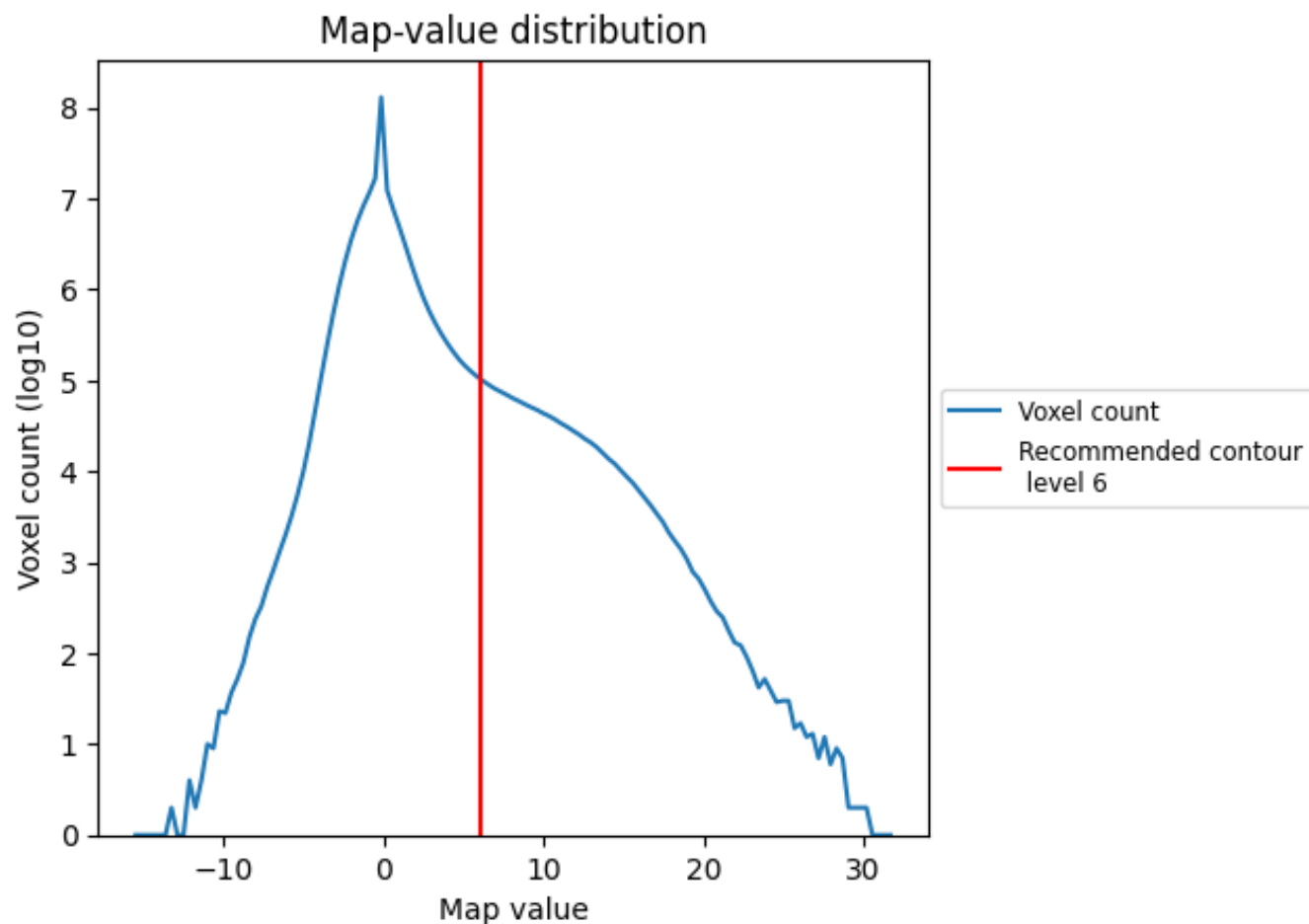
## 6.6 Mask visualisation

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

