



wwPDB EM Validation Summary Report ⓘ

Oct 22, 2024 – 06:26 AM JST

PDB ID : 8GYM
EMDB ID : EMD-34373
Title : Cryo-EM structure of Tetrahymena thermophila respiratory mega-complex
MC IV2+(I+III2+II)2
Authors : Wu, M.C.; Hu, Y.Q.; Han, F.Z.; Zhou, L.
Deposited on : 2022-09-23
Resolution : 2.96 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

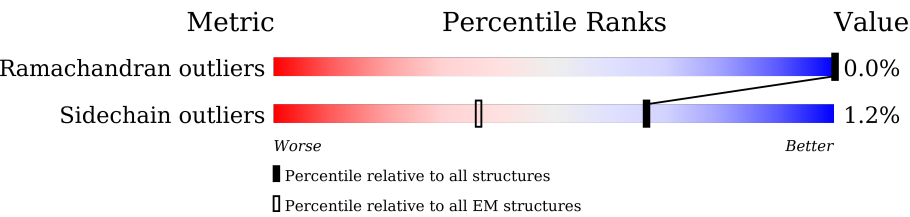
| | | |
|--------------------------------|---|--|
| EMDB validation analysis | : | 0.0.1.dev113 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.39 |

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 2.96 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.




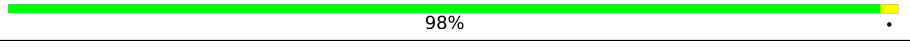
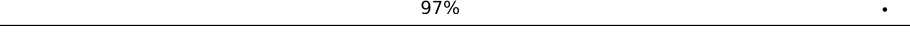
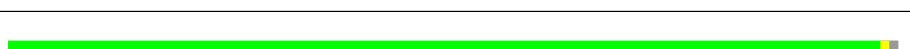

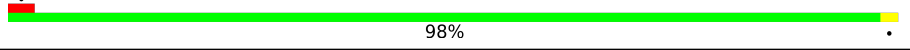
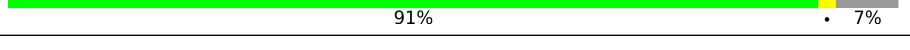
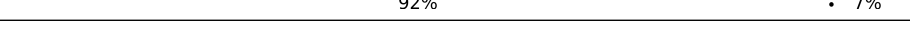
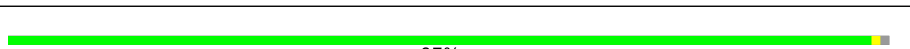
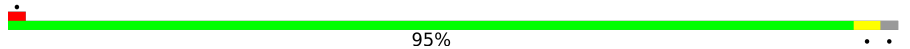
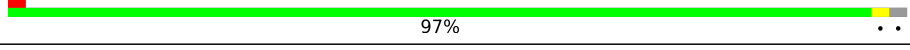
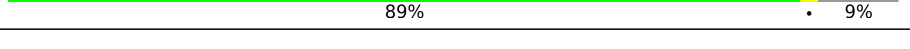

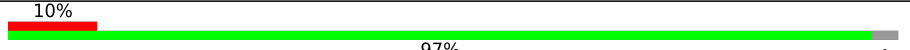


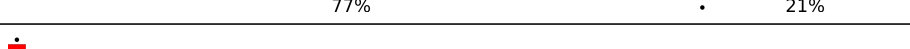







| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |

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 ≥ 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 | 1T | 72 | |
| 1 | 1t | 72 | |
| 2 | 2E | 322 | |
| 2 | 2e | 322 | |
| 3 | 2F | 296 | |
| 3 | 2f | 296 | |
| 4 | 2G | 198 | |
| 4 | 2g | 198 | |
| 5 | 2H | 195 | |

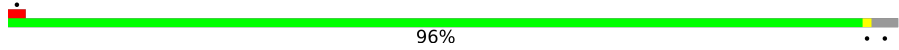
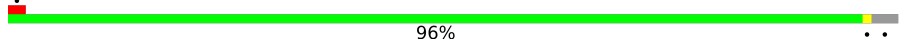
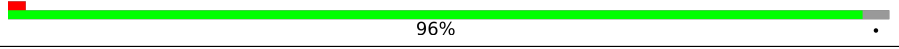
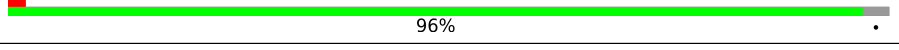
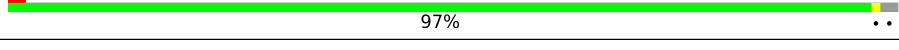
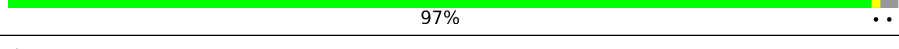
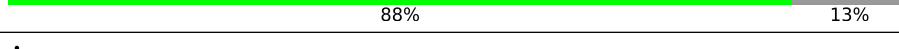
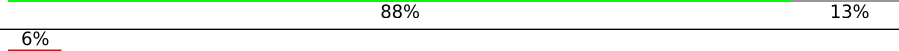
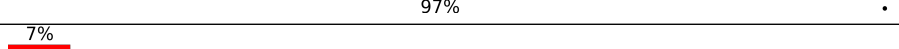
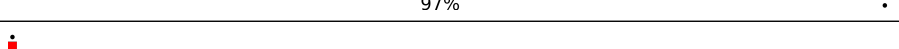
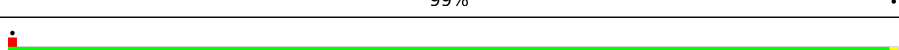
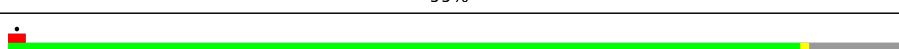
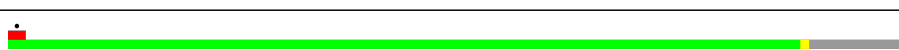







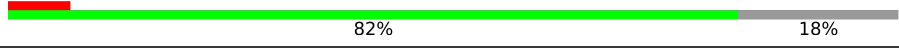
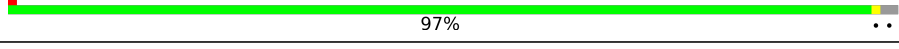
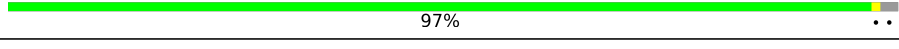
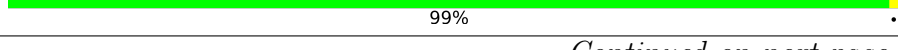

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 5 | 2h | 195 |  |
| 6 | 2I | 114 |  |
| 6 | 2i | 114 |  |
| 7 | 2J | 103 |  |
| 7 | 2j | 103 |  |
| 8 | 2K | 93 |  |
| 8 | 2k | 93 |  |
| 9 | 2L | 89 |  |
| 9 | 2l | 89 |  |
| 10 | 2M | 76 |  |
| 10 | 2m | 76 |  |
| 11 | 2N | 62 |  |
| 11 | 2n | 62 |  |
| 12 | 2O | 46 |  |
| 12 | 2o | 46 |  |
| 13 | 2T | 72 |  |
| 13 | 2t | 72 |  |
| 14 | 3T | 93 |  |
| 14 | 3t | 93 |  |
| 15 | 4A | 127 |  |
| 15 | 4a | 127 |  |
| 16 | 4T | 68 |  |
| 16 | 4t | 68 |  |
| 17 | 5T | 81 |  |
| 17 | 5t | 81 | |

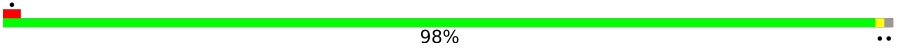
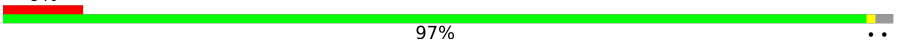
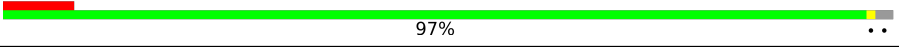


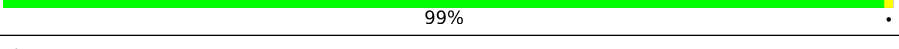
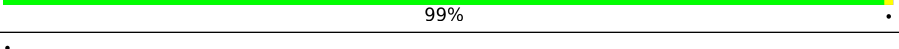
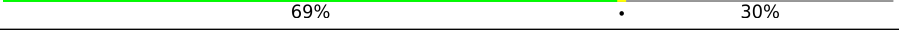
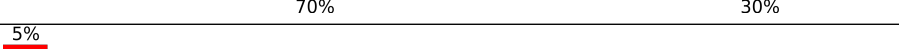
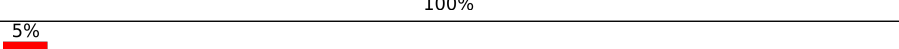
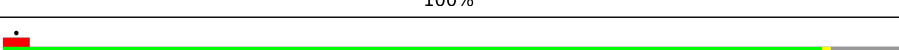
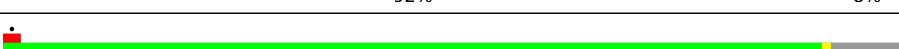
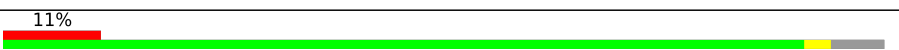







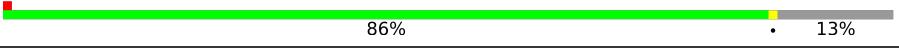
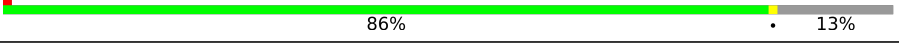
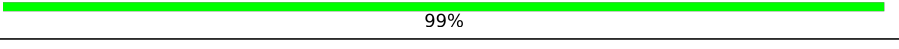
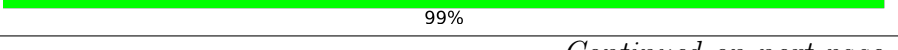

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 18 | 6A | 130 |  |
| 18 | 6a | 130 |  |
| 19 | 6B | 230 |  |
| 19 | 6b | 230 |  |
| 20 | 6C | 103 |  |
| 20 | 6c | 103 |  |
| 21 | 6L | 88 |  |
| 21 | 6l | 88 |  |
| 22 | 6T | 72 |  |
| 22 | 6t | 72 |  |
| 23 | 7A | 133 |  |
| 23 | 7a | 133 |  |
| 24 | 7C | 236 |  |
| 24 | 7c | 236 |  |
| 25 | 7L | 990 |  |
| 25 | 7l | 990 |  |
| 26 | A | 490 |  |
| 26 | a | 490 |  |
| 27 | B | 473 |  |
| 27 | b | 473 |  |
| 28 | BP | 462 |  |
| 28 | bp | 462 |  |
| 29 | C1 | 688 |  |
| 29 | c1 | 688 |  |
| 30 | C2 | 604 |  |

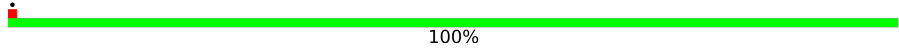
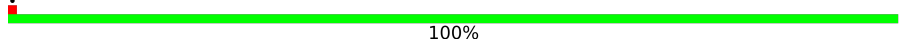
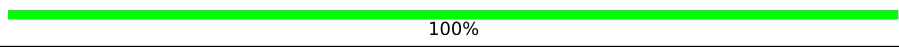
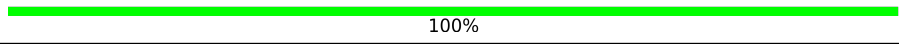
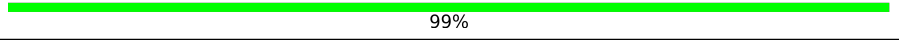
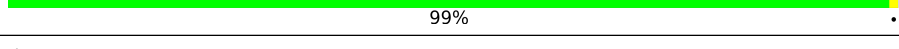
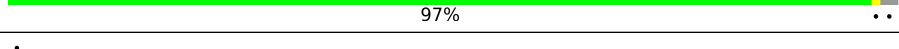
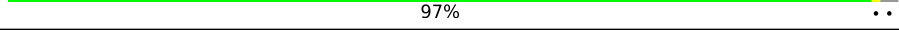
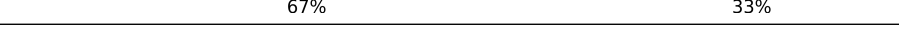
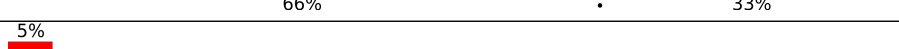
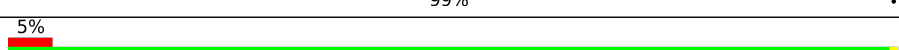
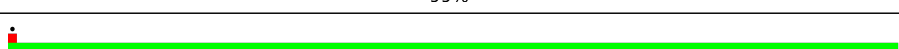
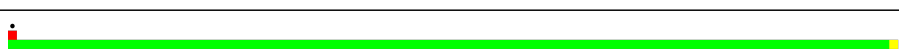
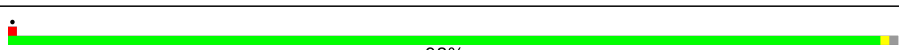
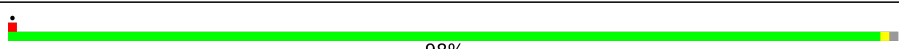
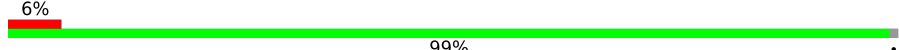
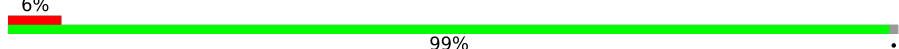
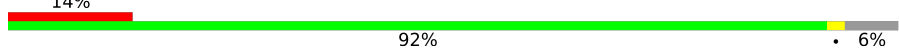
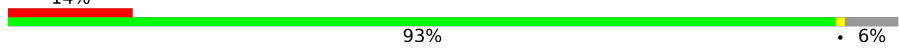

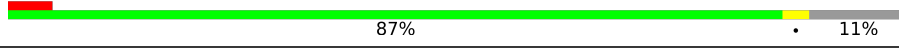
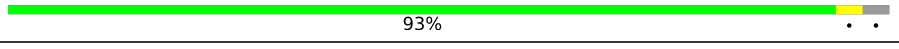
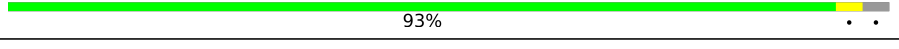
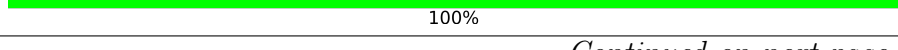

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 30 | c2 | 604 |  |
| 31 | C3 | 594 |  |
| 31 | c3 | 594 |  |
| 32 | D | 402 |  |
| 32 | d | 402 |  |
| 33 | E | 385 |  |
| 33 | e | 385 |  |
| 34 | F | 348 |  |
| 34 | f | 348 |  |
| 35 | FS | 188 |  |
| 35 | fs | 188 |  |
| 36 | G | 318 |  |
| 36 | g | 318 |  |
| 37 | H | 318 |  |
| 37 | h | 318 |  |
| 38 | I | 252 |  |
| 38 | i | 252 |  |
| 39 | J | 234 |  |
| 39 | j | 234 |  |
| 40 | K | 231 |  |
| 40 | k | 231 |  |
| 41 | L | 222 |  |
| 41 | l | 222 |  |
| 42 | M | 220 |  |
| 42 | m | 220 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 43 | M1 | 346 |  100% |
| 43 | m1 | 346 |  100% |
| 44 | M2 | 318 |  100% |
| 44 | m2 | 318 |  100% |
| 45 | M3 | 330 |  99% |
| 45 | m3 | 330 |  99% |
| 46 | N | 210 |  97% |
| 46 | n | 210 |  97% |
| 47 | O | 193 |  67% 33% |
| 47 | o | 193 |  66% 33% |
| 48 | P | 175 |  99% |
| 48 | p | 175 |  99% |
| 49 | Q | 173 |  100% |
| 49 | q | 173 |  99% |
| 50 | R | 173 |  98% |
| 50 | r | 173 |  98% |
| 51 | S | 170 |  99% |
| 51 | s | 170 |  99% |
| 52 | SA | 636 |  92% 6% |
| 52 | sa | 636 |  93% 6% |
| 53 | SB | 312 |  86% 11% |
| 53 | sb | 312 |  87% 11% |
| 54 | SC | 60 |  93% |
| 54 | sc | 60 |  93% |
| 55 | SD | 44 |  100% |

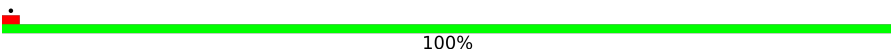
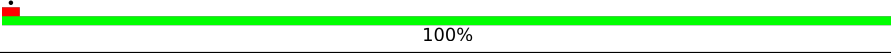
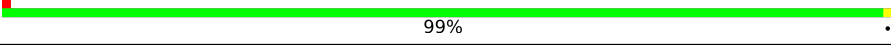
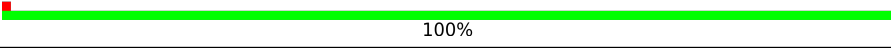
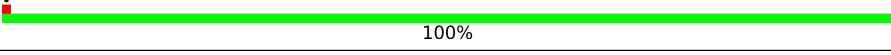
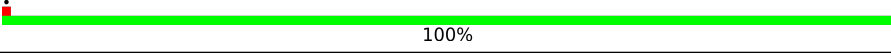
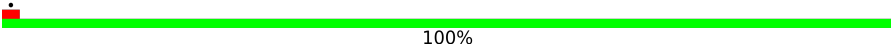
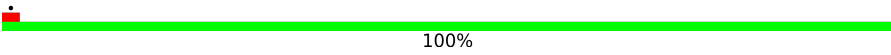
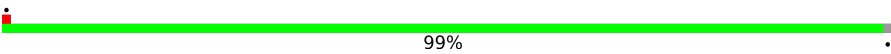
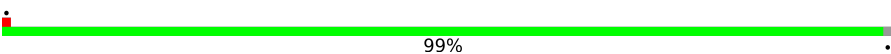
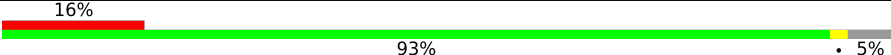
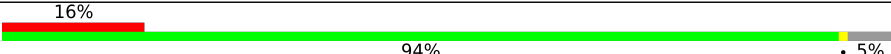
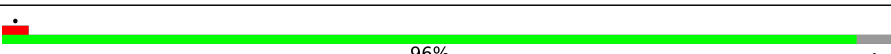
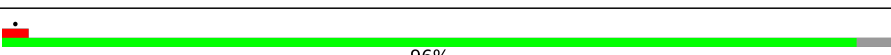
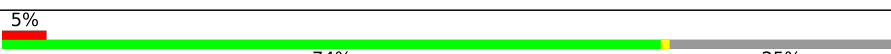
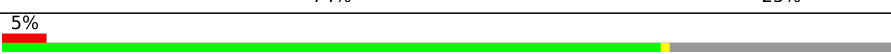

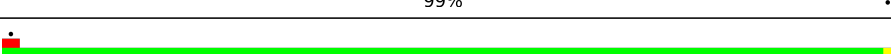
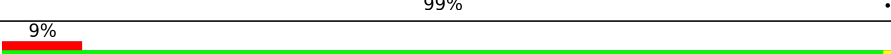
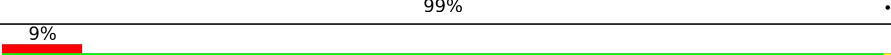
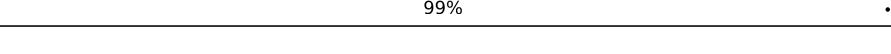
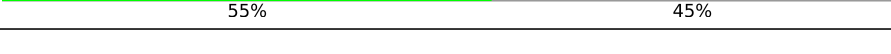