## 7 Map analysis [i](#)

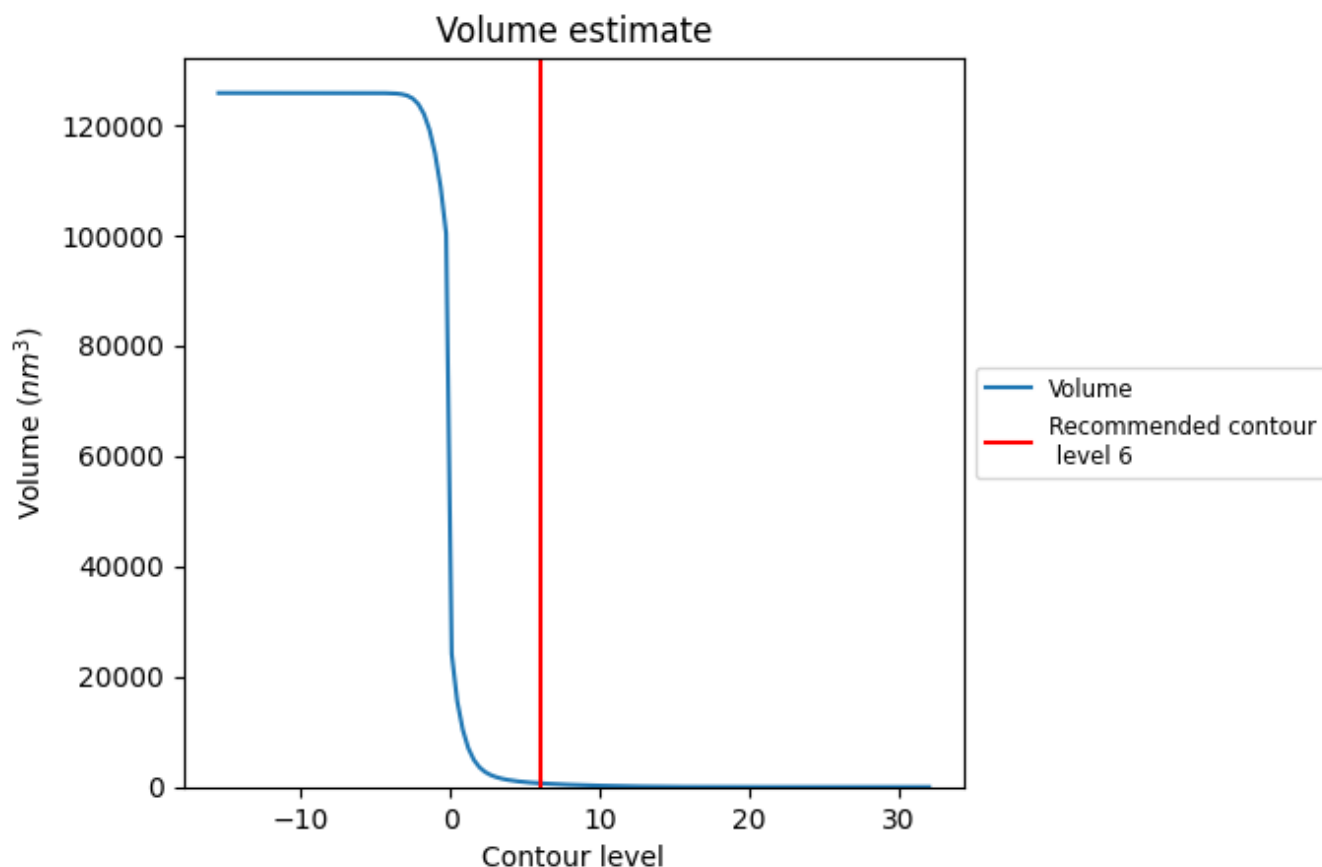
This section contains the results of statistical analysis of the map.