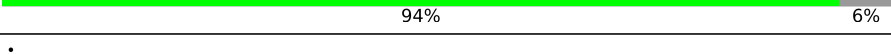
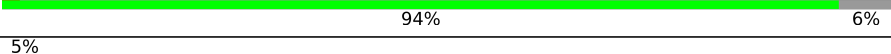
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 55 | sd | 44 | 100% |
| 56 | T | 158 | 98% |
| 56 | t | 158 | 98% |
| 57 | U | 154 | 98% |
| 57 | u | 154 | 98% |
| 58 | V | 149 | 98% |
| 58 | v | 149 | 98% |
| 59 | VB | 637 | 86% 13% |
| 59 | vb | 637 | 86% 13% |
| 60 | W | 124 | 98% |
| 60 | w | 124 | 98% |
| 61 | X | 122 | 99% |
| 61 | x | 122 | 99% |
| 62 | Y | 105 | 99% |
| 62 | y | 105 | 99% |
| 63 | Y0 | 89 | 100% |
| 63 | y0 | 89 | 100% |
| 64 | Y5 | 190 | 8% 100% |
| 64 | y5 | 190 | 8% 100% |
| 65 | Y7 | 453 | 7% 75% 24% |
| 65 | y7 | 453 | 7% 75% 24% |
| 66 | Z | 90 | 6% 94% |
| 66 | z | 90 | 6% 94% |
| 67 | Z1 | 100 | 97% |
| 67 | z1 | 100 | 97% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 68 | 1B | 59 |  100% |
| 68 | 1b | 59 |  100% |
| 69 | 2B | 178 |  99% |
| 69 | 2b | 178 |  100% |
| 70 | 4L | 116 |  100% |
| 70 | 4l | 116 |  100% |
| 71 | 5B | 100 |  100% |
| 71 | 5b | 100 |  100% |
| 72 | A1 | 94 |  99% |
| 72 | a1 | 94 |  99% |
| 73 | A2 | 103 |  16% 93% 5% |
| 73 | a2 | 103 |  16% 94% 5% |
| 74 | A3 | 135 |  96% |
| 74 | a3 | 135 |  96% |
| 75 | A5 | 206 |  5% 74% 25% |
| 75 | a5 | 206 |  5% 74% 25% |
| 76 | A6 | 172 |  99% |
| 76 | a6 | 172 |  99% |
| 77 | A7 | 282 |  9% 99% |
| 77 | a7 | 282 |  9% 99% |
| 78 | A8 | 238 |  55% 45% |
| 78 | a8 | 238 |  55% 45% |
| 79 | A9 | 362 |  94% 6% |
| 79 | a9 | 362 |  94% 6% |
| 80 | AB | 138 |  5% 80% 19% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 80 | ab | 138 | |
| 81 | AC | 133 | |
| 81 | ac | 133 | |
| 82 | AL | 194 | |
| 82 | al | 194 | |
| 83 | AM | 175 | |
| 83 | am | 175 | |
| 84 | AN | 231 | |
| 84 | an | 231 | |
| 85 | B2 | 126 | |
| 85 | b2 | 126 | |
| 86 | B3 | 83 | |
| 86 | b3 | 83 | |
| 87 | B4 | 147 | |
| 87 | b4 | 147 | |
| 88 | B6 | 129 | |
| 88 | b6 | 129 | |
| 89 | B7 | 120 | |
| 89 | b7 | 120 | |
| 90 | B8 | 207 | |
| 90 | b8 | 207 | |
| 91 | B9 | 189 | |
| 91 | b9 | 189 | |
| 92 | BL | 188 | |
| 92 | bl | 188 | |

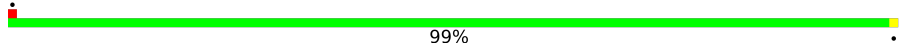

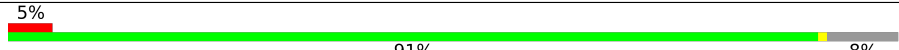
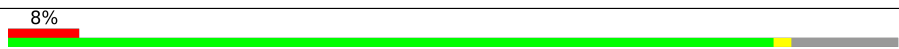

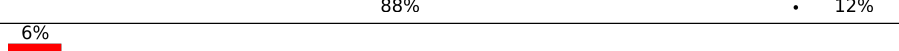
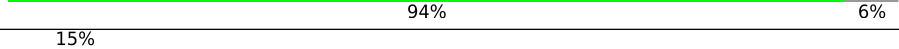
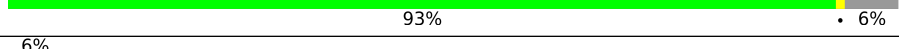
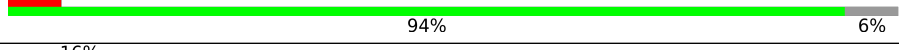
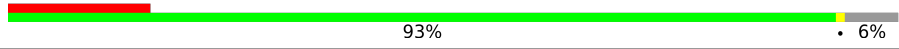
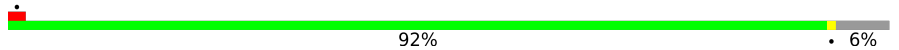
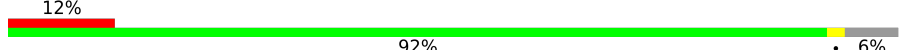
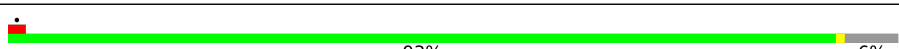

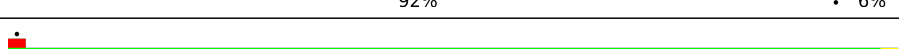
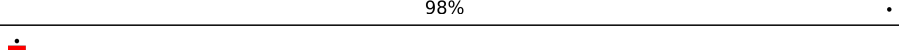
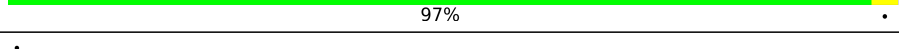
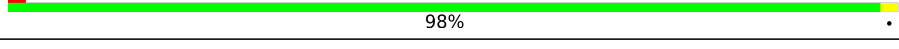
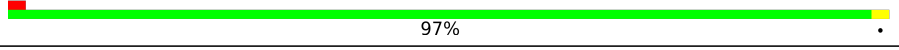
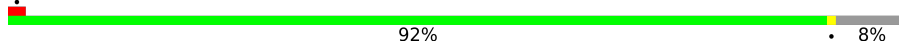
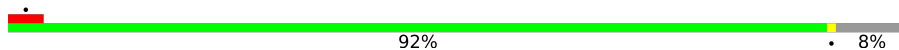
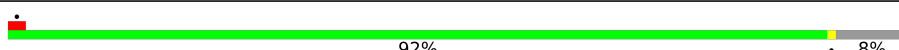

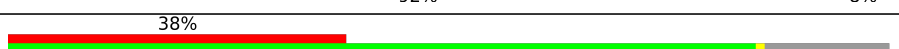
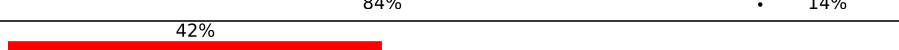
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 93 | BM | 214 | |
| 93 | bm | 214 | |
| 94 | C4 | 102 | |
| 94 | c4 | 102 | |
| 95 | FX | 172 | |
| 95 | fx | 172 | |
| 96 | G1 | 257 | |
| 96 | g1 | 257 | |
| 97 | G2 | 233 | |
| 97 | g2 | 233 | |
| 98 | G3 | 346 | |
| 98 | g3 | 346 | |
| 99 | J1 | 317 | |
| 99 | j1 | 317 | |
| 100 | N1 | 284 | |
| 100 | n1 | 284 | |
| 101 | N2 | 360 | |
| 101 | n2 | 360 | |
| 102 | N3 | 121 | |
| 102 | n3 | 121 | |
| 103 | N4 | 505 | |
| 103 | n4 | 505 | |
| 104 | N5 | 750 | |
| 104 | n5 | 750 | |
| 105 | N6 | 255 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 105 | n6 | 255 |  |
| 106 | P1 | 251 |  |
| 106 | p1 | 251 |  |
| 107 | P2 | 189 |  |
| 107 | p2 | 189 |  |
| 108 | QA | 482 |  |
| 108 | Qa | 482 |  |
| 108 | qA | 482 |  |
| 108 | qa | 482 |  |
| 109 | QB | 513 |  |
| 109 | Qb | 513 |  |
| 109 | qB | 513 |  |
| 109 | qb | 513 |  |
| 110 | QC | 426 |  |
| 110 | Qc | 426 |  |
| 110 | qC | 426 |  |
| 110 | qc | 426 |  |
| 111 | QD | 319 |  |
| 111 | Qd | 319 |  |
| 111 | qD | 319 |  |
| 111 | qd | 319 |  |
| 112 | QE | 269 |  |
| 112 | Qe | 269 |  |
| 112 | qE | 269 |  |
| 112 | qe | 269 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 113 | QF | 90 | |
| 113 | Qf | 90 | |
| 113 | qF | 90 | |
| 113 | qf | 90 | |
| 114 | QG | 328 | |
| 114 | Qg | 328 | |
| 114 | qG | 328 | |
| 114 | qg | 328 | |
| 115 | QH | 130 | |
| 115 | Qh | 130 | |
| 115 | qH | 130 | |
| 115 | qh | 130 | |
| 116 | QI | 119 | |
| 116 | Qi | 119 | |
| 116 | qI | 119 | |
| 116 | qi | 119 | |
| 117 | QJ | 62 | |
| 117 | Qj | 62 | |
| 117 | qJ | 62 | |
| 117 | qj | 62 | |
| 118 | QL | 41 | |
| 118 | Ql | 41 | |
| 118 | qL | 41 | |
| 118 | ql | 41 | |
| 119 | QM | 17 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 119 | Qm | 17 | 100% |
| 119 | U2 | 17 | 100% |
| 119 | qM | 17 | 100% |
| 119 | qm | 17 | 100% |
| 119 | u2 | 17 | 100% |
| 120 | S1 | 718 | 9% 95% . . |
| 120 | s1 | 718 | 8% 95% . . |
| 121 | S2 | 442 | . 97% . |
| 121 | s2 | 442 | . 98% . |
| 122 | S3 | 198 | . 98% . |
| 122 | s3 | 198 | . 98% . |
| 123 | S4 | 185 | 11% 96% . . |
| 123 | s4 | 185 | 11% 96% . . |
| 124 | S5 | 94 | 6% 96% . . |
| 124 | s5 | 94 | 6% 97% . . |
| 125 | S6 | 132 | 12% 68% . 30% |
| 125 | s6 | 132 | 11% 69% . 30% |
| 126 | S7 | 162 | . 95% . . |
| 126 | s7 | 162 | . 96% . . |
| 127 | S8 | 236 | 92% 8% |
| 127 | s8 | 236 | 92% 8% |
| 128 | T1 | 516 | 21% 96% . . |
| 128 | t1 | 516 | 21% 96% . . |
| 129 | T2 | 333 | 57% 82% . 16% |
| 129 | t2 | 333 | 57% 82% . 16% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 130 | T3 | 311 | |
| 130 | t3 | 311 | |
| 131 | T4 | 212 | |
| 131 | t4 | 212 | |
| 132 | T5 | 205 | |
| 132 | t5 | 205 | |
| 133 | T6 | 144 | |
| 133 | t6 | 144 | |
| 134 | T7 | 143 | |
| 134 | t7 | 143 | |
| 135 | T8 | 135 | |
| 135 | t8 | 135 | |
| 136 | T9 | 136 | |
| 136 | t9 | 136 | |
| 137 | TA | 127 | |
| 137 | ta | 127 | |
| 138 | TB | 113 | |
| 138 | tb | 113 | |
| 139 | TC | 93 | |
| 139 | tc | 93 | |
| 140 | TD | 73 | |
| 140 | td | 73 | |
| 141 | TE | 71 | |
| 141 | te | 71 | |
| 142 | TF | 236 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 142 | tf | 236 | |
| 143 | TG | 135 | |
| 143 | tg | 135 | |
| 144 | TH | 124 | |
| 144 | th | 124 | |
| 145 | TX | 166 | |
| 145 | tx | 166 | |
| 146 | V1 | 474 | |
| 146 | v1 | 474 | |
| 147 | V2 | 274 | |
| 147 | v2 | 274 | |
| 148 | X1 | 150 | |
| 148 | x1 | 150 | |
| 149 | C | 212 | |
| 149 | c | 212 | |
| 150 | U1 | 92 | |
| 150 | u1 | 92 | |

2 Entry composition

There are 171 unique types of molecules in this entry. The entry contains 568568 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 Tim10/DDP family zinc finger protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 1 | 1t | 70 | Total | C | N | O | S | 0 | 0 |
| | | | 540 | 329 | 98 | 109 | 4 | | |
| 1 | 1T | 70 | Total | C | N | O | S | 0 | 0 |
| | | | 540 | 329 | 98 | 109 | 4 | | |

- Molecule 2 is a protein called NmrA domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2 | 2e | 321 | Total | C | N | O | S | 0 | 0 |
| | | | 2560 | 1623 | 449 | 487 | 1 | | |
| 2 | 2E | 321 | Total | C | N | O | S | 0 | 0 |
| | | | 2560 | 1623 | 449 | 487 | 1 | | |

- Molecule 3 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3 | 2f | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1803 | 1166 | 305 | 328 | 4 | | |
| 3 | 2F | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1803 | 1166 | 305 | 328 | 4 | | |

- Molecule 4 is a protein called SDHTT3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4 | 2g | 198 | Total | C | N | O | S | 0 | 0 |
| | | | 1671 | 1083 | 276 | 307 | 5 | | |
| 4 | 2G | 198 | Total | C | N | O | S | 0 | 0 |
| | | | 1671 | 1083 | 276 | 307 | 5 | | |

- Molecule 5 is a protein called Diphthamide synthesis protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5 | 2h | 102 | Total | C | N | O | S | 0 | 0 |
| | | | 801 | 497 | 139 | 157 | 8 | | |
| 5 | 2H | 102 | Total | C | N | O | S | 0 | 0 |
| | | | 801 | 497 | 139 | 157 | 8 | | |

- Molecule 6 is a protein called DUF4885 domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6 | 2i | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 915 | 580 | 153 | 180 | 2 | | |
| 6 | 2I | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 915 | 580 | 153 | 180 | 2 | | |

- Molecule 7 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7 | 2j | 102 | Total | C | N | O | S | 0 | 0 |
| | | | 839 | 549 | 139 | 149 | 2 | | |
| 7 | 2J | 102 | Total | C | N | O | S | 0 | 0 |
| | | | 839 | 549 | 139 | 149 | 2 | | |

- Molecule 8 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8 | 2k | 93 | Total | C | N | O | S | 0 | 0 |
| | | | 795 | 530 | 129 | 134 | 2 | | |
| 8 | 2K | 93 | Total | C | N | O | S | 0 | 0 |
| | | | 795 | 530 | 129 | 134 | 2 | | |

- Molecule 9 is a protein called Transposase.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9 | 2l | 83 | Total | C | N | O | S | 0 | 0 |
| | | | 722 | 467 | 120 | 134 | 1 | | |
| 9 | 2L | 83 | Total | C | N | O | S | 0 | 0 |
| | | | 722 | 467 | 120 | 134 | 1 | | |

- Molecule 10 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10 | 2m | 75 | Total | C | N | O | S | 0 | 0 |
| | | | 640 | 412 | 116 | 110 | 2 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10 | 2M | 75 | Total | C | N | O | S | 0 | 0 |
| | | | 640 | 412 | 116 | 110 | 2 | | |

- Molecule 11 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 11 | 2n | 61 | Total | C | N | O | S | 0 | 0 |
| | | | 505 | 341 | 78 | 84 | 2 | | |
| 11 | 2N | 61 | Total | C | N | O | S | 0 | 0 |
| | | | 505 | 341 | 78 | 84 | 2 | | |

- Molecule 12 is a protein called SDHTT11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 12 | 2o | 42 | Total | C | N | O | S | 0 | 0 |
| | | | 356 | 239 | 59 | 56 | 2 | | |
| 12 | 2O | 42 | Total | C | N | O | S | 0 | 0 |
| | | | 356 | 239 | 59 | 56 | 2 | | |

- Molecule 13 is a protein called Zf-Tim10_DDP domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13 | 2t | 70 | Total | C | N | O | S | 0 | 0 |
| | | | 567 | 353 | 100 | 110 | 4 | | |
| 13 | 2T | 70 | Total | C | N | O | S | 0 | 0 |
| | | | 567 | 353 | 100 | 110 | 4 | | |

- Molecule 14 is a protein called Zf-Tim10_DDP domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14 | 3t | 83 | Total | C | N | O | S | 0 | 0 |
| | | | 655 | 412 | 109 | 128 | 6 | | |
| 14 | 3T | 83 | Total | C | N | O | S | 0 | 0 |
| | | | 655 | 412 | 109 | 128 | 6 | | |

- Molecule 15 is a protein called Phage protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15 | 4a | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 816 | 519 | 144 | 151 | 2 | | |
| 15 | 4A | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 816 | 519 | 144 | 151 | 2 | | |

- Molecule 16 is a protein called Transposase.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 16 | 4t | 57 | Total | C | N | O | S | 0 | 0 |
| | | | 481 | 308 | 80 | 90 | 3 | | |
| 16 | 4T | 57 | Total | C | N | O | S | 0 | 0 |
| | | | 481 | 308 | 80 | 90 | 3 | | |

- Molecule 17 is a protein called Cullin domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 17 | 5t | 62 | Total | C | N | O | S | 0 | 0 |
| | | | 506 | 322 | 89 | 93 | 2 | | |
| 17 | 5T | 62 | Total | C | N | O | S | 0 | 0 |
| | | | 506 | 322 | 89 | 93 | 2 | | |

- Molecule 18 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18 | 6a | 126 | Total | C | N | O | S | 0 | 0 |
| | | | 1083 | 698 | 184 | 199 | 2 | | |
| 18 | 6A | 126 | Total | C | N | O | S | 0 | 0 |
| | | | 1083 | 698 | 184 | 199 | 2 | | |

- Molecule 19 is a protein called Structural protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 19 | 6b | 222 | Total | C | N | O | S | 0 | 0 |
| | | | 1912 | 1238 | 312 | 349 | 13 | | |
| 19 | 6B | 222 | Total | C | N | O | S | 0 | 0 |
| | | | 1912 | 1238 | 312 | 349 | 13 | | |

- Molecule 20 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20 | 6c | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 891 | 580 | 158 | 150 | 3 | | |
| 20 | 6C | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 891 | 580 | 158 | 150 | 3 | | |

- Molecule 21 is a protein called Decapping nuclease.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21 | 6l | 77 | Total | C | N | O | S | 0 | 0 |
| | | | 636 | 407 | 108 | 115 | 6 | | |
| 21 | 6L | 77 | Total | C | N | O | S | 0 | 0 |
| | | | 636 | 407 | 108 | 115 | 6 | | |

- Molecule 22 is a protein called Annexin.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 22 | 6t | 70 | Total | C | N | O | S | 0 | 0 |
| | | | 561 | 362 | 90 | 105 | 4 | | |
| 22 | 6T | 70 | Total | C | N | O | S | 0 | 0 |
| | | | 561 | 362 | 90 | 105 | 4 | | |

- Molecule 23 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23 | 7a | 133 | Total | C | N | O | S | 0 | 0 |
| | | | 1166 | 769 | 197 | 199 | 1 | | |
| 23 | 7A | 133 | Total | C | N | O | S | 0 | 0 |
| | | | 1166 | 769 | 197 | 199 | 1 | | |

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---|---------|-------|
| 24 | 7c | 211 | Total | C | N | O | P | S | 0 | 0 |
| | | | 1825 | 1163 | 299 | 354 | 1 | 8 | | |
| 24 | 7C | 211 | Total | C | N | O | P | S | 0 | 0 |
| | | | 1825 | 1163 | 299 | 354 | 1 | 8 | | |

- Molecule 25 is a protein called CTF/NF-I domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25 | 7l | 131 | Total | C | N | O | S | 0 | 0 |
| | | | 1078 | 698 | 175 | 196 | 9 | | |
| 25 | 7L | 131 | Total | C | N | O | S | 0 | 0 |
| | | | 1078 | 698 | 175 | 196 | 9 | | |

- Molecule 26 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 26 | a | 449 | Total | C | N | O | S | 0 | 0 |
| | | | 3756 | 2408 | 638 | 701 | 9 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 26 | A | 449 | Total | C | N | O | S | 0 | 0 |
| | | | 3756 | 2408 | 638 | 701 | 9 | | |

- Molecule 27 is a protein called Protein phosphatase 2C, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 27 | b | 428 | Total | C | N | O | S | 0 | 0 |
| | | | 3398 | 2164 | 593 | 638 | 3 | | |
| 27 | B | 428 | Total | C | N | O | S | 0 | 0 |
| | | | 3398 | 2164 | 593 | 638 | 3 | | |

- Molecule 28 is a protein called Chromosome condensation regulator RCC1 repeat protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 28 | bp | 381 | Total | C | N | O | S | 0 | 0 |
| | | | 2920 | 1858 | 493 | 567 | 2 | | |
| 28 | BP | 381 | Total | C | N | O | S | 0 | 0 |
| | | | 2920 | 1858 | 493 | 567 | 2 | | |

- Molecule 29 is a protein called Cytochrome c oxidase subunit 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 29 | c1 | 674 | Total | C | N | O | S | 0 | 0 |
| | | | 5576 | 3730 | 910 | 900 | 36 | | |
| 29 | C1 | 674 | Total | C | N | O | S | 0 | 0 |
| | | | 5576 | 3730 | 910 | 900 | 36 | | |

- Molecule 30 is a protein called Cytochrome c oxidase subunit 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 30 | c2 | 599 | Total | C | N | O | S | 0 | 0 |
| | | | 5094 | 3322 | 881 | 880 | 11 | | |
| 30 | C2 | 599 | Total | C | N | O | S | 0 | 0 |
| | | | 5094 | 3322 | 881 | 880 | 11 | | |

- Molecule 31 is a protein called Ymf68.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 31 | c3 | 582 | Total | C | N | O | S | 0 | 0 |
| | | | 5084 | 3451 | 787 | 838 | 8 | | |
| 31 | C3 | 582 | Total | C | N | O | S | 0 | 0 |
| | | | 5084 | 3451 | 787 | 838 | 8 | | |

- Molecule 32 is a protein called SURF1-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 32 | d | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2366 | 1523 | 400 | 438 | 5 | | |
| 32 | D | 289 | Total | C | N | O | S | 0 | 0 |
| | | | 2366 | 1523 | 400 | 438 | 5 | | |

- Molecule 33 is a protein called TraB family protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 33 | e | 384 | Total | C | N | O | S | 0 | 0 |
| | | | 3176 | 2045 | 549 | 575 | 7 | | |
| 33 | E | 384 | Total | C | N | O | S | 0 | 0 |
| | | | 3176 | 2045 | 549 | 575 | 7 | | |

- Molecule 34 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 34 | f | 243 | Total | C | N | O | S | 0 | 0 |
| | | | 2024 | 1304 | 335 | 380 | 5 | | |
| 34 | F | 243 | Total | C | N | O | S | 0 | 0 |
| | | | 2024 | 1304 | 335 | 380 | 5 | | |

- Molecule 35 is a protein called Iron-binding zinc finger CDGSH type protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 35 | fs | 188 | Total | C | N | O | S | 0 | 0 |
| | | | 1509 | 978 | 260 | 257 | 14 | | |
| 35 | FS | 188 | Total | C | N | O | S | 0 | 0 |
| | | | 1509 | 978 | 260 | 257 | 14 | | |

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 36 | g | 293 | Total | C | N | O | S | 0 | 0 |
| | | | 2442 | 1555 | 410 | 465 | 12 | | |
| 36 | G | 293 | Total | C | N | O | S | 0 | 0 |
| | | | 2442 | 1555 | 410 | 465 | 12 | | |

- Molecule 37 is a protein called SURF1-like protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 37 | h | 298 | Total | C | N | O | S | 0 | 0 |
| | | | 2369 | 1500 | 409 | 450 | 10 | | |
| 37 | H | 298 | Total | C | N | O | S | 0 | 0 |
| | | | 2369 | 1500 | 409 | 450 | 10 | | |

- Molecule 38 is a protein called COXTT9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 38 | i | 231 | Total | C | N | O | S | 0 | 0 |
| | | | 1943 | 1253 | 340 | 346 | 4 | | |
| 38 | I | 231 | Total | C | N | O | S | 0 | 0 |
| | | | 1943 | 1253 | 340 | 346 | 4 | | |

- Molecule 39 is a protein called COXTT10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 39 | j | 187 | Total | C | N | O | S | 0 | 0 |
| | | | 1575 | 1024 | 276 | 274 | 1 | | |
| 39 | J | 187 | Total | C | N | O | S | 0 | 0 |
| | | | 1575 | 1024 | 276 | 274 | 1 | | |

- Molecule 40 is a protein called 39S ribosomal protein L9, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 40 | k | 208 | Total | C | N | O | S | 0 | 0 |
| | | | 1714 | 1090 | 302 | 319 | 3 | | |
| 40 | K | 208 | Total | C | N | O | S | 0 | 0 |
| | | | 1714 | 1090 | 302 | 319 | 3 | | |

- Molecule 41 is a protein called Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 41 | l | 194 | Total | C | N | O | S | 0 | 0 |
| | | | 1668 | 1089 | 284 | 293 | 2 | | |
| 41 | L | 194 | Total | C | N | O | S | 0 | 0 |
| | | | 1668 | 1089 | 284 | 293 | 2 | | |

- Molecule 42 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 42 | m | 219 | Total | C | N | O | S | 0 | 0 |
| | | | 1872 | 1218 | 315 | 328 | 11 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 42 | M | 219 | Total | C | N | O | S | 0 | 0 |
| | | | 1872 | 1218 | 315 | 328 | 11 | | |

- Molecule 43 is a protein called Oxoglutarate/malate translocator protein, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 43 | m1 | 346 | Total | C | N | O | S | 0 | 0 |
| | | | 2863 | 1890 | 469 | 491 | 13 | | |
| 43 | M1 | 346 | Total | C | N | O | S | 0 | 0 |
| | | | 2863 | 1890 | 469 | 491 | 13 | | |

- Molecule 44 is a protein called 2-oxoglutarate/malate carrier protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 44 | m2 | 318 | Total | C | N | O | S | 0 | 0 |
| | | | 2558 | 1665 | 440 | 449 | 4 | | |
| 44 | M2 | 318 | Total | C | N | O | S | 0 | 0 |
| | | | 2558 | 1665 | 440 | 449 | 4 | | |

- Molecule 45 is a protein called Carrier protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 45 | m3 | 329 | Total | C | N | O | S | 0 | 0 |
| | | | 2620 | 1700 | 446 | 470 | 4 | | |
| 45 | M3 | 329 | Total | C | N | O | S | 0 | 0 |
| | | | 2620 | 1700 | 446 | 470 | 4 | | |

- Molecule 46 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 46 | n | 206 | Total | C | N | O | S | 0 | 0 |
| | | | 1716 | 1117 | 286 | 306 | 7 | | |
| 46 | N | 206 | Total | C | N | O | S | 0 | 0 |
| | | | 1716 | 1117 | 286 | 306 | 7 | | |

- Molecule 47 is a protein called Mobilization protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47 | o | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1081 | 675 | 191 | 209 | 6 | | |
| 47 | O | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1081 | 675 | 191 | 209 | 6 | | |

- Molecule 48 is a protein called YftT domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48 | p | 175 | Total | C | N | O | S | 0 | 0 |
| | | | 1410 | 889 | 247 | 273 | 1 | | |
| 48 | P | 175 | Total | C | N | O | S | 0 | 0 |
| | | | 1410 | 889 | 247 | 273 | 1 | | |

- Molecule 49 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49 | q | 173 | Total | C | N | O | S | 0 | 0 |
| | | | 1434 | 927 | 243 | 255 | 9 | | |
| 49 | Q | 173 | Total | C | N | O | S | 0 | 0 |
| | | | 1434 | 927 | 243 | 255 | 9 | | |

- Molecule 50 is a protein called Transmembrane protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50 | r | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1407 | 921 | 231 | 252 | 3 | | |
| 50 | R | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1407 | 921 | 231 | 252 | 3 | | |

- Molecule 51 is a protein called Complex III subunit VII.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51 | s | 169 | Total | C | N | O | S | 0 | 0 |
| | | | 1388 | 878 | 243 | 263 | 4 | | |
| 51 | S | 169 | Total | C | N | O | S | 0 | 0 |
| | | | 1388 | 878 | 243 | 263 | 4 | | |

- Molecule 52 is a protein called Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 52 | sa | 599 | Total | C | N | O | S | 0 | 0 |
| | | | 4624 | 2907 | 825 | 866 | 26 | | |
| 52 | SA | 599 | Total | C | N | O | S | 0 | 0 |
| | | | 4624 | 2907 | 825 | 866 | 26 | | |

- Molecule 53 is a protein called Succinate dehydrogenase (quinone).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 53 | sb | 279 | Total | C | N | O | S | 0 | 0 |
| | | | 2260 | 1437 | 385 | 417 | 21 | | |
| 53 | SB | 279 | Total | C | N | O | S | 0 | 0 |
| | | | 2260 | 1437 | 385 | 417 | 21 | | |

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|-------|
| 54 | sc | 58 | Total | C | N | O | | 0 | 0 |
| | | | 481 | 314 | 85 | 82 | | | |
| 54 | SC | 58 | Total | C | N | O | | 0 | 0 |
| | | | 481 | 314 | 85 | 82 | | | |

- Molecule 55 is a protein called SDHD.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 55 | sd | 44 | Total | C | N | O | S | 0 | 0 |
| | | | 393 | 271 | 60 | 60 | 2 | | |
| 55 | SD | 44 | Total | C | N | O | S | 0 | 0 |
| | | | 393 | 271 | 60 | 60 | 2 | | |

- Molecule 56 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 56 | t | 156 | Total | C | N | O | S | 0 | 0 |
| | | | 1315 | 858 | 230 | 223 | 4 | | |
| 56 | T | 156 | Total | C | N | O | S | 0 | 0 |
| | | | 1315 | 858 | 230 | 223 | 4 | | |

- Molecule 57 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57 | u | 153 | Total | C | N | O | S | 0 | 0 |
| | | | 1304 | 848 | 221 | 230 | 5 | | |
| 57 | U | 153 | Total | C | N | O | S | 0 | 0 |
| | | | 1304 | 848 | 221 | 230 | 5 | | |

- Molecule 58 is a protein called COXTT22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 58 | v | 146 | Total | C | N | O | S | 0 | 0 |
| | | | 1234 | 802 | 217 | 213 | 2 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 58 | V | 146 | Total | C | N | O | S | 0 | 0 |
| | | | 1234 | 802 | 217 | 213 | 2 | | |

- Molecule 59 is a protein called Cytochrome C oxidase subunit Vb protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|------|---------|-------|
| 59 | vb | 555 | Total | C | N | O | P S | 0 | 0 |
| | | | 4630 | 2918 | 779 | 914 | 2 17 | | |
| 59 | VB | 555 | Total | C | N | O | P S | 0 | 0 |
| | | | 4630 | 2918 | 779 | 914 | 2 17 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 60 | w | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 1096 | 716 | 183 | 193 | 4 | | |
| 60 | W | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 1096 | 716 | 183 | 193 | 4 | | |

- Molecule 61 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61 | x | 122 | Total | C | N | O | S | 0 | 0 |
| | | | 1012 | 665 | 171 | 172 | 4 | | |
| 61 | X | 122 | Total | C | N | O | S | 0 | 0 |
| | | | 1012 | 665 | 171 | 172 | 4 | | |

- Molecule 62 is a protein called Lysozyme.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 62 | y | 105 | Total | C | N | O | S | 0 | 0 |
| | | | 859 | 540 | 157 | 153 | 9 | | |
| 62 | Y | 105 | Total | C | N | O | S | 0 | 0 |
| | | | 859 | 540 | 157 | 153 | 9 | | |

- Molecule 63 is a protein called Ymf70.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 63 | y0 | 89 | Total | C | N | O | S | 0 | 0 |
| | | | 775 | 535 | 115 | 123 | 2 | | |
| 63 | Y0 | 89 | Total | C | N | O | S | 0 | 0 |
| | | | 775 | 535 | 115 | 123 | 2 | | |

- Molecule 64 is a protein called Ymf75.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 64 | y5 | 190 | Total | C | N | O | S | 0 | 0 |
| | | | 1659 | 1141 | 249 | 265 | 4 | | |
| 64 | Y5 | 190 | Total | C | N | O | S | 0 | 0 |
| | | | 1659 | 1141 | 249 | 265 | 4 | | |

- Molecule 65 is a protein called Ymf67.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 65 | y7 | 343 | Total | C | N | O | S | 0 | 0 |
| | | | 2938 | 1964 | 468 | 500 | 6 | | |
| 65 | Y7 | 343 | Total | C | N | O | S | 0 | 0 |
| | | | 2938 | 1964 | 468 | 500 | 6 | | |

- Molecule 66 is a protein called ABC transporter.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 66 | z | 87 | Total | C | N | O | 0 | 0 |
| | | | 717 | 459 | 130 | 128 | | |
| 66 | Z | 87 | Total | C | N | O | 0 | 0 |
| | | | 717 | 459 | 130 | 128 | | |

- Molecule 67 is a protein called COXTT28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 67 | z1 | 97 | Total | C | N | O | S | 0 | 0 |
| | | | 766 | 489 | 135 | 140 | 2 | | |
| 67 | Z1 | 97 | Total | C | N | O | S | 0 | 0 |
| | | | 766 | 489 | 135 | 140 | 2 | | |

- Molecule 68 is a protein called NADH dehydrogenase subunit 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 68 | 1b | 59 | Total | C | N | O | S | 0 | 0 |
| | | | 516 | 362 | 78 | 73 | 3 | | |
| 68 | 1B | 59 | Total | C | N | O | S | 0 | 0 |
| | | | 516 | 362 | 78 | 73 | 3 | | |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| 1b | 49 | VAL | LEU | conflict | UNP Q09FB0 |

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

- Molecule 69 is a protein called NADH dehydrogenase subunit 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 69 | 2b | 178 | Total | C | N | O | S | 0 | 0 |
| | | | 1483 | 1015 | 215 | 248 | 5 | | |
| 69 | 2B | 178 | Total | C | N | O | S | 0 | 0 |
| | | | 1483 | 1015 | 215 | 248 | 5 | | |

- Molecule 70 is a protein called Ymf58.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 70 | 4l | 116 | Total | C | N | O | S | 0 | 0 |
| | | | 957 | 648 | 142 | 163 | 4 | | |
| 70 | 4L | 116 | Total | C | N | O | S | 0 | 0 |
| | | | 957 | 648 | 142 | 163 | 4 | | |

- Molecule 71 is a protein called Ymf57.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 71 | 5b | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 888 | 620 | 128 | 137 | 3 | | |
| 71 | 5B | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 888 | 620 | 128 | 137 | 3 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 72 | a1 | 93 | Total | C | N | O | | 0 | 0 |
| | | | 806 | 531 | 139 | 136 | | | |
| 72 | A1 | 93 | Total | C | N | O | | 0 | 0 |
| | | | 806 | 531 | 139 | 136 | | | |

- Molecule 73 is a protein called Ribosomal protein L51/S25/CI-B8 domain protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 73 | a2 | 98 | Total | C | N | O | S | 0 | 0 |
| | | | 811 | 512 | 146 | 151 | 2 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 73 | A2 | 98 | Total | C | N | O | S | 0 | 0 |
| | | | 811 | 512 | 146 | 151 | 2 | | |

- Molecule 74 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 74 | a3 | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1077 | 697 | 195 | 182 | 3 | | |
| 74 | A3 | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1077 | 697 | 195 | 182 | 3 | | |

- Molecule 75 is a protein called ETC complex I subunit motif protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 75 | a5 | 155 | Total | C | N | O | S | 0 | 0 |
| | | | 1307 | 838 | 219 | 244 | 6 | | |
| 75 | A5 | 155 | Total | C | N | O | S | 0 | 0 |
| | | | 1307 | 838 | 219 | 244 | 6 | | |

- Molecule 76 is a protein called NADH dehydrogenase, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 76 | a6 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1421 | 903 | 253 | 257 | 8 | | |
| 76 | A6 | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1421 | 903 | 253 | 257 | 8 | | |

- Molecule 77 is a protein called 37S ribosomal protein S25, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 77 | a7 | 282 | Total | C | N | O | S | 0 | 0 |
| | | | 2347 | 1478 | 413 | 453 | 3 | | |
| 77 | A7 | 282 | Total | C | N | O | S | 0 | 0 |
| | | | 2347 | 1478 | 413 | 453 | 3 | | |

- Molecule 78 is a protein called CX9C domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 78 | a8 | 132 | Total | C | N | O | S | 0 | 0 |
| | | | 1075 | 676 | 180 | 208 | 11 | | |
| 78 | A8 | 132 | Total | C | N | O | S | 0 | 0 |
| | | | 1075 | 676 | 180 | 208 | 11 | | |

- Molecule 79 is a protein called NAD-dependent epimerase/dehydratase family protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 79 | a9 | 340 | Total | C | N | O | S | 0 | 0 |
| | | | 2736 | 1747 | 479 | 498 | 12 | | |
| 79 | A9 | 340 | Total | C | N | O | S | 0 | 0 |
| | | | 2736 | 1747 | 479 | 498 | 12 | | |

- Molecule 80 is a protein called Acyl carrier protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 80 | ab | 112 | Total | C | N | O | | 0 | 0 |
| | | | 926 | 586 | 158 | 182 | | | |
| 80 | AB | 112 | Total | C | N | O | | 0 | 0 |
| | | | 926 | 586 | 158 | 182 | | | |

- Molecule 81 is a protein called Acyl carrier protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 81 | ac | 98 | Total | C | N | O | S | 0 | 0 |
| | | | 806 | 513 | 134 | 158 | 1 | | |
| 81 | AC | 98 | Total | C | N | O | S | 0 | 0 |
| | | | 806 | 513 | 134 | 158 | 1 | | |

- Molecule 82 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 82 | al | 193 | Total | C | N | O | S | 0 | 0 |
| | | | 1612 | 1019 | 303 | 285 | 5 | | |
| 82 | AL | 193 | Total | C | N | O | S | 0 | 0 |
| | | | 1612 | 1019 | 303 | 285 | 5 | | |

- Molecule 83 is a protein called NDUA13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 83 | am | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1349 | 858 | 256 | 227 | 8 | | |
| 83 | AM | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1349 | 858 | 256 | 227 | 8 | | |

- Molecule 84 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 84 | an | 231 | Total | C | N | O | S | 0 | 0 |
| | | | 1879 | 1219 | 317 | 336 | 7 | | |
| 84 | AN | 231 | Total | C | N | O | S | 0 | 0 |
| | | | 1879 | 1219 | 317 | 336 | 7 | | |

- Molecule 85 is a protein called NDUB2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 85 | b2 | 120 | Total | C | N | O | S | 0 | 0 |
| | | | 966 | 621 | 167 | 175 | 3 | | |
| 85 | B2 | 120 | Total | C | N | O | S | 0 | 0 |
| | | | 966 | 621 | 167 | 175 | 3 | | |

- Molecule 86 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 86 | b3 | 69 | Total | C | N | O | S | 0 | 0 |
| | | | 602 | 396 | 105 | 100 | 1 | | |
| 86 | B3 | 69 | Total | C | N | O | S | 0 | 0 |
| | | | 602 | 396 | 105 | 100 | 1 | | |

- Molecule 87 is a protein called NDUB4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 87 | b4 | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 976 | 641 | 156 | 175 | 4 | | |
| 87 | B4 | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 976 | 641 | 156 | 175 | 4 | | |

- Molecule 88 is a protein called NDUB6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 88 | b6 | 70 | Total | C | N | O | S | 0 | 0 |
| | | | 596 | 400 | 98 | 94 | 4 | | |
| 88 | B6 | 70 | Total | C | N | O | S | 0 | 0 |
| | | | 596 | 400 | 98 | 94 | 4 | | |

- Molecule 89 is a protein called CHCH domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 89 | b7 | 116 | Total | C | N | O | S | 0 | 0 |
| | | | 941 | 595 | 163 | 177 | 6 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 89 | B7 | 116 | Total | C | N | O | S | 0 | 0 |
| | | | 941 | 595 | 163 | 177 | 6 | | |

- Molecule 90 is a protein called NDUB8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 90 | b8 | 175 | Total | C | N | O | S | 0 | 0 |
| | | | 1456 | 936 | 248 | 266 | 6 | | |
| 90 | B8 | 175 | Total | C | N | O | S | 0 | 0 |
| | | | 1456 | 936 | 248 | 266 | 6 | | |

- Molecule 91 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 91 | b9 | 188 | Total | C | N | O | S | 0 | 0 |
| | | | 1596 | 1032 | 255 | 304 | 5 | | |
| 91 | B9 | 188 | Total | C | N | O | S | 0 | 0 |
| | | | 1596 | 1032 | 255 | 304 | 5 | | |

- Molecule 92 is a protein called NDUB10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 92 | bl | 175 | Total | C | N | O | S | 0 | 0 |
| | | | 1461 | 925 | 264 | 268 | 4 | | |
| 92 | BL | 175 | Total | C | N | O | S | 0 | 0 |
| | | | 1461 | 925 | 264 | 268 | 4 | | |

- Molecule 93 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 93 | bm | 164 | Total | C | N | O | S | 0 | 0 |
| | | | 1321 | 834 | 223 | 259 | 5 | | |
| 93 | BM | 164 | Total | C | N | O | S | 0 | 0 |
| | | | 1321 | 834 | 223 | 259 | 5 | | |

- Molecule 94 is a protein called Complex I-MNLL.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 94 | c4 | 102 | Total | C | N | O | S | 0 | 0 |
| | | | 850 | 553 | 139 | 150 | 8 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 94 | C4 | 102 | Total | C | N | O | S | 0 | 0 |
| | | | 850 | 553 | 139 | 150 | 8 | | |

- Molecule 95 is a protein called 2 iron, 2 sulfur cluster-binding protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 95 | fx | 146 | Total | C | N | O | S | 0 | 0 |
| | | | 1162 | 722 | 207 | 223 | 10 | | |
| 95 | FX | 146 | Total | C | N | O | S | 0 | 0 |
| | | | 1162 | 722 | 207 | 223 | 10 | | |

- Molecule 96 is a protein called Gamma-carbonic anhydrase.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 96 | g1 | 229 | Total | C | N | O | S | 0 | 0 |
| | | | 1773 | 1113 | 305 | 350 | 5 | | |
| 96 | G1 | 229 | Total | C | N | O | S | 0 | 0 |
| | | | 1773 | 1113 | 305 | 350 | 5 | | |

- Molecule 97 is a protein called Gamma-carbonic anhydrase.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 97 | g2 | 230 | Total | C | N | O | S | 0 | 0 |
| | | | 1762 | 1106 | 315 | 334 | 7 | | |
| 97 | G2 | 230 | Total | C | N | O | S | 0 | 0 |
| | | | 1762 | 1106 | 315 | 334 | 7 | | |

- Molecule 98 is a protein called Transcription factor apfi protein, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 98 | g3 | 346 | Total | C | N | O | S | 0 | 0 |
| | | | 2804 | 1766 | 481 | 549 | 8 | | |
| 98 | G3 | 346 | Total | C | N | O | S | 0 | 0 |
| | | | 2804 | 1766 | 481 | 549 | 8 | | |