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



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

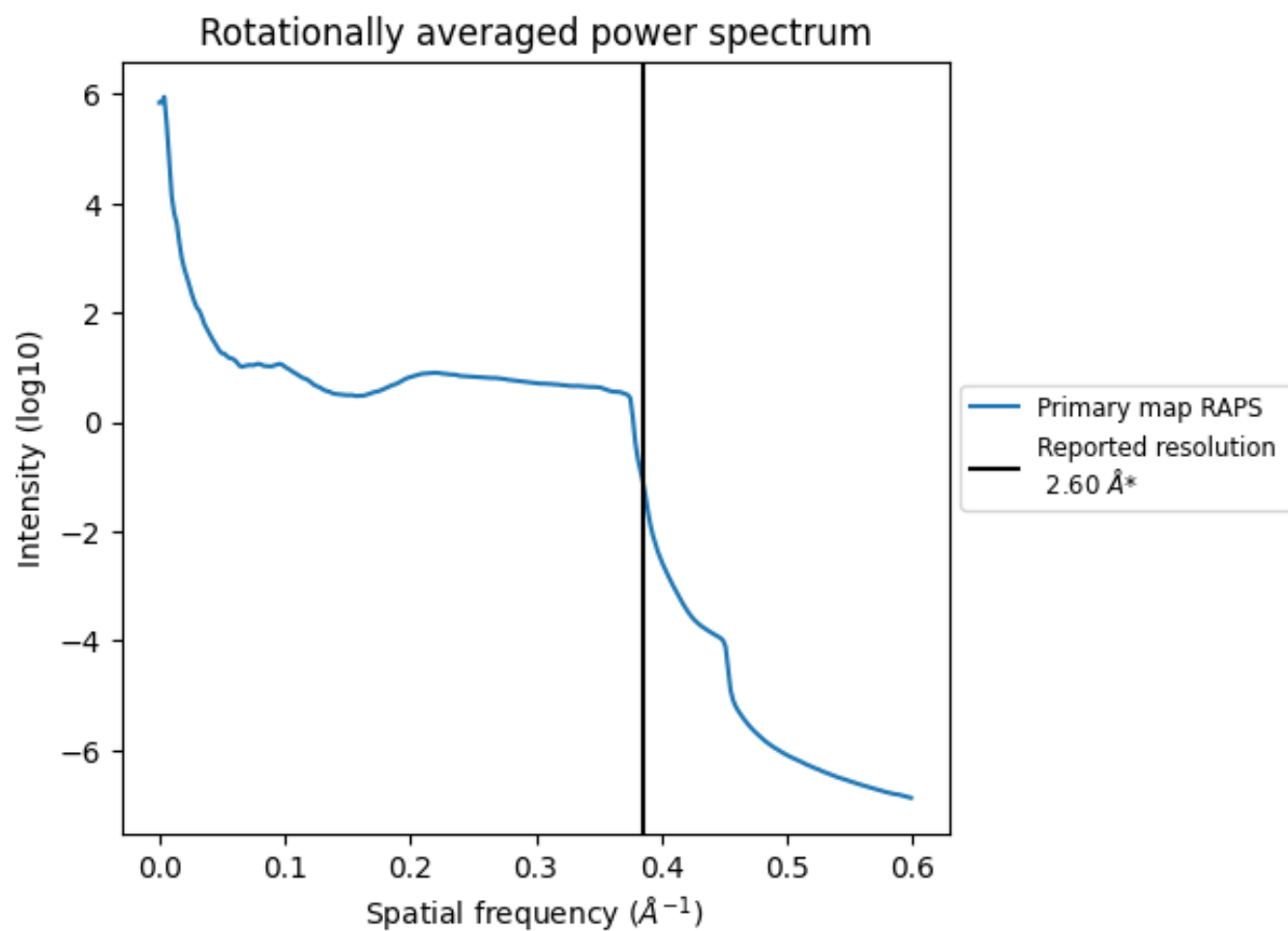
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 673 nm<sup>3</sup>; this corresponds to an approximate mass of 608 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

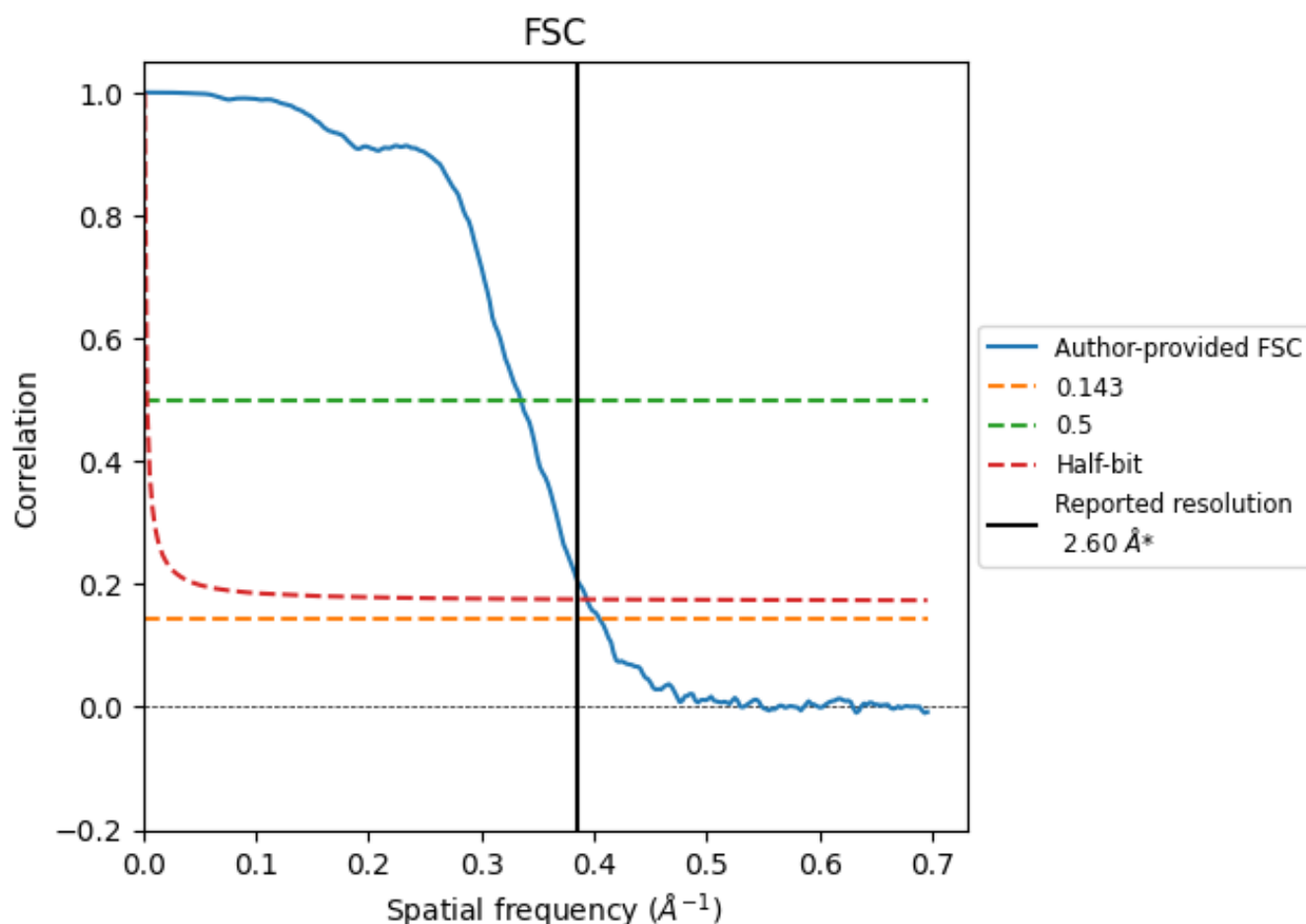


\*Reported resolution corresponds to spatial frequency of 0.385 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.385 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.60                               | -    | -        |
| Author-provided FSC curve | 2.47                               | 2.99 | 2.54     |
| Unmasked-calculated*      | -                                  | -    | -        |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