- Molecule 99 is a protein called DnaJ domain protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 99 | j1 | 265 | Total | C | N | O | S | 0 | 0 |
| | | | 2170 | 1375 | 402 | 390 | 3 | | |
| 99 | J1 | 265 | Total | C | N | O | S | 0 | 0 |
| | | | 2170 | 1375 | 402 | 390 | 3 | | |

- Molecule 100 is a protein called NADH-ubiquinone oxidoreductase chain 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 100 | n1 | 283 | Total | C | N | O | S | 0 | 0 |
| | | | 2305 | 1581 | 334 | 378 | 12 | | |
| 100 | N1 | 283 | Total | C | N | O | S | 0 | 0 |
| | | | 2305 | 1581 | 334 | 378 | 12 | | |

- Molecule 101 is a protein called Ymf65.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 101 | n2 | 360 | Total | C | N | O | S | 0 | 0 |
| | | | 3073 | 2134 | 436 | 495 | 8 | | |
| 101 | N2 | 360 | Total | C | N | O | S | 0 | 0 |
| | | | 3073 | 2134 | 436 | 495 | 8 | | |

- Molecule 102 is a protein called NADH-ubiquinone oxidoreductase chain 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 102 | n3 | 120 | Total | C | N | O | S | 0 | 0 |
| | | | 1017 | 705 | 142 | 166 | 4 | | |
| 102 | N3 | 120 | Total | C | N | O | S | 0 | 0 |
| | | | 1017 | 705 | 142 | 166 | 4 | | |

- Molecule 103 is a protein called NADH-ubiquinone oxidoreductase chain 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 103 | n4 | 505 | Total | C | N | O | S | 0 | 0 |
| | | | 4170 | 2859 | 601 | 692 | 18 | | |
| 103 | N4 | 505 | Total | C | N | O | S | 0 | 0 |
| | | | 4170 | 2859 | 601 | 692 | 18 | | |

- Molecule 104 is a protein called NADH dehydrogenase subunit 5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 104 | n5 | 709 | Total | C | N | O | S | 0 | 0 |
| | | | 5908 | 4044 | 850 | 998 | 16 | | |
| 104 | N5 | 709 | Total | C | N | O | S | 0 | 0 |
| | | | 5908 | 4044 | 850 | 998 | 16 | | |

- Molecule 105 is a protein called Ymf62.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 105 | n6 | 255 | Total | C | N | O | S | 0 | 0 |
| | | | 2168 | 1483 | 306 | 374 | 5 | | |
| 105 | N6 | 255 | Total | C | N | O | S | 0 | 0 |
| | | | 2168 | 1483 | 306 | 374 | 5 | | |

- Molecule 106 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 106 | p1 | 230 | Total | C | N | O | S | 0 | 0 |
| | | | 1908 | 1241 | 322 | 340 | 5 | | |
| 106 | P1 | 230 | Total | C | N | O | S | 0 | 0 |
| | | | 1908 | 1241 | 322 | 340 | 5 | | |

- Molecule 107 is a protein called NDUPH2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 107 | p2 | 167 | Total | C | N | O | S | 0 | 0 |
| | | | 1414 | 926 | 225 | 258 | 5 | | |
| 107 | P2 | 167 | Total | C | N | O | S | 0 | 0 |
| | | | 1414 | 926 | 225 | 258 | 5 | | |

- Molecule 108 is a protein called M16 family peptidase, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 108 | qA | 454 | Total | C | N | O | S | 0 | 0 |
| | | | 3517 | 2213 | 599 | 699 | 6 | | |
| 108 | qa | 454 | Total | C | N | O | S | 0 | 0 |
| | | | 3517 | 2213 | 599 | 699 | 6 | | |
| 108 | QA | 454 | Total | C | N | O | S | 0 | 0 |
| | | | 3517 | 2213 | 599 | 699 | 6 | | |
| 108 | Qa | 454 | Total | C | N | O | S | 0 | 0 |
| | | | 3517 | 2213 | 599 | 699 | 6 | | |

- Molecule 109 is a protein called Peptidase M16 inactive domain protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 109 | qB | 480 | Total | C | N | O | S | 0 | 0 |
| | | | 3835 | 2431 | 668 | 731 | 5 | | |
| 109 | qb | 480 | Total | C | N | O | S | 0 | 0 |
| | | | 3835 | 2431 | 668 | 731 | 5 | | |
| 109 | QB | 480 | Total | C | N | O | S | 0 | 0 |
| | | | 3835 | 2431 | 668 | 731 | 5 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 109 | Qb | 480 | Total | C | N | O | S | 0 | 0 |
| | | | 3835 | 2431 | 668 | 731 | 5 | | |

- Molecule 110 is a protein called Apocytochrome b.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 110 | qC | 426 | Total | C | N | O | S | 0 | 0 |
| | | | 3589 | 2417 | 541 | 609 | 22 | | |
| 110 | qc | 425 | Total | C | N | O | S | 0 | 0 |
| | | | 3580 | 2411 | 539 | 608 | 22 | | |
| 110 | QC | 426 | Total | C | N | O | S | 0 | 0 |
| | | | 3589 | 2417 | 541 | 609 | 22 | | |
| 110 | Qc | 425 | Total | C | N | O | S | 0 | 0 |
| | | | 3580 | 2411 | 539 | 608 | 22 | | |

- Molecule 111 is a protein called Cytochrome protein c1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 111 | qD | 295 | Total | C | N | O | S | 0 | 0 |
| | | | 2489 | 1627 | 418 | 431 | 13 | | |
| 111 | qd | 295 | Total | C | N | O | S | 0 | 0 |
| | | | 2489 | 1627 | 418 | 431 | 13 | | |
| 111 | QD | 295 | Total | C | N | O | S | 0 | 0 |
| | | | 2489 | 1627 | 418 | 431 | 13 | | |
| 111 | Qd | 295 | Total | C | N | O | S | 0 | 0 |
| | | | 2489 | 1627 | 418 | 431 | 13 | | |

- Molecule 112 is a protein called Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 112 | qE | 230 | Total | C | N | O | S | 0 | 0 |
| | | | 1559 | 971 | 294 | 292 | 2 | | |
| 112 | qe | 219 | Total | C | N | O | S | 0 | 0 |
| | | | 1471 | 917 | 278 | 274 | 2 | | |
| 112 | QE | 230 | Total | C | N | O | S | 0 | 0 |
| | | | 1559 | 971 | 294 | 292 | 2 | | |
| 112 | Qe | 219 | Total | C | N | O | S | 0 | 0 |
| | | | 1471 | 917 | 278 | 274 | 2 | | |

- Molecule 113 is a protein called Ubiquinol-cytochrome C reductase hinge protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 113 | qF | 89 | Total | C | N | O | S | 0 | 0 |
| | | | 702 | 439 | 125 | 129 | 9 | | |
| 113 | qf | 80 | Total | C | N | O | S | 0 | 0 |
| | | | 630 | 393 | 112 | 116 | 9 | | |
| 113 | QF | 89 | Total | C | N | O | S | 0 | 0 |
| | | | 702 | 439 | 125 | 129 | 9 | | |
| 113 | Qf | 80 | Total | C | N | O | S | 0 | 0 |
| | | | 630 | 393 | 112 | 116 | 9 | | |

- Molecule 114 is a protein called Sulphotransf domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 114 | qG | 327 | Total | C | N | O | S | 0 | 0 |
| | | | 2767 | 1789 | 482 | 490 | 6 | | |
| 114 | qg | 326 | Total | C | N | O | S | 0 | 0 |
| | | | 2760 | 1784 | 481 | 489 | 6 | | |
| 114 | QG | 327 | Total | C | N | O | S | 0 | 0 |
| | | | 2767 | 1789 | 482 | 490 | 6 | | |
| 114 | Qg | 326 | Total | C | N | O | S | 0 | 0 |
| | | | 2760 | 1784 | 481 | 489 | 6 | | |

- Molecule 115 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 115 | qH | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1098 | 708 | 195 | 187 | 8 | | |
| 115 | qh | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1098 | 708 | 195 | 187 | 8 | | |
| 115 | QH | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1098 | 708 | 195 | 187 | 8 | | |
| 115 | Qh | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1098 | 708 | 195 | 187 | 8 | | |

- Molecule 116 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 116 | qI | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 971 | 651 | 161 | 158 | 1 | | |
| 116 | qi | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 971 | 651 | 161 | 158 | 1 | | |
| 116 | QI | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 971 | 651 | 161 | 158 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 116 | Qi | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 971 | 651 | 161 | 158 | 1 | | |

- Molecule 117 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 117 | qJ | 56 | Total | C | N | O | S | 0 | 0 |
| | | | 481 | 329 | 73 | 77 | 2 | | |
| 117 | qj | 58 | Total | C | N | O | S | 0 | 0 |
| | | | 501 | 341 | 79 | 79 | 2 | | |
| 117 | QJ | 56 | Total | C | N | O | S | 0 | 0 |
| | | | 481 | 329 | 73 | 77 | 2 | | |
| 117 | Qj | 58 | Total | C | N | O | S | 0 | 0 |
| | | | 501 | 341 | 79 | 79 | 2 | | |

- Molecule 118 is a protein called UQCRTT2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 118 | qL | 32 | Total | C | N | O | S | 0 | 0 |
| | | | 266 | 181 | 41 | 42 | 2 | | |
| 118 | ql | 32 | Total | C | N | O | S | 0 | 0 |
| | | | 266 | 181 | 41 | 42 | 2 | | |
| 118 | QL | 32 | Total | C | N | O | S | 0 | 0 |
| | | | 266 | 181 | 41 | 42 | 2 | | |
| 118 | Ql | 32 | Total | C | N | O | S | 0 | 0 |
| | | | 266 | 181 | 41 | 42 | 2 | | |

- Molecule 119 is a protein called Unknown peptide.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 119 | qM | 17 | Total | C | N | O | 0 | 0 |
| | | | 85 | 51 | 17 | 17 | | |
| 119 | qm | 17 | Total | C | N | O | 0 | 0 |
| | | | 85 | 51 | 17 | 17 | | |
| 119 | Qm | 17 | Total | C | N | O | 0 | 0 |
| | | | 85 | 51 | 17 | 17 | | |
| 119 | u2 | 17 | Total | C | N | O | 0 | 0 |
| | | | 85 | 51 | 17 | 17 | | |
| 119 | U2 | 17 | Total | C | N | O | 0 | 0 |
| | | | 85 | 51 | 17 | 17 | | |
| 119 | QM | 17 | Total | C | N | O | 0 | 0 |
| | | | 85 | 51 | 17 | 17 | | |

- Molecule 120 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 120 | s1 | 689 | Total | C | N | O | S | 0 | 0 |
| | | | 5410 | 3414 | 937 | 1031 | 28 | | |
| 120 | S1 | 689 | Total | C | N | O | S | 0 | 0 |
| | | | 5410 | 3414 | 937 | 1031 | 28 | | |

- Molecule 121 is a protein called NADH dehydrogenase subunit 7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 121 | s2 | 442 | Total | C | N | O | S | 0 | 0 |
| | | | 3598 | 2291 | 624 | 659 | 24 | | |
| 121 | S2 | 442 | Total | C | N | O | S | 0 | 0 |
| | | | 3598 | 2291 | 624 | 659 | 24 | | |

- Molecule 122 is a protein called NADH dehydrogenase subunit 9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 122 | s3 | 198 | Total | C | N | O | S | 0 | 0 |
| | | | 1681 | 1096 | 267 | 312 | 6 | | |
| 122 | S3 | 198 | Total | C | N | O | S | 0 | 0 |
| | | | 1681 | 1096 | 267 | 312 | 6 | | |

- Molecule 123 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 123 | s4 | 182 | Total | C | N | O | S | 0 | 0 |
| | | | 1500 | 952 | 268 | 272 | 8 | | |
| 123 | S4 | 182 | Total | C | N | O | S | 0 | 0 |
| | | | 1500 | 952 | 268 | 272 | 8 | | |

- Molecule 124 is a protein called GRAM domain protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 124 | s5 | 93 | Total | C | N | O | S | 0 | 0 |
| | | | 756 | 480 | 129 | 141 | 6 | | |
| 124 | S5 | 93 | Total | C | N | O | S | 0 | 0 |
| | | | 756 | 480 | 129 | 141 | 6 | | |

- Molecule 125 is a protein called Zinc-finger protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 125 | s6 | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 738 | 464 | 131 | 139 | 4 | | |
| 125 | S6 | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 738 | 464 | 131 | 139 | 4 | | |

- Molecule 126 is a protein called NADH dehydrogenase subunit 10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 126 | s7 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1278 | 822 | 220 | 226 | 10 | | |
| 126 | S7 | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1278 | 822 | 220 | 226 | 10 | | |

- Molecule 127 is a protein called NADH-ubiquinone oxidoreductase 1, chain, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 127 | s8 | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1812 | 1155 | 299 | 347 | 11 | | |
| 127 | S8 | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1812 | 1155 | 299 | 347 | 11 | | |

- Molecule 128 is a protein called Lipid-A-disaccharide synthase.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 128 | t1 | 502 | Total | C | N | O | S | 0 | 0 |
| | | | 4059 | 2600 | 698 | 748 | 13 | | |
| 128 | T1 | 502 | Total | C | N | O | S | 0 | 0 |
| | | | 4059 | 2600 | 698 | 748 | 13 | | |

- Molecule 129 is a protein called Acyl-CoA synthetase (AMP-forming)/AMP-acid ligase II.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 129 | t2 | 279 | Total | C | N | O | S | 0 | 0 |
| | | | 2180 | 1386 | 375 | 418 | 1 | | |
| 129 | T2 | 279 | Total | C | N | O | S | 0 | 0 |
| | | | 2180 | 1386 | 375 | 418 | 1 | | |

- Molecule 130 is a protein called RNase III domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 130 | t3 | 310 | Total | C | N | O | S | 0 | 0 |
| | | | 2479 | 1576 | 432 | 464 | 7 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 130 | T3 | 310 | Total | C | N | O | S | 0 | 0 |
| | | | 2479 | 1576 | 432 | 464 | 7 | | |

- Molecule 131 is a protein called Transmembrane protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 131 | t4 | 198 | Total | C | N | O | S | 0 | 0 |
| | | | 1644 | 1068 | 284 | 289 | 3 | | |
| 131 | T4 | 198 | Total | C | N | O | S | 0 | 0 |
| | | | 1644 | 1068 | 284 | 289 | 3 | | |

- Molecule 132 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 132 | t5 | 141 | Total | C | N | O | S | 0 | 0 |
| | | | 1138 | 730 | 202 | 204 | 2 | | |
| 132 | T5 | 141 | Total | C | N | O | S | 0 | 0 |
| | | | 1138 | 730 | 202 | 204 | 2 | | |

- Molecule 133 is a protein called COX assembly mitochondrial protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 133 | t6 | 109 | Total | C | N | O | S | 0 | 0 |
| | | | 903 | 562 | 161 | 174 | 6 | | |
| 133 | T6 | 109 | Total | C | N | O | S | 0 | 0 |
| | | | 903 | 562 | 161 | 174 | 6 | | |

- Molecule 134 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 134 | t7 | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1187 | 770 | 202 | 209 | 6 | | |
| 134 | T7 | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1187 | 770 | 202 | 209 | 6 | | |

- Molecule 135 is a protein called PH domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 135 | t8 | 131 | Total | C | N | O | 0 | 0 |
| | | | 1084 | 705 | 191 | 188 | | |
| 135 | T8 | 131 | Total | C | N | O | 0 | 0 |
| | | | 1084 | 705 | 191 | 188 | | |

- Molecule 136 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 136 | t9 | 132 | Total | C | N | O | S | 0 | 0 |
| | | | 1066 | 670 | 185 | 201 | 10 | | |
| 136 | T9 | 132 | Total | C | N | O | S | 0 | 0 |
| | | | 1066 | 670 | 185 | 201 | 10 | | |

- Molecule 137 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 137 | ta | 102 | Total | C | N | O | S | 0 | 0 |
| | | | 854 | 553 | 141 | 155 | 5 | | |
| 137 | TA | 102 | Total | C | N | O | S | 0 | 0 |
| | | | 854 | 553 | 141 | 155 | 5 | | |

- Molecule 138 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 138 | tb | 96 | Total | C | N | O | | 0 | 0 |
| | | | 801 | 515 | 139 | 147 | | | |
| 138 | TB | 96 | Total | C | N | O | | 0 | 0 |
| | | | 801 | 515 | 139 | 147 | | | |

- Molecule 139 is a protein called ATP synthase subunit e, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 139 | tc | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 789 | 497 | 146 | 145 | 1 | | |
| 139 | TC | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 789 | 497 | 146 | 145 | 1 | | |

- Molecule 140 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 140 | td | 72 | Total | C | N | O | | 0 | 0 |
| | | | 616 | 403 | 110 | 103 | | | |
| 140 | TD | 72 | Total | C | N | O | | 0 | 0 |
| | | | 616 | 403 | 110 | 103 | | | |

- Molecule 141 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 141 | te | 50 | Total | C | N | O | S | 0 | 0 |
| | | | 420 | 282 | 64 | 72 | 2 | | |
| 141 | TE | 50 | Total | C | N | O | S | 0 | 0 |
| | | | 420 | 282 | 64 | 72 | 2 | | |

- Molecule 142 is a protein called NDUTT15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 142 | tf | 216 | Total | C | N | O | S | 0 | 0 |
| | | | 1789 | 1150 | 304 | 327 | 8 | | |
| 142 | TF | 216 | Total | C | N | O | S | 0 | 0 |
| | | | 1789 | 1150 | 304 | 327 | 8 | | |

- Molecule 143 is a protein called NDUTT16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 143 | tg | 134 | Total | C | N | O | S | 0 | 0 |
| | | | 1081 | 683 | 194 | 203 | 1 | | |
| 143 | TG | 134 | Total | C | N | O | S | 0 | 0 |
| | | | 1081 | 683 | 194 | 203 | 1 | | |

- Molecule 144 is a protein called NDUTT17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 144 | th | 124 | Total | C | N | O | S | 0 | 0 |
| | | | 996 | 639 | 178 | 177 | 2 | | |
| 144 | TH | 124 | Total | C | N | O | S | 0 | 0 |
| | | | 996 | 639 | 178 | 177 | 2 | | |

- Molecule 145 is a protein called Thioredoxin.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 145 | tx | 144 | Total | C | N | O | S | 0 | 0 |
| | | | 1206 | 767 | 205 | 227 | 7 | | |
| 145 | TX | 144 | Total | C | N | O | S | 0 | 0 |
| | | | 1206 | 767 | 205 | 227 | 7 | | |

- Molecule 146 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 146 | v1 | 442 | Total | C | N | O | S | 0 | 0 |
| | | | 3410 | 2146 | 600 | 640 | 24 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 146 | V1 | 442 | Total | C | N | O | S | 0 | 0 |
| | | | 3410 | 2146 | 600 | 640 | 24 | | |

- Molecule 147 is a protein called NADH-ubiquinone oxidoreductase 24 kDa subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 147 | v2 | 231 | Total | C | N | O | S | 0 | 0 |
| | | | 1858 | 1173 | 318 | 357 | 10 | | |
| 147 | V2 | 231 | Total | C | N | O | S | 0 | 0 |
| | | | 1858 | 1173 | 318 | 357 | 10 | | |

- Molecule 148 is a protein called NADH-ubiquinone oxidoreductase complex I, 21 kDa subunit.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 148 | x1 | 149 | Total | C | N | O | 0 | 0 |
| | | | 1227 | 800 | 213 | 214 | | |
| 148 | X1 | 149 | Total | C | N | O | 0 | 0 |
| | | | 1227 | 800 | 213 | 214 | | |

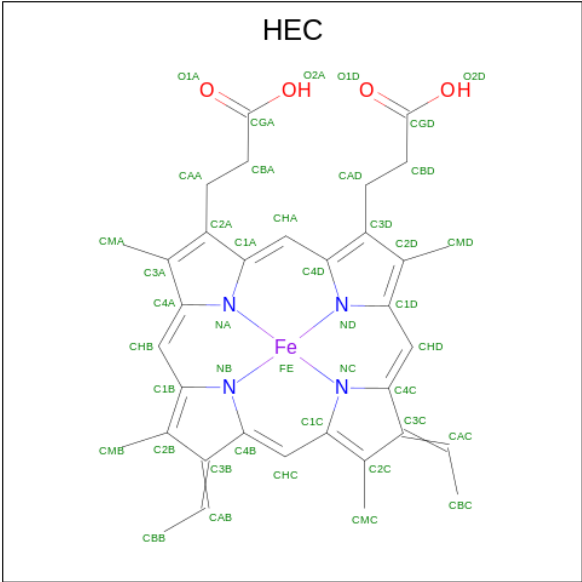
- Molecule 149 is a protein called COXTT3.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 149 | C | 203 | Total | C | N | O | 0 | 0 |
| | | | 1368 | 851 | 246 | 271 | | |
| 149 | c | 203 | Total | C | N | O | 0 | 0 |
| | | | 1368 | 851 | 246 | 271 | | |

- Molecule 150 is a protein called Unknown peptide.

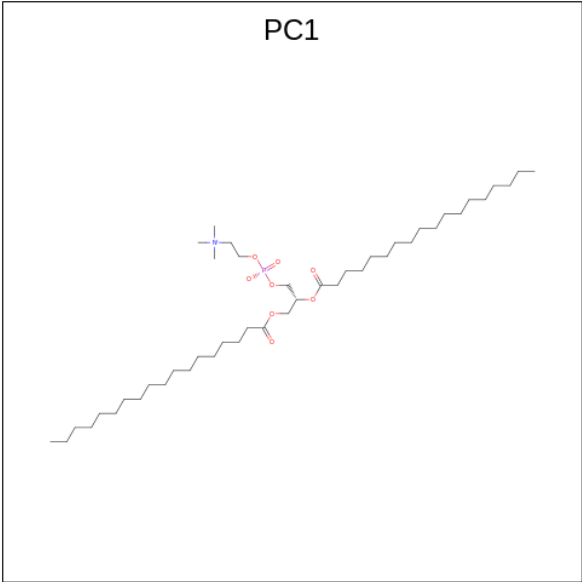
| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 150 | u1 | 92 | Total | C | N | O | 0 | 0 |
| | | | 460 | 276 | 92 | 92 | | |
| 150 | U1 | 92 | Total | C | N | O | 0 | 0 |
| | | | 460 | 276 | 92 | 92 | | |

- Molecule 151 is HEME C (three-letter code: HEC) (formula: C₃₄H₃₄FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 151 | 2e | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 151 | qD | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 151 | qd | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 151 | 2E | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 151 | QD | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 151 | Qd | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |

- Molecule 152 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: C₄₄H₈₈NO₈P).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 152 | 2f | 1 | Total | C | N | O | P | 0 |
| | | | 47 | 37 | 1 | 8 | 1 | |
| 152 | 2f | 1 | Total | C | N | O | P | 0 |
| | | | 42 | 32 | 1 | 8 | 1 | |
| 152 | 2f | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 22 | 1 | 8 | 1 | |
| 152 | 2g | 1 | Total | C | N | O | P | 0 |
| | | | 50 | 40 | 1 | 8 | 1 | |
| 152 | 2j | 1 | Total | C | N | O | P | 0 |
| | | | 42 | 32 | 1 | 8 | 1 | |
| 152 | 6a | 1 | Total | C | N | O | P | 0 |
| | | | 35 | 25 | 1 | 8 | 1 | |
| 152 | 6c | 1 | Total | C | N | O | P | 0 |
| | | | 33 | 23 | 1 | 8 | 1 | |
| 152 | 7a | 1 | Total | C | N | O | P | 0 |
| | | | 45 | 35 | 1 | 8 | 1 | |
| 152 | 7c | 1 | Total | C | N | O | P | 0 |
| | | | 43 | 33 | 1 | 8 | 1 | |
| 152 | a | 1 | Total | C | N | O | P | 0 |
| | | | 41 | 31 | 1 | 8 | 1 | |
| 152 | a | 1 | Total | C | N | O | P | 0 |
| | | | 41 | 31 | 1 | 8 | 1 | |
| 152 | c1 | 1 | Total | C | N | O | P | 0 |
| | | | 49 | 39 | 1 | 8 | 1 | |
| 152 | c1 | 1 | Total | C | N | O | P | 0 |
| | | | 45 | 35 | 1 | 8 | 1 | |
| 152 | c1 | 1 | Total | C | N | O | P | 0 |
| | | | 38 | 28 | 1 | 8 | 1 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 152 | c1 | 1 | Total | C | N | O | P | 0 |
| | | | 39 | 29 | 1 | 8 | 1 | |
| 152 | c2 | 1 | Total | C | N | O | P | 0 |
| | | | 36 | 26 | 1 | 8 | 1 | |
| 152 | c3 | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 152 | c3 | 1 | Total | C | N | O | P | 0 |
| | | | 39 | 29 | 1 | 8 | 1 | |
| 152 | c3 | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 21 | 1 | 8 | 1 | |
| 152 | c3 | 1 | Total | C | N | O | P | 0 |
| | | | 39 | 29 | 1 | 8 | 1 | |
| 152 | c3 | 1 | Total | C | N | O | P | 0 |
| | | | 49 | 39 | 1 | 8 | 1 | |
| 152 | d | 1 | Total | C | N | O | P | 0 |
| | | | 35 | 25 | 1 | 8 | 1 | |
| 152 | f | 1 | Total | C | N | O | P | 0 |
| | | | 38 | 28 | 1 | 8 | 1 | |
| 152 | fs | 1 | Total | C | N | O | P | 0 |
| | | | 40 | 30 | 1 | 8 | 1 | |
| 152 | i | 1 | Total | C | N | O | P | 0 |
| | | | 39 | 29 | 1 | 8 | 1 | |
| 152 | j | 1 | Total | C | N | O | P | 0 |
| | | | 37 | 27 | 1 | 8 | 1 | |
| 152 | m | 1 | Total | C | N | O | P | 0 |
| | | | 45 | 35 | 1 | 8 | 1 | |
| 152 | m | 1 | Total | C | N | O | P | 0 |
| | | | 35 | 25 | 1 | 8 | 1 | |
| 152 | m | 1 | Total | C | N | O | P | 0 |
| | | | 36 | 26 | 1 | 8 | 1 | |
| 152 | m1 | 1 | Total | C | N | O | P | 0 |
| | | | 54 | 44 | 1 | 8 | 1 | |
| 152 | m1 | 1 | Total | C | N | O | P | 0 |
| | | | 42 | 32 | 1 | 8 | 1 | |
| 152 | m2 | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 22 | 1 | 8 | 1 | |
| 152 | m2 | 1 | Total | C | N | O | P | 0 |
| | | | 54 | 44 | 1 | 8 | 1 | |
| 152 | m2 | 1 | Total | C | N | O | P | 0 |
| | | | 46 | 36 | 1 | 8 | 1 | |
| 152 | n | 1 | Total | C | N | O | P | 0 |
| | | | 41 | 31 | 1 | 8 | 1 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 152 | n | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 22 | 1 | 8 | 1 | |
| 152 | n | 1 | Total | C | N | O | P | 0 |
| | | | 36 | 26 | 1 | 8 | 1 | |
| 152 | v | 1 | Total | C | N | O | P | 0 |
| | | | 35 | 25 | 1 | 8 | 1 | |
| 152 | v | 1 | Total | C | N | O | P | 0 |
| | | | 49 | 39 | 1 | 8 | 1 | |
| 152 | w | 1 | Total | C | N | O | P | 0 |
| | | | 49 | 39 | 1 | 8 | 1 | |
| 152 | w | 1 | Total | C | N | O | P | 0 |
| | | | 34 | 24 | 1 | 8 | 1 | |
| 152 | w | 1 | Total | C | N | O | P | 0 |
| | | | 43 | 33 | 1 | 8 | 1 | |
| 152 | 5b | 1 | Total | C | N | O | P | 0 |
| | | | 47 | 37 | 1 | 8 | 1 | |
| 152 | al | 1 | Total | C | N | O | P | 0 |
| | | | 26 | 16 | 1 | 8 | 1 | |
| 152 | am | 1 | Total | C | N | O | P | 0 |
| | | | 39 | 29 | 1 | 8 | 1 | |
| 152 | an | 1 | Total | C | N | O | P | 0 |
| | | | 36 | 26 | 1 | 8 | 1 | |
| 152 | b9 | 1 | Total | C | N | O | P | 0 |
| | | | 34 | 24 | 1 | 8 | 1 | |
| 152 | c4 | 1 | Total | C | N | O | P | 0 |
| | | | 41 | 31 | 1 | 8 | 1 | |
| 152 | j1 | 1 | Total | C | N | O | P | 0 |
| | | | 40 | 30 | 1 | 8 | 1 | |
| 152 | n1 | 1 | Total | C | N | O | P | 0 |
| | | | 36 | 26 | 1 | 8 | 1 | |
| 152 | n3 | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 21 | 1 | 8 | 1 | |
| 152 | n5 | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 152 | n5 | 1 | Total | C | N | O | P | 0 |
| | | | 53 | 43 | 1 | 8 | 1 | |
| 152 | n5 | 1 | Total | C | N | O | P | 0 |
| | | | 39 | 29 | 1 | 8 | 1 | |
| 152 | n5 | 1 | Total | C | N | O | P | 0 |
| | | | 54 | 44 | 1 | 8 | 1 | |
| 152 | n6 | 1 | Total | C | N | O | P | 0 |
| | | | 54 | 44 | 1 | 8 | 1 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|--------|---------|
| 152 | p1 | 1 | Total 40 | C 30 | N 1 | O 8 | P 1 | 0 |
| 152 | qB | 1 | Total 44 | C 34 | N 1 | O 8 | P 1 | 0 |
| 152 | qC | 1 | Total 38 | C 28 | N 1 | O 8 | P 1 | 0 |
| 152 | qC | 1 | Total 50 | C 40 | N 1 | O 8 | P 1 | 0 |
| 152 | qC | 1 | Total 36 | C 26 | N 1 | O 8 | P 1 | 0 |
| 152 | qE | 1 | Total 24 | C 14 | N 1 | O 8 | P 1 | 0 |
| 152 | qE | 1 | Total 39 | C 29 | N 1 | O 8 | P 1 | 0 |
| 152 | qE | 1 | Total 28 | C 18 | N 1 | O 8 | P 1 | 0 |
| 152 | qG | 1 | Total 32 | C 22 | N 1 | O 8 | P 1 | 0 |
| 152 | qI | 1 | Total 30 | C 20 | N 1 | O 8 | P 1 | 0 |
| 152 | qI | 1 | Total 43 | C 33 | N 1 | O 8 | P 1 | 0 |
| 152 | qJ | 1 | Total 38 | C 28 | N 1 | O 8 | P 1 | 0 |
| 152 | qb | 1 | Total 43 | C 33 | N 1 | O 8 | P 1 | 0 |
| 152 | qc | 1 | Total 38 | C 28 | N 1 | O 8 | P 1 | 0 |
| 152 | qc | 1 | Total 47 | C 37 | N 1 | O 8 | P 1 | 0 |
| 152 | qe | 1 | Total 33 | C 23 | N 1 | O 8 | P 1 | 0 |
| 152 | qe | 1 | Total 43 | C 33 | N 1 | O 8 | P 1 | 0 |
| 152 | qg | 1 | Total 32 | C 22 | N 1 | O 8 | P 1 | 0 |
| 152 | qi | 1 | Total 30 | C 20 | N 1 | O 8 | P 1 | 0 |
| 152 | qi | 1 | Total 42 | C 32 | N 1 | O 8 | P 1 | 0 |
| 152 | qj | 1 | Total 36 | C 26 | N 1 | O 8 | P 1 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 152 | s8 | 1 | Total | C | N | O | P | 0 |
| | | | 30 | 20 | 1 | 8 | 1 | |
| 152 | t1 | 1 | Total | C | N | O | P | 0 |
| | | | 33 | 23 | 1 | 8 | 1 | |
| 152 | t4 | 1 | Total | C | N | O | P | 0 |
| | | | 48 | 38 | 1 | 8 | 1 | |
| 152 | t4 | 1 | Total | C | N | O | P | 0 |
| | | | 54 | 44 | 1 | 8 | 1 | |
| 152 | tc | 1 | Total | C | N | O | P | 0 |
| | | | 42 | 32 | 1 | 8 | 1 | |
| 152 | tc | 1 | Total | C | N | O | P | 0 |
| | | | 47 | 37 | 1 | 8 | 1 | |
| 152 | te | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 22 | 1 | 8 | 1 | |
| 152 | 2F | 1 | Total | C | N | O | P | 0 |
| | | | 47 | 37 | 1 | 8 | 1 | |
| 152 | 2F | 1 | Total | C | N | O | P | 0 |
| | | | 42 | 32 | 1 | 8 | 1 | |
| 152 | 2F | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 22 | 1 | 8 | 1 | |
| 152 | 2G | 1 | Total | C | N | O | P | 0 |
| | | | 50 | 40 | 1 | 8 | 1 | |
| 152 | 2J | 1 | Total | C | N | O | P | 0 |
| | | | 42 | 32 | 1 | 8 | 1 | |
| 152 | 6A | 1 | Total | C | N | O | P | 0 |
| | | | 35 | 25 | 1 | 8 | 1 | |
| 152 | 6C | 1 | Total | C | N | O | P | 0 |
| | | | 33 | 23 | 1 | 8 | 1 | |
| 152 | 7A | 1 | Total | C | N | O | P | 0 |
| | | | 45 | 35 | 1 | 8 | 1 | |
| 152 | 7C | 1 | Total | C | N | O | P | 0 |
| | | | 43 | 33 | 1 | 8 | 1 | |
| 152 | A | 1 | Total | C | N | O | P | 0 |
| | | | 41 | 31 | 1 | 8 | 1 | |
| 152 | A | 1 | Total | C | N | O | P | 0 |
| | | | 41 | 31 | 1 | 8 | 1 | |
| 152 | C1 | 1 | Total | C | N | O | P | 0 |
| | | | 49 | 39 | 1 | 8 | 1 | |
| 152 | C1 | 1 | Total | C | N | O | P | 0 |
| | | | 45 | 35 | 1 | 8 | 1 | |
| 152 | C1 | 1 | Total | C | N | O | P | 0 |
| | | | 38 | 28 | 1 | 8 | 1 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 152 | C1 | 1 | Total | C | N | O | P | 0 |
| | | | 39 | 29 | 1 | 8 | 1 | |
| 152 | C2 | 1 | Total | C | N | O | P | 0 |
| | | | 36 | 26 | 1 | 8 | 1 | |
| 152 | C3 | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 152 | C3 | 1 | Total | C | N | O | P | 0 |
| | | | 39 | 29 | 1 | 8 | 1 | |
| 152 | C3 | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 21 | 1 | 8 | 1 | |
| 152 | C3 | 1 | Total | C | N | O | P | 0 |
| | | | 39 | 29 | 1 | 8 | 1 | |
| 152 | C3 | 1 | Total | C | N | O | P | 0 |
| | | | 49 | 39 | 1 | 8 | 1 | |
| 152 | D | 1 | Total | C | N | O | P | 0 |
| | | | 35 | 25 | 1 | 8 | 1 | |
| 152 | F | 1 | Total | C | N | O | P | 0 |
| | | | 38 | 28 | 1 | 8 | 1 | |
| 152 | FS | 1 | Total | C | N | O | P | 0 |
| | | | 40 | 30 | 1 | 8 | 1 | |
| 152 | I | 1 | Total | C | N | O | P | 0 |
| | | | 39 | 29 | 1 | 8 | 1 | |
| 152 | J | 1 | Total | C | N | O | P | 0 |
| | | | 37 | 27 | 1 | 8 | 1 | |
| 152 | M | 1 | Total | C | N | O | P | 0 |
| | | | 36 | 26 | 1 | 8 | 1 | |
| 152 | M | 1 | Total | C | N | O | P | 0 |
| | | | 45 | 35 | 1 | 8 | 1 | |
| 152 | M | 1 | Total | C | N | O | P | 0 |
| | | | 35 | 25 | 1 | 8 | 1 | |
| 152 | M1 | 1 | Total | C | N | O | P | 0 |
| | | | 54 | 44 | 1 | 8 | 1 | |
| 152 | M1 | 1 | Total | C | N | O | P | 0 |
| | | | 42 | 32 | 1 | 8 | 1 | |
| 152 | M2 | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 22 | 1 | 8 | 1 | |
| 152 | M2 | 1 | Total | C | N | O | P | 0 |
| | | | 54 | 44 | 1 | 8 | 1 | |
| 152 | M2 | 1 | Total | C | N | O | P | 0 |
| | | | 46 | 36 | 1 | 8 | 1 | |
| 152 | N | 1 | Total | C | N | O | P | 0 |
| | | | 41 | 31 | 1 | 8 | 1 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|--------|---------|
| 152 | N | 1 | Total 32 | C 22 | N 1 | O 8 | P 1 | 0 |
| 152 | N | 1 | Total 36 | C 26 | N 1 | O 8 | P 1 | 0 |
| 152 | V | 1 | Total 35 | C 25 | N 1 | O 8 | P 1 | 0 |
| 152 | V | 1 | Total 49 | C 39 | N 1 | O 8 | P 1 | 0 |
| 152 | W | 1 | Total 49 | C 39 | N 1 | O 8 | P 1 | 0 |
| 152 | W | 1 | Total 34 | C 24 | N 1 | O 8 | P 1 | 0 |
| 152 | W | 1 | Total 43 | C 33 | N 1 | O 8 | P 1 | 0 |
| 152 | 5B | 1 | Total 47 | C 37 | N 1 | O 8 | P 1 | 0 |
| 152 | AL | 1 | Total 26 | C 16 | N 1 | O 8 | P 1 | 0 |
| 152 | AM | 1 | Total 39 | C 29 | N 1 | O 8 | P 1 | 0 |
| 152 | AN | 1 | Total 36 | C 26 | N 1 | O 8 | P 1 | 0 |
| 152 | B9 | 1 | Total 34 | C 24 | N 1 | O 8 | P 1 | 0 |
| 152 | C4 | 1 | Total 41 | C 31 | N 1 | O 8 | P 1 | 0 |
| 152 | J1 | 1 | Total 40 | C 30 | N 1 | O 8 | P 1 | 0 |
| 152 | N1 | 1 | Total 36 | C 26 | N 1 | O 8 | P 1 | 0 |
| 152 | N3 | 1 | Total 31 | C 21 | N 1 | O 8 | P 1 | 0 |
| 152 | N5 | 1 | Total 52 | C 42 | N 1 | O 8 | P 1 | 0 |
| 152 | N5 | 1 | Total 53 | C 43 | N 1 | O 8 | P 1 | 0 |
| 152 | N5 | 1 | Total 39 | C 29 | N 1 | O 8 | P 1 | 0 |
| 152 | N5 | 1 | Total 54 | C 44 | N 1 | O 8 | P 1 | 0 |
| 152 | N6 | 1 | Total 54 | C 44 | N 1 | O 8 | P 1 | 0 |

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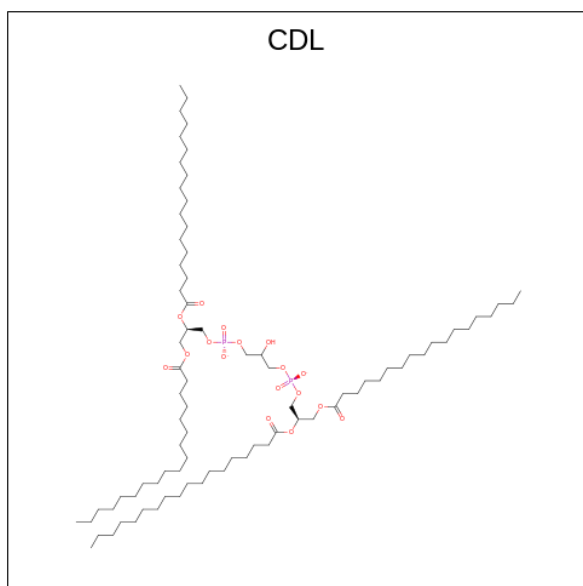
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|--------|---------|
| 152 | P1 | 1 | Total 40 | C 30 | N 1 | O 8 | P 1 | 0 |
| 152 | QB | 1 | Total 44 | C 34 | N 1 | O 8 | P 1 | 0 |
| 152 | QC | 1 | Total 38 | C 28 | N 1 | O 8 | P 1 | 0 |
| 152 | QC | 1 | Total 50 | C 40 | N 1 | O 8 | P 1 | 0 |
| 152 | QC | 1 | Total 36 | C 26 | N 1 | O 8 | P 1 | 0 |
| 152 | QE | 1 | Total 24 | C 14 | N 1 | O 8 | P 1 | 0 |
| 152 | QE | 1 | Total 39 | C 29 | N 1 | O 8 | P 1 | 0 |
| 152 | QG | 1 | Total 32 | C 22 | N 1 | O 8 | P 1 | 0 |
| 152 | QI | 1 | Total 30 | C 20 | N 1 | O 8 | P 1 | 0 |
| 152 | QI | 1 | Total 43 | C 33 | N 1 | O 8 | P 1 | 0 |
| 152 | QJ | 1 | Total 28 | C 18 | N 1 | O 8 | P 1 | 0 |
| 152 | QJ | 1 | Total 38 | C 28 | N 1 | O 8 | P 1 | 0 |
| 152 | Qb | 1 | Total 43 | C 33 | N 1 | O 8 | P 1 | 0 |
| 152 | Qc | 1 | Total 38 | C 28 | N 1 | O 8 | P 1 | 0 |
| 152 | Qc | 1 | Total 47 | C 37 | N 1 | O 8 | P 1 | 0 |
| 152 | Qe | 1 | Total 33 | C 23 | N 1 | O 8 | P 1 | 0 |
| 152 | Qe | 1 | Total 43 | C 33 | N 1 | O 8 | P 1 | 0 |
| 152 | Qg | 1 | Total 32 | C 22 | N 1 | O 8 | P 1 | 0 |
| 152 | Qi | 1 | Total 30 | C 20 | N 1 | O 8 | P 1 | 0 |
| 152 | Qi | 1 | Total 42 | C 32 | N 1 | O 8 | P 1 | 0 |
| 152 | Qj | 1 | Total 36 | C 26 | N 1 | O 8 | P 1 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 152 | S8 | 1 | Total | C | N | O | P | 0 |
| | | | 30 | 20 | 1 | 8 | 1 | |
| 152 | T1 | 1 | Total | C | N | O | P | 0 |
| | | | 33 | 23 | 1 | 8 | 1 | |
| 152 | T4 | 1 | Total | C | N | O | P | 0 |
| | | | 48 | 38 | 1 | 8 | 1 | |
| 152 | T4 | 1 | Total | C | N | O | P | 0 |
| | | | 54 | 44 | 1 | 8 | 1 | |
| 152 | TC | 1 | Total | C | N | O | P | 0 |
| | | | 42 | 32 | 1 | 8 | 1 | |
| 152 | TC | 1 | Total | C | N | O | P | 0 |
| | | | 47 | 37 | 1 | 8 | 1 | |
| 152 | TE | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 22 | 1 | 8 | 1 | |