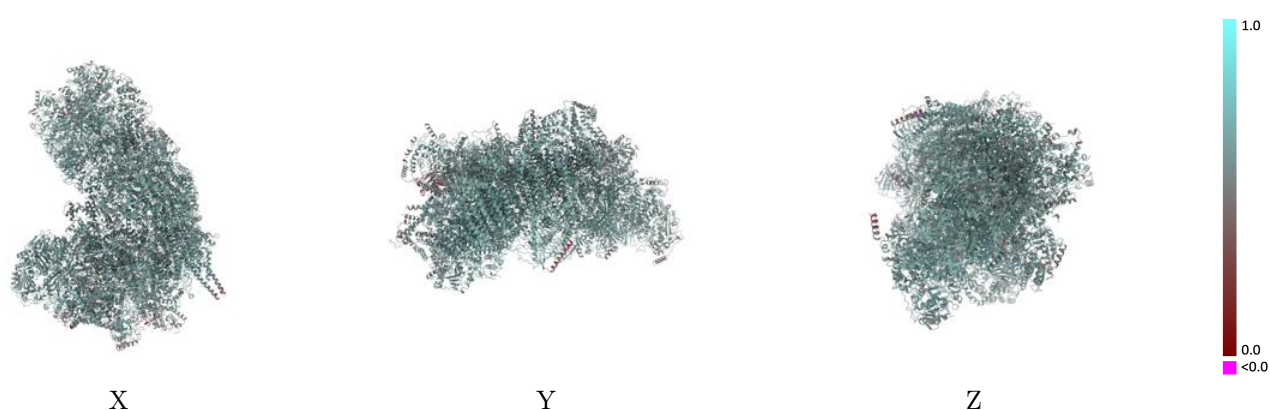
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25882 and PDB model 7TGH. Per-residue inclusion information can be found in section 3 on page 31.

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

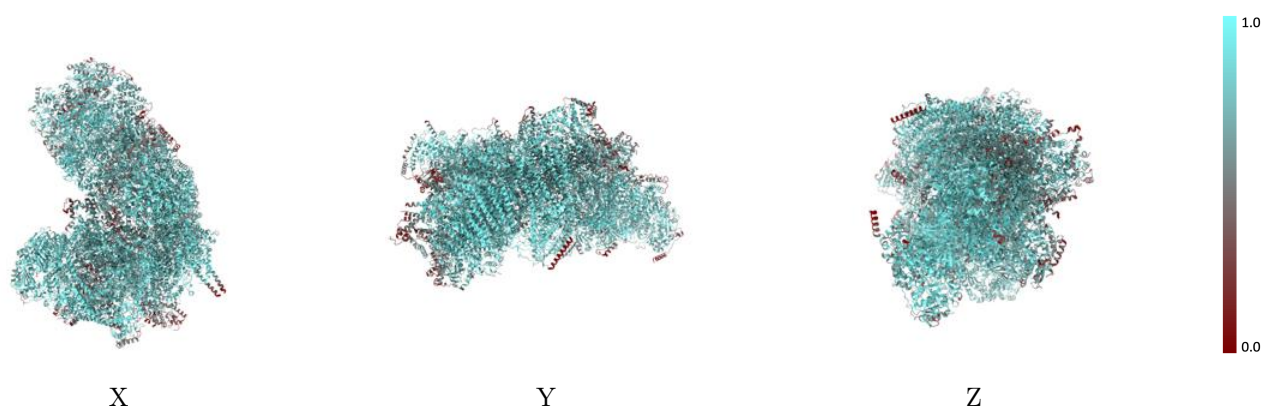
This section was not generated.