- Molecule 153 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 153 | 2g | 1 | Total | C | O | P | 0 |
| | | | 89 | 70 | 17 | 2 | |
| 153 | 2g | 1 | Total | C | O | P | 0 |
| | | | 55 | 36 | 17 | 2 | |
| 153 | 2g | 1 | Total | C | O | P | 0 |
| | | | 63 | 44 | 17 | 2 | |
| 153 | 2k | 1 | Total | C | O | P | 0 |
| | | | 98 | 79 | 17 | 2 | |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 153 | 2m | 1 | Total | C | O | P | 0 |
| | | | 96 | 77 | 17 | 2 | |
| 153 | 2o | 1 | Total | C | O | P | 0 |
| | | | 50 | 31 | 17 | 2 | |
| 153 | 6a | 1 | Total | C | O | P | 0 |
| | | | 74 | 55 | 17 | 2 | |
| 153 | 6c | 1 | Total | C | O | P | 0 |
| | | | 75 | 56 | 17 | 2 | |
| 153 | 6c | 1 | Total | C | O | P | 0 |
| | | | 82 | 63 | 17 | 2 | |
| 153 | 7a | 1 | Total | C | O | P | 0 |
| | | | 100 | 81 | 17 | 2 | |
| 153 | 7a | 1 | Total | C | O | P | 0 |
| | | | 62 | 43 | 17 | 2 | |
| 153 | 7c | 1 | Total | C | O | P | 0 |
| | | | 85 | 66 | 17 | 2 | |
| 153 | 7c | 1 | Total | C | O | P | 0 |
| | | | 51 | 32 | 17 | 2 | |
| 153 | a | 1 | Total | C | O | P | 0 |
| | | | 51 | 32 | 17 | 2 | |
| 153 | a | 1 | Total | C | O | P | 0 |
| | | | 94 | 75 | 17 | 2 | |
| 153 | a | 1 | Total | C | O | P | 0 |
| | | | 82 | 63 | 17 | 2 | |
| 153 | b | 1 | Total | C | O | P | 0 |
| | | | 62 | 43 | 17 | 2 | |
| 153 | c1 | 1 | Total | C | O | P | 0 |
| | | | 79 | 60 | 17 | 2 | |
| 153 | c1 | 1 | Total | C | O | P | 0 |
| | | | 65 | 46 | 17 | 2 | |
| 153 | c1 | 1 | Total | C | O | P | 0 |
| | | | 63 | 44 | 17 | 2 | |
| 153 | c1 | 1 | Total | C | O | P | 0 |
| | | | 95 | 76 | 17 | 2 | |
| 153 | c3 | 1 | Total | C | O | P | 0 |
| | | | 68 | 49 | 17 | 2 | |
| 153 | e | 1 | Total | C | O | P | 0 |
| | | | 60 | 41 | 17 | 2 | |
| 153 | e | 1 | Total | C | O | P | 0 |
| | | | 72 | 53 | 17 | 2 | |
| 153 | e | 1 | Total | C | O | P | 0 |
| | | | 63 | 44 | 17 | 2 | |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|--------------|---------|---------|--------|---------|
| 153 | f | 1 | Total 100 | C 81 | O 17 | P 2 | 0 |
| 153 | fs | 1 | Total 47 | C 28 | O 17 | P 2 | 0 |
| 153 | i | 1 | Total 77 | C 58 | O 17 | P 2 | 0 |
| 153 | i | 1 | Total 75 | C 56 | O 17 | P 2 | 0 |
| 153 | j | 1 | Total 70 | C 51 | O 17 | P 2 | 0 |
| 153 | l | 1 | Total 74 | C 55 | O 17 | P 2 | 0 |
| 153 | m | 1 | Total 64 | C 45 | O 17 | P 2 | 0 |
| 153 | m | 1 | Total 83 | C 64 | O 17 | P 2 | 0 |
| 153 | m | 1 | Total 64 | C 45 | O 17 | P 2 | 0 |
| 153 | m | 1 | Total 66 | C 47 | O 17 | P 2 | 0 |
| 153 | m1 | 1 | Total 66 | C 47 | O 17 | P 2 | 0 |
| 153 | m1 | 1 | Total 91 | C 72 | O 17 | P 2 | 0 |
| 153 | m1 | 1 | Total 57 | C 38 | O 17 | P 2 | 0 |
| 153 | m2 | 1 | Total 54 | C 35 | O 17 | P 2 | 0 |
| 153 | m2 | 1 | Total 66 | C 47 | O 17 | P 2 | 0 |
| 153 | m2 | 1 | Total 74 | C 55 | O 17 | P 2 | 0 |
| 153 | m3 | 1 | Total 63 | C 44 | O 17 | P 2 | 0 |
| 153 | m3 | 1 | Total 55 | C 36 | O 17 | P 2 | 0 |
| 153 | n | 1 | Total 84 | C 65 | O 17 | P 2 | 0 |
| 153 | q | 1 | Total 63 | C 44 | O 17 | P 2 | 0 |
| 153 | q | 1 | Total 72 | C 53 | O 17 | P 2 | 0 |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 153 | q | 1 | Total | C | O | P | 0 |
| | | | 86 | 67 | 17 | 2 | |
| 153 | r | 1 | Total | C | O | P | 0 |
| | | | 65 | 46 | 17 | 2 | |
| 153 | sd | 1 | Total | C | O | P | 0 |
| | | | 76 | 57 | 17 | 2 | |
| 153 | t | 1 | Total | C | O | P | 0 |
| | | | 59 | 40 | 17 | 2 | |
| 153 | t | 1 | Total | C | O | P | 0 |
| | | | 75 | 56 | 17 | 2 | |
| 153 | t | 1 | Total | C | O | P | 0 |
| | | | 71 | 52 | 17 | 2 | |
| 153 | t | 1 | Total | C | O | P | 0 |
| | | | 90 | 71 | 17 | 2 | |
| 153 | u | 1 | Total | C | O | P | 0 |
| | | | 60 | 41 | 17 | 2 | |
| 153 | vb | 1 | Total | C | O | P | 0 |
| | | | 62 | 43 | 17 | 2 | |
| 153 | vb | 1 | Total | C | O | P | 0 |
| | | | 67 | 48 | 17 | 2 | |
| 153 | w | 1 | Total | C | O | P | 0 |
| | | | 84 | 65 | 17 | 2 | |
| 153 | y5 | 1 | Total | C | O | P | 0 |
| | | | 70 | 51 | 17 | 2 | |
| 153 | y7 | 1 | Total | C | O | P | 0 |
| | | | 65 | 46 | 17 | 2 | |
| 153 | z | 1 | Total | C | O | P | 0 |
| | | | 67 | 48 | 17 | 2 | |
| 153 | 2b | 1 | Total | C | O | P | 0 |
| | | | 87 | 68 | 17 | 2 | |
| 153 | 5b | 1 | Total | C | O | P | 0 |
| | | | 81 | 62 | 17 | 2 | |
| 153 | a1 | 1 | Total | C | O | P | 0 |
| | | | 67 | 48 | 17 | 2 | |
| 153 | a9 | 1 | Total | C | O | P | 0 |
| | | | 76 | 57 | 17 | 2 | |
| 153 | a9 | 1 | Total | C | O | P | 0 |
| | | | 87 | 68 | 17 | 2 | |
| 153 | al | 1 | Total | C | O | P | 0 |
| | | | 53 | 34 | 17 | 2 | |
| 153 | am | 1 | Total | C | O | P | 0 |
| | | | 56 | 37 | 17 | 2 | |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 153 | an | 1 | Total | C | O | P | 0 |
| | | | 87 | 68 | 17 | 2 | |
| 153 | b3 | 1 | Total | C | O | P | 0 |
| | | | 58 | 39 | 17 | 2 | |
| 153 | b3 | 1 | Total | C | O | P | 0 |
| | | | 82 | 63 | 17 | 2 | |
| 153 | b4 | 1 | Total | C | O | P | 0 |
| | | | 37 | 18 | 17 | 2 | |
| 153 | b8 | 1 | Total | C | O | P | 0 |
| | | | 69 | 50 | 17 | 2 | |
| 153 | bm | 1 | Total | C | O | P | 0 |
| | | | 86 | 67 | 17 | 2 | |
| 153 | c4 | 1 | Total | C | O | P | 0 |
| | | | 98 | 79 | 17 | 2 | |
| 153 | n5 | 1 | Total | C | O | P | 0 |
| | | | 90 | 71 | 17 | 2 | |
| 153 | n6 | 1 | Total | C | O | P | 0 |
| | | | 90 | 71 | 17 | 2 | |
| 153 | p1 | 1 | Total | C | O | P | 0 |
| | | | 63 | 44 | 17 | 2 | |
| 153 | p1 | 1 | Total | C | O | P | 0 |
| | | | 58 | 39 | 17 | 2 | |
| 153 | qB | 1 | Total | C | O | P | 0 |
| | | | 68 | 49 | 17 | 2 | |
| 153 | qC | 1 | Total | C | O | P | 0 |
| | | | 64 | 45 | 17 | 2 | |
| 153 | qC | 1 | Total | C | O | P | 0 |
| | | | 56 | 37 | 17 | 2 | |
| 153 | qD | 1 | Total | C | O | P | 0 |
| | | | 61 | 42 | 17 | 2 | |
| 153 | qG | 1 | Total | C | O | P | 0 |
| | | | 86 | 67 | 17 | 2 | |
| 153 | qH | 1 | Total | C | O | P | 0 |
| | | | 94 | 75 | 17 | 2 | |
| 153 | qI | 1 | Total | C | O | P | 0 |
| | | | 71 | 52 | 17 | 2 | |
| 153 | qb | 1 | Total | C | O | P | 0 |
| | | | 68 | 49 | 17 | 2 | |
| 153 | qc | 1 | Total | C | O | P | 0 |
| | | | 64 | 45 | 17 | 2 | |
| 153 | qc | 1 | Total | C | O | P | 0 |
| | | | 56 | 37 | 17 | 2 | |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|--------------|---------|---------|--------|---------|
| 153 | qc | 1 | Total 47 | C 28 | O 17 | P 2 | 0 |
| 153 | qg | 1 | Total 100 | C 81 | O 17 | P 2 | 0 |
| 153 | qi | 1 | Total 71 | C 52 | O 17 | P 2 | 0 |
| 153 | t1 | 1 | Total 55 | C 36 | O 17 | P 2 | 0 |
| 153 | t5 | 1 | Total 96 | C 77 | O 17 | P 2 | 0 |
| 153 | t7 | 1 | Total 73 | C 54 | O 17 | P 2 | 0 |
| 153 | td | 1 | Total 66 | C 47 | O 17 | P 2 | 0 |
| 153 | te | 1 | Total 53 | C 34 | O 17 | P 2 | 0 |
| 153 | th | 1 | Total 84 | C 65 | O 17 | P 2 | 0 |
| 153 | 2G | 1 | Total 89 | C 70 | O 17 | P 2 | 0 |
| 153 | 2G | 1 | Total 55 | C 36 | O 17 | P 2 | 0 |
| 153 | 2G | 1 | Total 63 | C 44 | O 17 | P 2 | 0 |
| 153 | 2K | 1 | Total 98 | C 79 | O 17 | P 2 | 0 |
| 153 | 2M | 1 | Total 96 | C 77 | O 17 | P 2 | 0 |
| 153 | 2O | 1 | Total 50 | C 31 | O 17 | P 2 | 0 |
| 153 | 6A | 1 | Total 74 | C 55 | O 17 | P 2 | 0 |
| 153 | 6C | 1 | Total 75 | C 56 | O 17 | P 2 | 0 |
| 153 | 6C | 1 | Total 82 | C 63 | O 17 | P 2 | 0 |
| 153 | 7A | 1 | Total 100 | C 81 | O 17 | P 2 | 0 |
| 153 | 7A | 1 | Total 62 | C 43 | O 17 | P 2 | 0 |
| 153 | 7C | 1 | Total 85 | C 66 | O 17 | P 2 | 0 |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 153 | 7C | 1 | Total | C | O | P | 0 |
| | | | 51 | 32 | 17 | 2 | |
| 153 | A | 1 | Total | C | O | P | 0 |
| | | | 51 | 32 | 17 | 2 | |
| 153 | A | 1 | Total | C | O | P | 0 |
| | | | 94 | 75 | 17 | 2 | |
| 153 | B | 1 | Total | C | O | P | 0 |
| | | | 62 | 43 | 17 | 2 | |
| 153 | C1 | 1 | Total | C | O | P | 0 |
| | | | 79 | 60 | 17 | 2 | |
| 153 | C1 | 1 | Total | C | O | P | 0 |
| | | | 65 | 46 | 17 | 2 | |
| 153 | C1 | 1 | Total | C | O | P | 0 |
| | | | 63 | 44 | 17 | 2 | |
| 153 | C1 | 1 | Total | C | O | P | 0 |
| | | | 95 | 76 | 17 | 2 | |
| 153 | C3 | 1 | Total | C | O | P | 0 |
| | | | 68 | 49 | 17 | 2 | |
| 153 | E | 1 | Total | C | O | P | 0 |
| | | | 60 | 41 | 17 | 2 | |
| 153 | E | 1 | Total | C | O | P | 0 |
| | | | 72 | 53 | 17 | 2 | |
| 153 | E | 1 | Total | C | O | P | 0 |
| | | | 63 | 44 | 17 | 2 | |
| 153 | F | 1 | Total | C | O | P | 0 |
| | | | 100 | 81 | 17 | 2 | |
| 153 | FS | 1 | Total | C | O | P | 0 |
| | | | 47 | 28 | 17 | 2 | |
| 153 | I | 1 | Total | C | O | P | 0 |
| | | | 77 | 58 | 17 | 2 | |
| 153 | I | 1 | Total | C | O | P | 0 |
| | | | 75 | 56 | 17 | 2 | |
| 153 | J | 1 | Total | C | O | P | 0 |
| | | | 70 | 51 | 17 | 2 | |
| 153 | L | 1 | Total | C | O | P | 0 |
| | | | 74 | 55 | 17 | 2 | |
| 153 | M | 1 | Total | C | O | P | 0 |
| | | | 66 | 47 | 17 | 2 | |
| 153 | M | 1 | Total | C | O | P | 0 |
| | | | 64 | 45 | 17 | 2 | |
| 153 | M | 1 | Total | C | O | P | 0 |
| | | | 83 | 64 | 17 | 2 | |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 153 | M | 1 | Total | C | O | P | 0 |
| | | | 64 | 45 | 17 | 2 | |
| 153 | M1 | 1 | Total | C | O | P | 0 |
| | | | 66 | 47 | 17 | 2 | |
| 153 | M1 | 1 | Total | C | O | P | 0 |
| | | | 91 | 72 | 17 | 2 | |
| 153 | M1 | 1 | Total | C | O | P | 0 |
| | | | 57 | 38 | 17 | 2 | |
| 153 | M2 | 1 | Total | C | O | P | 0 |
| | | | 54 | 35 | 17 | 2 | |
| 153 | M2 | 1 | Total | C | O | P | 0 |
| | | | 66 | 47 | 17 | 2 | |
| 153 | M2 | 1 | Total | C | O | P | 0 |
| | | | 74 | 55 | 17 | 2 | |
| 153 | M3 | 1 | Total | C | O | P | 0 |
| | | | 63 | 44 | 17 | 2 | |
| 153 | M3 | 1 | Total | C | O | P | 0 |
| | | | 55 | 36 | 17 | 2 | |
| 153 | N | 1 | Total | C | O | P | 0 |
| | | | 84 | 65 | 17 | 2 | |
| 153 | Q | 1 | Total | C | O | P | 0 |
| | | | 63 | 44 | 17 | 2 | |
| 153 | Q | 1 | Total | C | O | P | 0 |
| | | | 72 | 53 | 17 | 2 | |
| 153 | R | 1 | Total | C | O | P | 0 |
| | | | 65 | 46 | 17 | 2 | |
| 153 | SD | 1 | Total | C | O | P | 0 |
| | | | 76 | 57 | 17 | 2 | |
| 153 | T | 1 | Total | C | O | P | 0 |
| | | | 59 | 40 | 17 | 2 | |
| 153 | T | 1 | Total | C | O | P | 0 |
| | | | 75 | 56 | 17 | 2 | |
| 153 | T | 1 | Total | C | O | P | 0 |
| | | | 71 | 52 | 17 | 2 | |
| 153 | T | 1 | Total | C | O | P | 0 |
| | | | 90 | 71 | 17 | 2 | |
| 153 | U | 1 | Total | C | O | P | 0 |
| | | | 60 | 41 | 17 | 2 | |
| 153 | VB | 1 | Total | C | O | P | 0 |
| | | | 62 | 43 | 17 | 2 | |
| 153 | VB | 1 | Total | C | O | P | 0 |
| | | | 86 | 67 | 17 | 2 | |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 153 | VB | 1 | Total | C | O | P | 0 |
| | | | 82 | 63 | 17 | 2 | |
| 153 | VB | 1 | Total | C | O | P | 0 |
| | | | 67 | 48 | 17 | 2 | |
| 153 | W | 1 | Total | C | O | P | 0 |
| | | | 84 | 65 | 17 | 2 | |
| 153 | Y5 | 1 | Total | C | O | P | 0 |
| | | | 70 | 51 | 17 | 2 | |
| 153 | Y7 | 1 | Total | C | O | P | 0 |
| | | | 65 | 46 | 17 | 2 | |
| 153 | Z | 1 | Total | C | O | P | 0 |
| | | | 67 | 48 | 17 | 2 | |
| 153 | 2B | 1 | Total | C | O | P | 0 |
| | | | 87 | 68 | 17 | 2 | |
| 153 | 5B | 1 | Total | C | O | P | 0 |
| | | | 81 | 62 | 17 | 2 | |
| 153 | A1 | 1 | Total | C | O | P | 0 |
| | | | 66 | 47 | 17 | 2 | |
| 153 | A1 | 1 | Total | C | O | P | 0 |
| | | | 67 | 48 | 17 | 2 | |
| 153 | A9 | 1 | Total | C | O | P | 0 |
| | | | 76 | 57 | 17 | 2 | |
| 153 | A9 | 1 | Total | C | O | P | 0 |
| | | | 87 | 68 | 17 | 2 | |
| 153 | AL | 1 | Total | C | O | P | 0 |
| | | | 53 | 34 | 17 | 2 | |
| 153 | AM | 1 | Total | C | O | P | 0 |
| | | | 56 | 37 | 17 | 2 | |
| 153 | AN | 1 | Total | C | O | P | 0 |
| | | | 87 | 68 | 17 | 2 | |
| 153 | B3 | 1 | Total | C | O | P | 0 |
| | | | 58 | 39 | 17 | 2 | |
| 153 | B3 | 1 | Total | C | O | P | 0 |
| | | | 82 | 63 | 17 | 2 | |
| 153 | B4 | 1 | Total | C | O | P | 0 |
| | | | 37 | 18 | 17 | 2 | |
| 153 | B8 | 1 | Total | C | O | P | 0 |
| | | | 69 | 50 | 17 | 2 | |
| 153 | BM | 1 | Total | C | O | P | 0 |
| | | | 86 | 67 | 17 | 2 | |
| 153 | C4 | 1 | Total | C | O | P | 0 |
| | | | 98 | 79 | 17 | 2 | |

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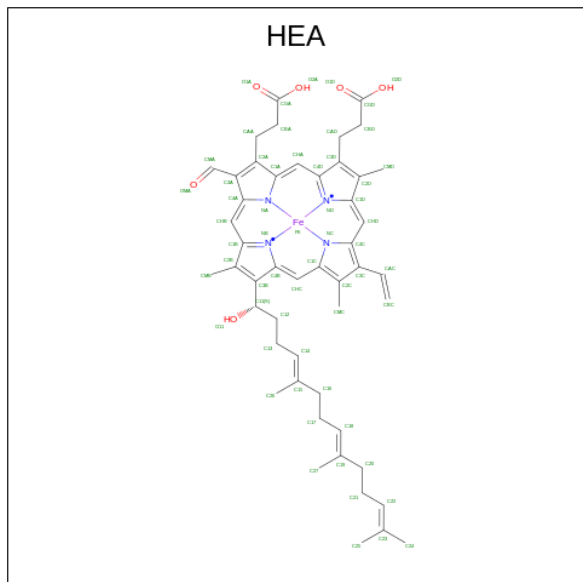
| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 153 | N5 | 1 | Total | C | O | P | 0 |
| | | | 90 | 71 | 17 | 2 | |
| 153 | N6 | 1 | Total | C | O | P | 0 |
| | | | 90 | 71 | 17 | 2 | |
| 153 | P1 | 1 | Total | C | O | P | 0 |
| | | | 63 | 44 | 17 | 2 | |
| 153 | P1 | 1 | Total | C | O | P | 0 |
| | | | 58 | 39 | 17 | 2 | |
| 153 | QB | 1 | Total | C | O | P | 0 |
| | | | 68 | 49 | 17 | 2 | |
| 153 | QC | 1 | Total | C | O | P | 0 |
| | | | 64 | 45 | 17 | 2 | |
| 153 | QC | 1 | Total | C | O | P | 0 |
| | | | 56 | 37 | 17 | 2 | |
| 153 | QD | 1 | Total | C | O | P | 0 |
| | | | 61 | 42 | 17 | 2 | |
| 153 | QG | 1 | Total | C | O | P | 0 |
| | | | 86 | 67 | 17 | 2 | |
| 153 | QH | 1 | Total | C | O | P | 0 |
| | | | 94 | 75 | 17 | 2 | |
| 153 | QI | 1 | Total | C | O | P | 0 |
| | | | 71 | 52 | 17 | 2 | |
| 153 | Qb | 1 | Total | C | O | P | 0 |
| | | | 68 | 49 | 17 | 2 | |
| 153 | Qc | 1 | Total | C | O | P | 0 |
| | | | 64 | 45 | 17 | 2 | |
| 153 | Qc | 1 | Total | C | O | P | 0 |
| | | | 56 | 37 | 17 | 2 | |
| 153 | Qc | 1 | Total | C | O | P | 0 |
| | | | 47 | 28 | 17 | 2 | |
| 153 | Qg | 1 | Total | C | O | P | 0 |
| | | | 100 | 81 | 17 | 2 | |
| 153 | Qi | 1 | Total | C | O | P | 0 |
| | | | 71 | 52 | 17 | 2 | |
| 153 | T1 | 1 | Total | C | O | P | 0 |
| | | | 55 | 36 | 17 | 2 | |
| 153 | T5 | 1 | Total | C | O | P | 0 |
| | | | 96 | 77 | 17 | 2 | |
| 153 | T7 | 1 | Total | C | O | P | 0 |
| | | | 73 | 54 | 17 | 2 | |
| 153 | TE | 1 | Total | C | O | P | 0 |
| | | | 53 | 34 | 17 | 2 | |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 153 | TH | 1 | Total | C | O | P | 0 |
| | | | 84 | 65 | 17 | 2 | |
| 153 | C | 1 | Total | C | O | P | 0 |
| | | | 64 | 45 | 17 | 2 | |
| 153 | c | 1 | Total | C | O | P | 0 |
| | | | 64 | 45 | 17 | 2 | |
| 153 | u1 | 1 | Total | C | O | P | 0 |
| | | | 57 | 38 | 17 | 2 | |
| 153 | U1 | 1 | Total | C | O | P | 0 |
| | | | 57 | 38 | 17 | 2 | |

- Molecule 154 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 154 | c1 | 1 | Total | C | Fe | N | O | 0 |
| | | | 60 | 49 | 1 | 4 | 6 | |
| 154 | c1 | 1 | Total | C | Fe | N | O | 0 |
| | | | 60 | 49 | 1 | 4 | 6 | |
| 154 | C1 | 1 | Total | C | Fe | N | O | 0 |
| | | | 60 | 49 | 1 | 4 | 6 | |
| 154 | C1 | 1 | Total | C | Fe | N | O | 0 |
| | | | 60 | 49 | 1 | 4 | 6 | |

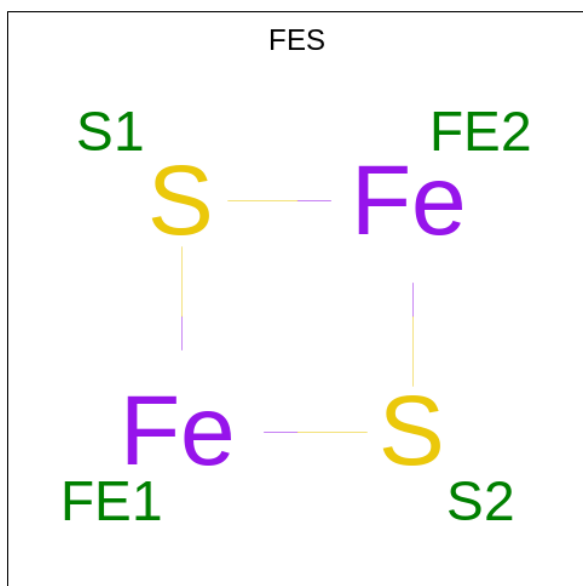
- Molecule 155 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|---------|---------|
| 155 | c1 | 1 | Total 1 | Cu 1 | 0 |
| 155 | c2 | 2 | Total 2 | Cu 2 | 0 |
| 155 | C1 | 1 | Total 1 | Cu 1 | 0 |
| 155 | C2 | 2 | Total 2 | Cu 2 | 0 |

- Molecule 156 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|---------|---------|
| 156 | c1 | 1 | Total 1 | Mg 1 | 0 |
| 156 | C1 | 1 | Total 1 | Mg 1 | 0 |

- Molecule 157 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).



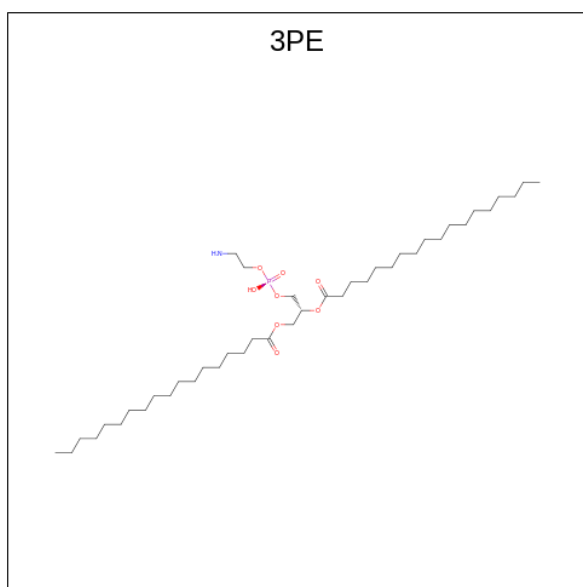
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|------------|---------|--------|---------|
| 157 | fs | 1 | Total 4 | Fe 2 | S 2 | 0 |
| 157 | fs | 1 | Total 4 | Fe 2 | S 2 | 0 |
| 157 | sb | 1 | Total 4 | Fe 2 | S 2 | 0 |

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| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|------------|---------|--------|---------|
| 157 | fx | 1 | Total 4 | Fe 2 | S 2 | 0 |
| 157 | qE | 1 | Total 4 | Fe 2 | S 2 | 0 |
| 157 | qe | 1 | Total 4 | Fe 2 | S 2 | 0 |
| 157 | s1 | 1 | Total 4 | Fe 2 | S 2 | 0 |
| 157 | v2 | 1 | Total 4 | Fe 2 | S 2 | 0 |
| 157 | FS | 1 | Total 4 | Fe 2 | S 2 | 0 |
| 157 | FS | 1 | Total 4 | Fe 2 | S 2 | 0 |
| 157 | SB | 1 | Total 4 | Fe 2 | S 2 | 0 |
| 157 | FX | 1 | Total 4 | Fe 2 | S 2 | 0 |
| 157 | QE | 1 | Total 4 | Fe 2 | S 2 | 0 |
| 157 | Qe | 1 | Total 4 | Fe 2 | S 2 | 0 |
| 157 | S1 | 1 | Total 4 | Fe 2 | S 2 | 0 |
| 157 | V2 | 1 | Total 4 | Fe 2 | S 2 | 0 |

- Molecule 158 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: C₄₁H₈₂NO₈P).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 158 | i | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 22 | 1 | 8 | 1 | |
| 158 | m2 | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 21 | 1 | 8 | 1 | |
| 158 | m3 | 1 | Total | C | N | O | P | 0 |
| | | | 38 | 28 | 1 | 8 | 1 | |
| 158 | sc | 1 | Total | C | N | O | P | 0 |
| | | | 40 | 30 | 1 | 8 | 1 | |
| 158 | vb | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 18 | 1 | 8 | 1 | |
| 158 | w | 1 | Total | C | N | O | P | 0 |
| | | | 34 | 24 | 1 | 8 | 1 | |
| 158 | y5 | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 18 | 1 | 8 | 1 | |
| 158 | a3 | 1 | Total | C | N | O | P | 0 |
| | | | 45 | 35 | 1 | 8 | 1 | |
| 158 | a3 | 1 | Total | C | N | O | P | 0 |
| | | | 44 | 34 | 1 | 8 | 1 | |
| 158 | an | 1 | Total | C | N | O | P | 0 |
| | | | 45 | 35 | 1 | 8 | 1 | |
| 158 | an | 1 | Total | C | N | O | P | 0 |
| | | | 45 | 35 | 1 | 8 | 1 | |
| 158 | an | 1 | Total | C | N | O | P | 0 |
| | | | 33 | 23 | 1 | 8 | 1 | |
| 158 | an | 1 | Total | C | N | O | P | 0 |
| | | | 29 | 19 | 1 | 8 | 1 | |
| 158 | b4 | 1 | Total | C | N | O | P | 0 |
| | | | 48 | 38 | 1 | 8 | 1 | |

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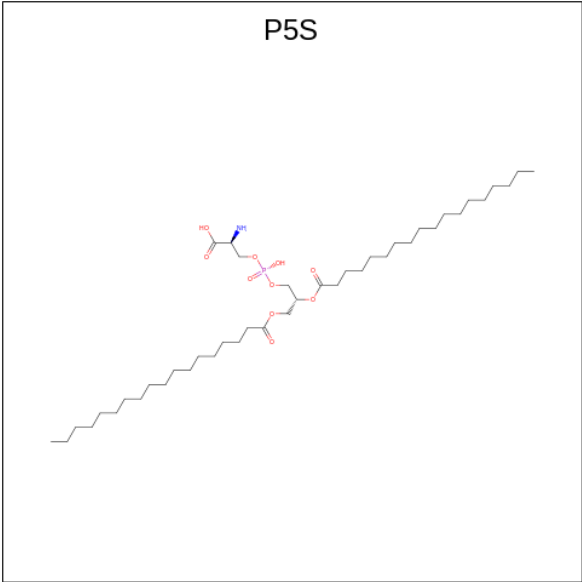
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 158 | bm | 1 | Total | C | N | O | P | 0 |
| | | | 30 | 20 | 1 | 8 | 1 | |
| 158 | c4 | 1 | Total | C | N | O | P | 0 |
| | | | 51 | 41 | 1 | 8 | 1 | |
| 158 | g2 | 1 | Total | C | N | O | P | 0 |
| | | | 51 | 41 | 1 | 8 | 1 | |
| 158 | n4 | 1 | Total | C | N | O | P | 0 |
| | | | 36 | 26 | 1 | 8 | 1 | |
| 158 | n5 | 1 | Total | C | N | O | P | 0 |
| | | | 36 | 26 | 1 | 8 | 1 | |
| 158 | s8 | 1 | Total | C | N | O | P | 0 |
| | | | 41 | 31 | 1 | 8 | 1 | |
| 158 | t4 | 1 | Total | C | N | O | P | 0 |
| | | | 25 | 15 | 1 | 8 | 1 | |
| 158 | t8 | 1 | Total | C | N | O | P | 0 |
| | | | 47 | 37 | 1 | 8 | 1 | |
| 158 | t8 | 1 | Total | C | N | O | P | 0 |
| | | | 39 | 29 | 1 | 8 | 1 | |
| 158 | ta | 1 | Total | C | N | O | P | 0 |
| | | | 26 | 16 | 1 | 8 | 1 | |
| 158 | I | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 22 | 1 | 8 | 1 | |
| 158 | M2 | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 21 | 1 | 8 | 1 | |
| 158 | M3 | 1 | Total | C | N | O | P | 0 |
| | | | 38 | 28 | 1 | 8 | 1 | |
| 158 | SC | 1 | Total | C | N | O | P | 0 |
| | | | 40 | 30 | 1 | 8 | 1 | |
| 158 | VB | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 18 | 1 | 8 | 1 | |
| 158 | W | 1 | Total | C | N | O | P | 0 |
| | | | 34 | 24 | 1 | 8 | 1 | |
| 158 | Y5 | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 18 | 1 | 8 | 1 | |
| 158 | A3 | 1 | Total | C | N | O | P | 0 |
| | | | 45 | 35 | 1 | 8 | 1 | |
| 158 | A3 | 1 | Total | C | N | O | P | 0 |
| | | | 44 | 34 | 1 | 8 | 1 | |
| 158 | AN | 1 | Total | C | N | O | P | 0 |
| | | | 45 | 35 | 1 | 8 | 1 | |
| 158 | AN | 1 | Total | C | N | O | P | 0 |
| | | | 45 | 35 | 1 | 8 | 1 | |

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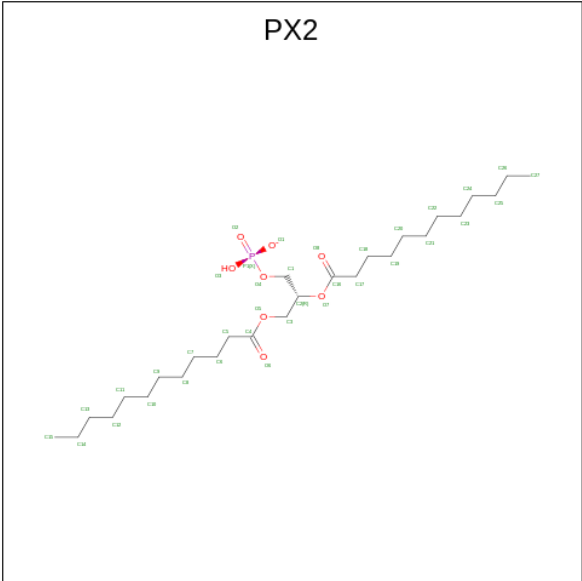
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 158 | AN | 1 | Total | C | N | O | P | 0 |
| | | | 33 | 23 | 1 | 8 | 1 | |
| 158 | AN | 1 | Total | C | N | O | P | 0 |
| | | | 29 | 19 | 1 | 8 | 1 | |
| 158 | B4 | 1 | Total | C | N | O | P | 0 |
| | | | 48 | 38 | 1 | 8 | 1 | |
| 158 | BM | 1 | Total | C | N | O | P | 0 |
| | | | 30 | 20 | 1 | 8 | 1 | |
| 158 | C4 | 1 | Total | C | N | O | P | 0 |
| | | | 51 | 41 | 1 | 8 | 1 | |
| 158 | G2 | 1 | Total | C | N | O | P | 0 |
| | | | 51 | 41 | 1 | 8 | 1 | |
| 158 | N4 | 1 | Total | C | N | O | P | 0 |
| | | | 36 | 26 | 1 | 8 | 1 | |
| 158 | N5 | 1 | Total | C | N | O | P | 0 |
| | | | 36 | 26 | 1 | 8 | 1 | |
| 158 | S8 | 1 | Total | C | N | O | P | 0 |
| | | | 41 | 31 | 1 | 8 | 1 | |
| 158 | T4 | 1 | Total | C | N | O | P | 0 |
| | | | 25 | 15 | 1 | 8 | 1 | |
| 158 | T8 | 1 | Total | C | N | O | P | 0 |
| | | | 47 | 37 | 1 | 8 | 1 | |
| 158 | T8 | 1 | Total | C | N | O | P | 0 |
| | | | 39 | 29 | 1 | 8 | 1 | |
| 158 | TA | 1 | Total | C | N | O | P | 0 |
| | | | 26 | 16 | 1 | 8 | 1 | |

- Molecule 159 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy} (hydroxy)phosphoryl]-L-serine (three-letter code: P5S) (formula: C₄₂H₈₂NO₁₀P).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 159 | m2 | 1 | Total | C | N | O | P | 0 |
| | | | 36 | 24 | 1 | 10 | 1 | |
| 159 | M2 | 1 | Total | C | N | O | P | 0 |
| | | | 36 | 24 | 1 | 10 | 1 | |

- Molecule 160 is 1,2-DILAUROYL-SN-GLYCERO-3-PHOSPHATE (three-letter code: PX2) (formula: C₂₇H₅₂O₈P).



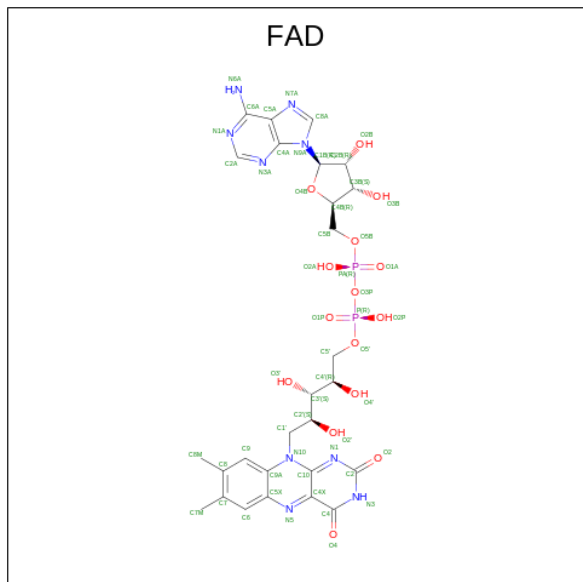
| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 160 | r | 1 | Total | C | O | P | 0 |
| | | | 33 | 24 | 8 | 1 | |

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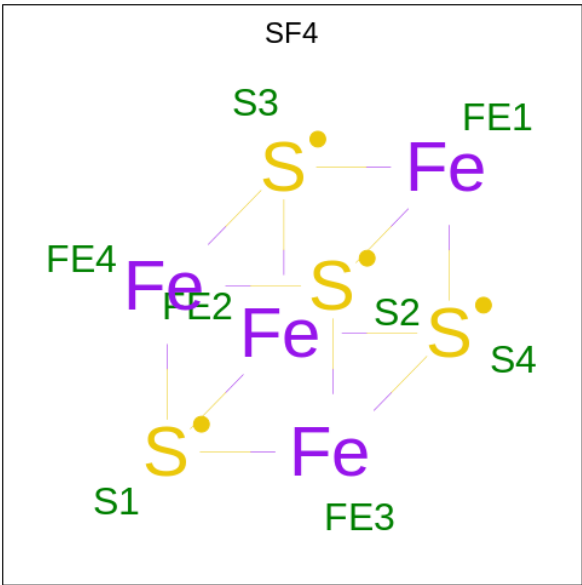
| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 160 | y5 | 1 | Total | C | O | P | 0 |
| | | | 21 | 12 | 8 | 1 | |
| 160 | qh | 1 | Total | C | O | P | 0 |
| | | | 36 | 27 | 8 | 1 | |
| 160 | R | 1 | Total | C | O | P | 0 |
| | | | 33 | 24 | 8 | 1 | |
| 160 | Y5 | 1 | Total | C | O | P | 0 |
| | | | 21 | 12 | 8 | 1 | |
| 160 | Qh | 1 | Total | C | O | P | 0 |
| | | | 36 | 27 | 8 | 1 | |

- Molecule 161 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



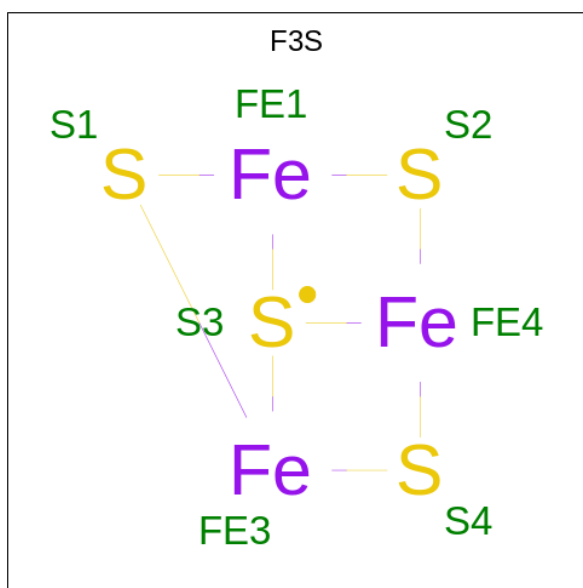
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 161 | sa | 1 | Total 53 | C 27 | N 9 | O 15 | P 2 | 0 |
| 161 | SA | 1 | Total 53 | C 27 | N 9 | O 15 | P 2 | 0 |

- Molecule 162 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



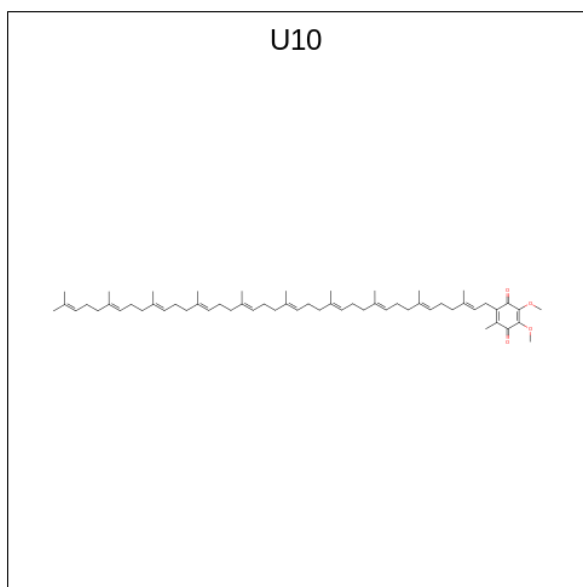
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 162 | sb | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 162 | s1 | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 162 | s1 | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 162 | s7 | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 162 | s8 | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 162 | s8 | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 162 | v1 | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 162 | SB | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 162 | S1 | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 162 | S1 | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 162 | S7 | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 162 | S8 | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 162 | S8 | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 162 | V1 | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |

- Molecule 163 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 163 | sb | 1 | Total | Fe | S | 0 |
| | | | 7 | 3 | 4 | |
| 163 | SB | 1 | Total | Fe | S | 0 |
| | | | 7 | 3 | 4 | |

- Molecule 164 is UBIQUINONE-10 (three-letter code: U10) (formula: $\text{C}_{59}\text{H}_{90}\text{O}_4$) (labeled as "Ligand of Interest" by depositor).