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



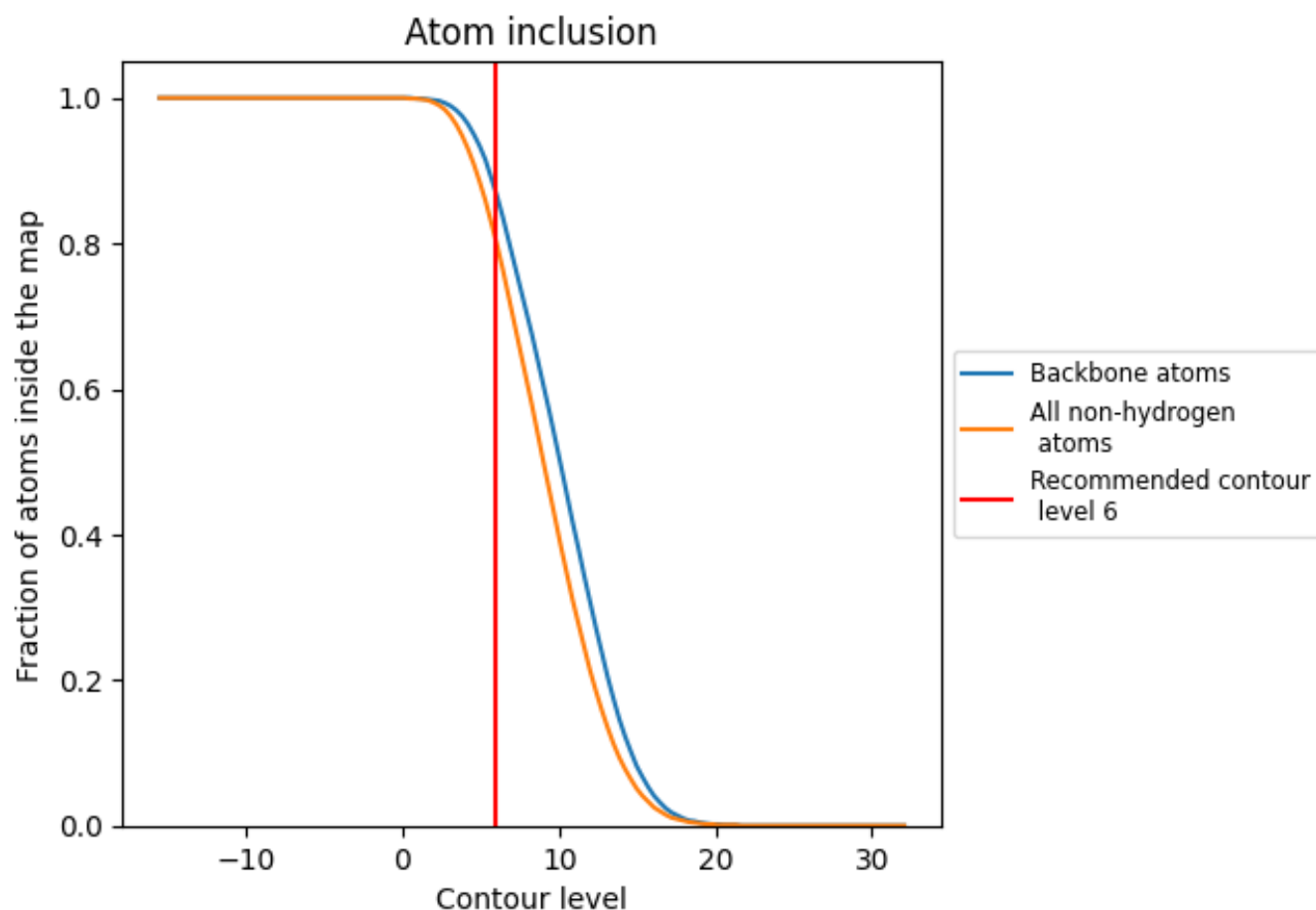
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (6) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8020   |  0.6050   |
| 1     |  0.7560   |  0.6000   |
| 1B    |  0.8320   |  0.6230   |
| 2     |  0.9050   |  0.6450   |
| 2B    |  0.9020   |  0.6420   |
| 3     |  0.8080   |  0.6230   |
| 3A    |  0.8860   |  0.6160   |
| 3B    |  0.9010   |  0.6320   |
| 3C    |  0.7980   |  0.5920   |
| 3D    |  0.9260   |  0.6340   |
| 3E    |  0.6380   |  0.5290   |
| 3F    |  0.7560   |  0.5760   |
| 3G    |  0.7280   |  0.5750   |
| 3H    |  0.8030   |  0.6080   |
| 3I    |  0.8340  |  0.6220  |
| 3J    |  0.8060 |  0.6210 |
| 3M    |  0.7720 |  0.5900 |
| 3a    |  0.8340 |  0.6060 |
| 3b    |  0.8590 |  0.6030 |
| 3c    |  0.7600 |  0.5770 |
| 3d    |  0.8820 |  0.6020 |
| 3e    |  0.8320 |  0.5980 |
| 3f    |  0.5320 |  0.4700 |
| 3g    |  0.7150 |  0.5560 |
| 3h    |  0.7450 |  0.5700 |
| 3i    |  0.7890 |  0.5870 |
| 3j    |  0.7850 |  0.5630 |
| 3l    |  0.4350 |  0.4300 |
| 3m    |  0.8710 |  0.6070 |
| 4     |  0.9010 |  0.6390 |
| 4L    |  0.8760 |  0.6250 |
| 5     |  0.9060 |  0.6420 |
| 5B    |  0.8430 |  0.6410 |
| 6     |  0.8340 |  0.6270 |
| A1    |  0.7800 |  0.6080 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| A2    |  0.7560   |  0.5850   |
| A3    |  0.8090   |  0.6140   |
| A5    |  0.7690   |  0.5900   |
| A6    |  0.9140   |  0.6430   |
| A7    |  0.6990   |  0.5830   |
| A8    |  0.8040   |  0.5990   |
| A9    |  0.9040   |  0.6420   |
| AB    |  0.7690   |  0.6210   |
| AC    |  0.8360   |  0.6250   |
| AL    |  0.8330   |  0.6240   |
| AM    |  0.7340   |  0.5920   |
| AN    |  0.7350   |  0.6020   |
| B2    |  0.7240   |  0.5860   |
| B3    |  0.8300   |  0.6310   |
| B4    |  0.8500   |  0.6380   |
| B6    |  0.9310   |  0.6580   |
| B7    |  0.8550   |  0.6170   |
| B8    |  0.8420  |  0.6290  |
| B9    |  0.8390 |  0.6230 |
| BL    |  0.8960 |  0.6330 |
| BM    |  0.7830 |  0.6100 |
| C     |  0.7170 |  0.5510 |
| C1    |  0.8850 |  0.6350 |
| C2    |  0.8060 |  0.5960 |
| C3    |  0.7680 |  0.6020 |
| C4    |  0.8080 |  0.6180 |
| FX    |  0.8640 |  0.6390 |
| J1    |  0.6580 |  0.5900 |
| P1    |  0.7600 |  0.6040 |
| P2    |  0.6870 |  0.5940 |
| R     |  0.8150 |  0.5970 |
| S1    |  0.8850 |  0.6300 |
| S2    |  0.8860 |  0.6270 |
| S3    |  0.8910 |  0.6330 |
| S4    |  0.8630 |  0.6280 |
| S5    |  0.8470 |  0.6230 |
| S6    |  0.8810 |  0.6330 |
| S7    |  0.9160 |  0.6390 |
| S8    |  0.7870 |  0.6150 |
| T1    |  0.6840 |  0.5720 |
| T2    |  0.7770 |  0.5890 |
| T3    |  0.4530 |  0.5160 |

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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| T4    |  0.4930 |  0.5340 |
| T5    |  0.8230 |  0.5990 |
| T6    |  0.8250 |  0.6030 |
| T7    |  0.5040 |  0.5310 |
| T8    |  0.7910 |  0.6090 |
| T9    |  0.8080 |  0.6010 |
| TA    |  0.6410 |  0.5690 |
| TB    |  0.8380 |  0.6220 |
| TC    |  0.7950 |  0.6130 |
| TD    |  0.4560 |  0.5450 |
| TE    |  0.6210 |  0.5920 |
| TX    |  0.7130 |  0.6110 |
| V1    |  0.7910 |  0.5870 |
| V2    |  0.7040 |  0.5690 |
| X1    |  0.8380 |  0.6200 |