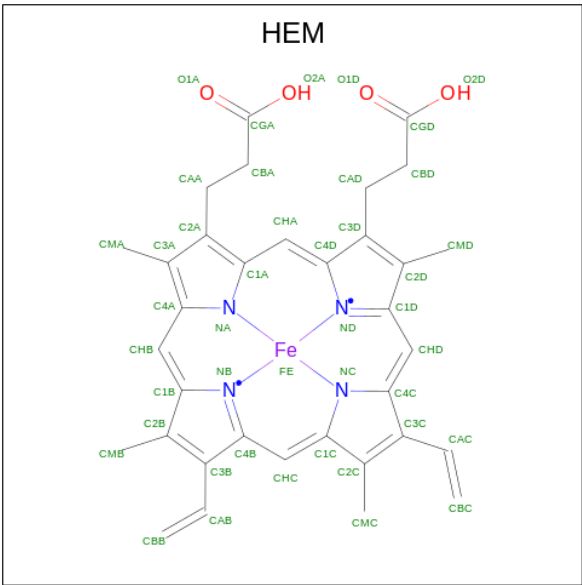


| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 164 | sc | 1 | Total | C | O | 0 |
| | | | 63 | 59 | 4 | |
| 164 | b8 | 1 | Total | C | O | 0 |
| | | | 63 | 59 | 4 | |
| 164 | qC | 1 | Total | C | O | 0 |
| | | | 29 | 25 | 4 | |
| 164 | qc | 1 | Total | C | | 0 |
| | | | 26 | 26 | | |
| 164 | qc | 1 | Total | C | O | 0 |
| | | | 29 | 25 | 4 | |
| 164 | SC | 1 | Total | C | O | 0 |
| | | | 63 | 59 | 4 | |
| 164 | B8 | 1 | Total | C | O | 0 |
| | | | 63 | 59 | 4 | |
| 164 | QC | 1 | Total | C | O | 0 |
| | | | 29 | 25 | 4 | |
| 164 | Qc | 1 | Total | C | | 0 |
| | | | 26 | 26 | | |
| 164 | Qc | 1 | Total | C | O | 0 |
| | | | 29 | 25 | 4 | |

- Molecule 165 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 165 | vb | 2 | Total | Zn | 0 |
| | | | 2 | 2 | |
| 165 | s6 | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 165 | VB | 2 | Total | Zn | 0 |
| | | | 2 | 2 | |
| 165 | S6 | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

- Molecule 166 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 166 | y5 | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 166 | qC | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 166 | qC | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 166 | qc | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 166 | qc | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 166 | Y5 | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 166 | QC | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 166 | QC | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 166 | Qc | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 166 | Qc | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |

- Molecule 167 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 167 | a9 | 1 | Total 48 | C 21 | N 7 | O 17 | P 3 | 0 |
| 167 | A9 | 1 | Total 48 | C 21 | N 7 | O 17 | P 3 | 0 |

- Molecule 168 is S-[2-($\{N-[(2S)-2\text{-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-\beta\text{-alaninyl}\}$ amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



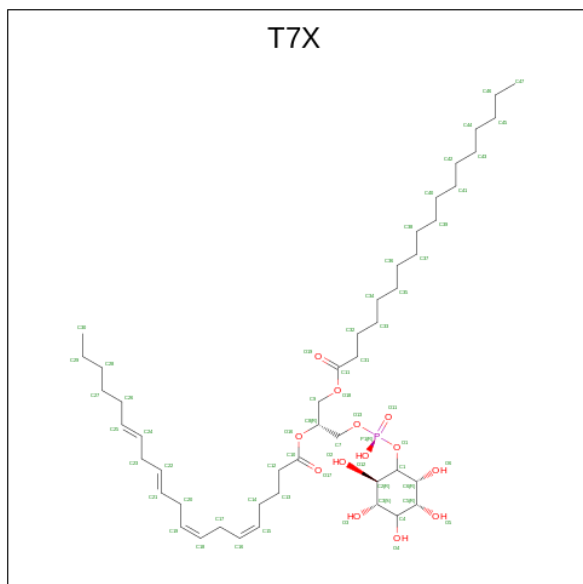
| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---|---------|
| 168 | ab | 1 | Total | C | N | O | P | S | 0 |
| | | | 37 | 25 | 2 | 8 | 1 | 1 | |

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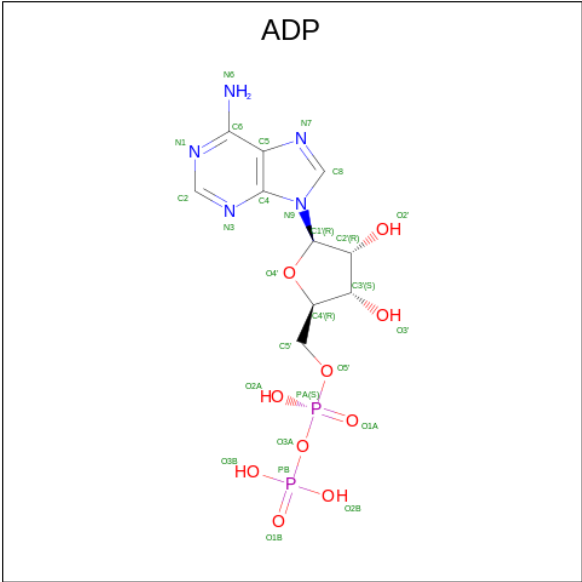
| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---|---------|
| | | | Total | C | N | O | P | S | |
| 168 | AB | 1 | 37 | 25 | 2 | 8 | 1 | 1 | 0 |

- Molecule 169 is Phosphatidylinositol (three-letter code: T7X) (formula: $C_{47}H_{83}O_{13}P$).



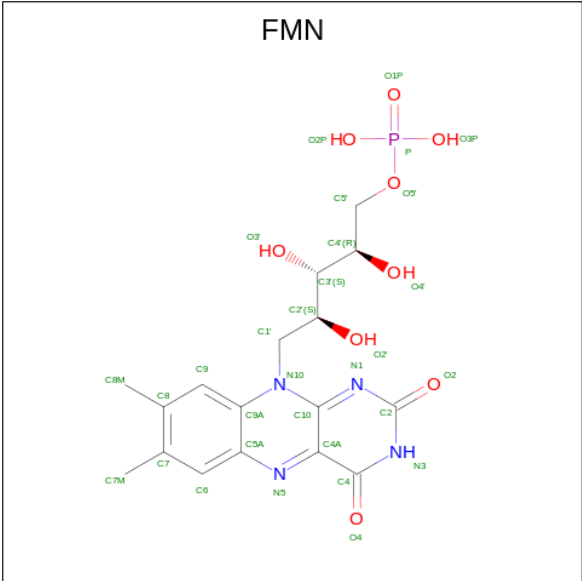
| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| | | | Total | C | O | P | |
| 169 | b6 | 1 | 55 | 41 | 13 | 1 | 0 |
| 169 | B6 | 1 | 55 | 41 | 13 | 1 | 0 |

- Molecule 170 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 170 | b9 | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 170 | B9 | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |

- Molecule 171 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 171 | v1 | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 17 | 4 | 9 | 1 | |

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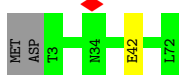
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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| | | | Total | C | N | O | P | |
| 171 | V1 | 1 | 31 | 17 | 4 | 9 | 1 | 0 |

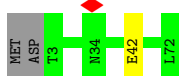
3 Residue-property plots [i](#)

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

- Molecule 1: Tim10/DDP family zinc finger protein



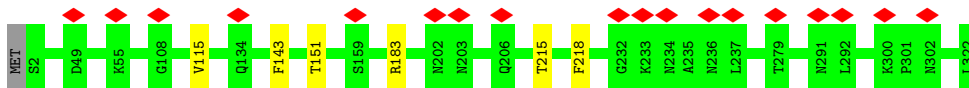
- Molecule 1: Tim10/DDP family zinc finger protein



- Molecule 2: NmrA domain-containing protein



- Molecule 2: NmrA domain-containing protein

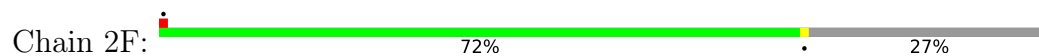


- Molecule 3: Transmembrane protein, putative





- Molecule 3: Transmembrane protein, putative



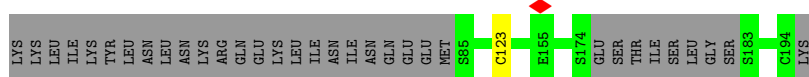
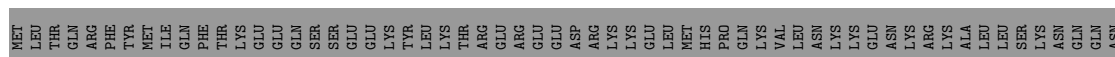
- Molecule 4: SDHTT3



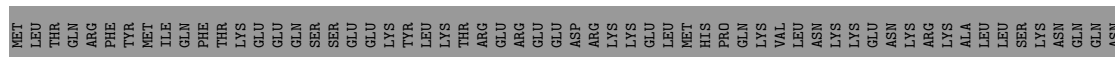
- Molecule 4: SDHTT3



- Molecule 5: Diphthamide synthesis protein



- Molecule 5: Diphthamide synthesis protein



- Molecule 6: DUF4885 domain-containing protein

Chain 2i:  97% .



- Molecule 6: DUF4885 domain-containing protein

Chain 2I:  98% .



- Molecule 7: Transmembrane protein, putative

Chain 2j:  98% ..



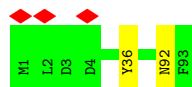
- Molecule 7: Transmembrane protein, putative

Chain 2J:  98% ..



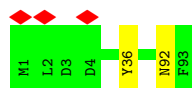
- Molecule 8: Transmembrane protein, putative

Chain 2k:  98% .



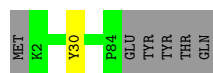
- Molecule 8: Transmembrane protein, putative

Chain 2K:  98% .



- Molecule 9: Transposase

Chain 2l:  92% . 7%



- Molecule 9: Transposase

Chain 2L:  91% • 7%



- Molecule 10: Transmembrane protein, putative

Chain 2m:  97% ..



- Molecule 10: Transmembrane protein, putative

Chain 2M:  97% ..



- Molecule 11: Transmembrane protein, putative

Chain 2n:  97% ..



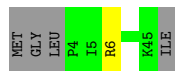
- Molecule 11: Transmembrane protein, putative

Chain 2N:  95% ..



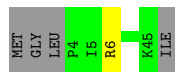
- Molecule 12: SDHTT11

Chain 2o:  89% • 9%



- Molecule 12: SDHTT11

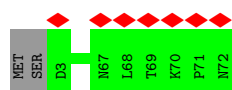
Chain 2O:  89% • 9%



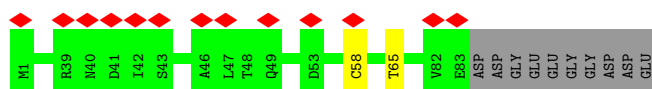
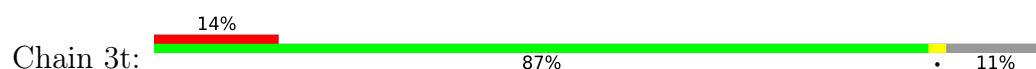
- Molecule 13: Zf-Tim10_DDP domain-containing protein



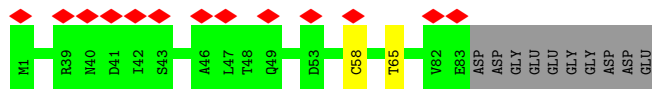
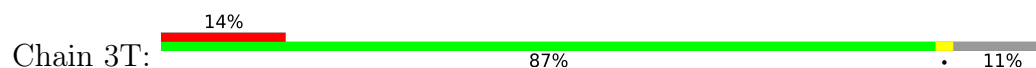
- Molecule 13: Zf-Tim10_DDP domain-containing protein



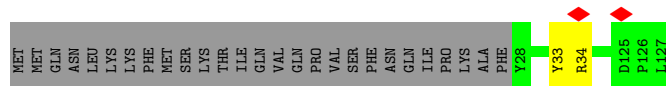
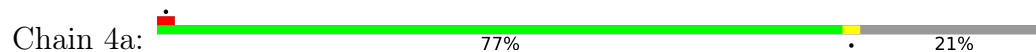
- Molecule 14: Zf-Tim10_DDP domain-containing protein



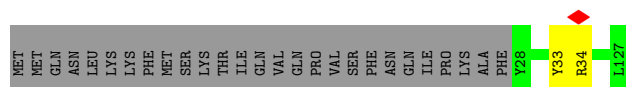
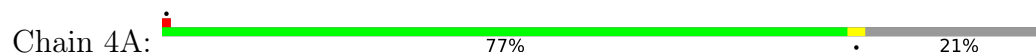
- Molecule 14: Zf-Tim10_DDP domain-containing protein



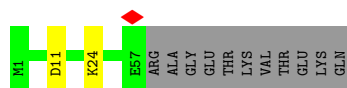
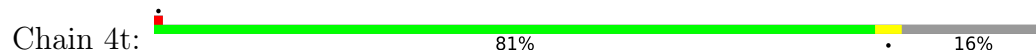
- Molecule 15: Phage protein



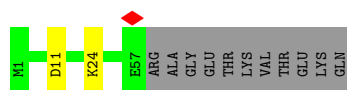
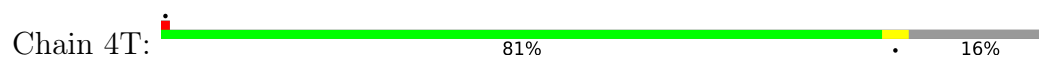
- Molecule 15: Phage protein



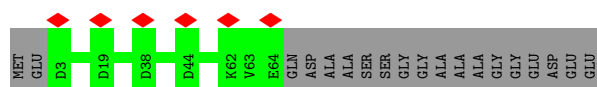
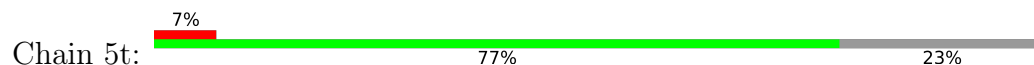
- Molecule 16: Transposase



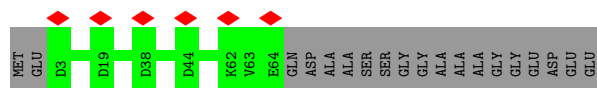
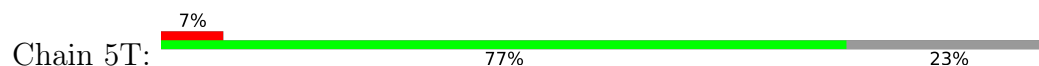
- Molecule 16: Transposase



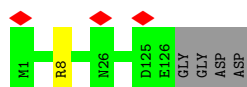
- Molecule 17: Cullin domain-containing protein



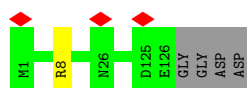
- Molecule 17: Cullin domain-containing protein



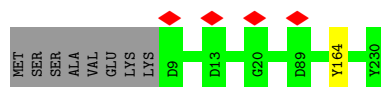
- Molecule 18: Transmembrane protein, putative



- Molecule 18: Transmembrane protein, putative

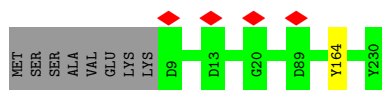


- Molecule 19: Structural protein

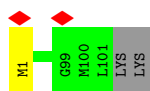


- Molecule 19: Structural protein

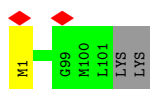




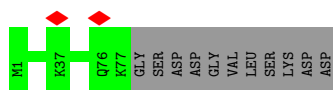
- Molecule 20: Transmembrane protein, putative



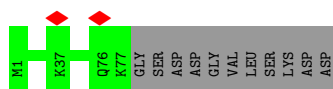
- Molecule 20: Transmembrane protein, putative



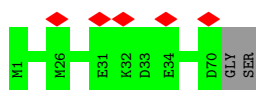
- Molecule 21: Decapping nuclease



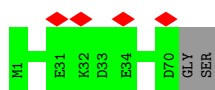
- Molecule 21: Decapping nuclease



- Molecule 22: Annexin



- Molecule 22: Annexin



- Molecule 23: Transmembrane protein, putative

-

- MET
 ILE
 SER
 LYS
 TYR
 ARG
 TYR
 LEU
 HIS
 CYS
 ALA
 ARG
 LYS
 LEU
 VAL
 GLN
 SER
 VAL
 GLN
 ALA
 PHE
 GLY
 GLY
 GLY
 H296
 H27
 H28
 H29
 Q77
 W106
 K196
 I236

- MET
 ILE
 SER
 LYS
 TYR
 ARG
 TYR
 LEU
 HIS
 CYS
 VAL
 ARG
 LYS
 LEU
 VAL
 LYS
 GLN
 SER
 VAL
 GLN
 ALA
 PHE
 GLY
 GLY
 H26
 H27
 H28
 H29
 Q77
 W106
 K196
 I236

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| MET | ASN | LYS | SER | GLN | ASP | GLU | VAL | GLU | LYS | ASP | PHE | SER | ILE | LYS | LYS | LYS | LYS | TYR | ASN | SER | LEU | ASP | CYS | VAL | LEU | SER | PRO | ILE | VAL | THR | ARG | LYS | LYS | GLN | GLU | SER | SER | ASN | PHE | GLN | ALA | GLY | LEU | GLN | GLN | ASP | GLN | ASN | SER | THR | ALA | VAL | PRO | GLU | SER | SER | PRO | PHE |
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| ILE | ARG | ASN | CYS | SER | GLU | THR | LEU | ASN | ARG | SER | GLN | HIS | LYS | ILE | LEU | LEU | ASP | HIS | TYR | PHE | GLU | TYR | ASP | SER | LEU | LYS | LYS | ILE | GLU | LYS | ILE | LYS | ILE | SER | LEU | GLN | ASN | LYS | THR | THR | ASP | SER | SER | GLN | SER | LEU | VAL | GLN | LYS | ARG | LEU | ASP | ASP | LEU | ARG | LYS | LYS |
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| THR | LEU | TYR | GLN | PHE | ASN | ILE | GLN | LYS | ASN | ASN | ASN | ASN | ASN | ASN | THR | GLY | PHE | PHE | ILE | GLU | LYS | ASP | GLN | ASN | ASN | LEU | LEU | SER | GLN | HIS | GLN | ILE | ILE | LYS | SER | LYS | GLN | GLY | LYS | HIS | ARG | SER | PHE | THR | THR | LEU | TYR | CYS | SER | SER | ASN |
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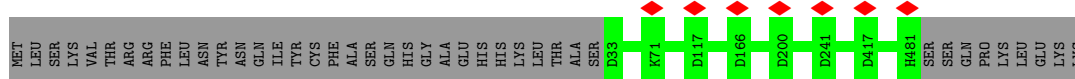
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| Met | GLN | GLN | ASP | ALA | GLU | ARG | GLN | PHE | LYS | SER | ASN | SER | ASP | LYS | SER | LYS | SER | ILE | THR | GLN | ILE | LEU | GLU | ASN | ASN | CYS | GLU | ASN | ALA | ILE | VAL | LEU | LEU | LEU | ASN | HIS | LEU | ILE | GLN | ILE | ILE | THR | ASP | SER | ILE | PRO | SER | ILE | SER | LYS | ASN | SER | ILE | LEU | LEU | ASP | GLU | LYS | SER | GLN |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

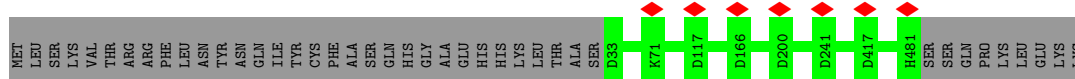
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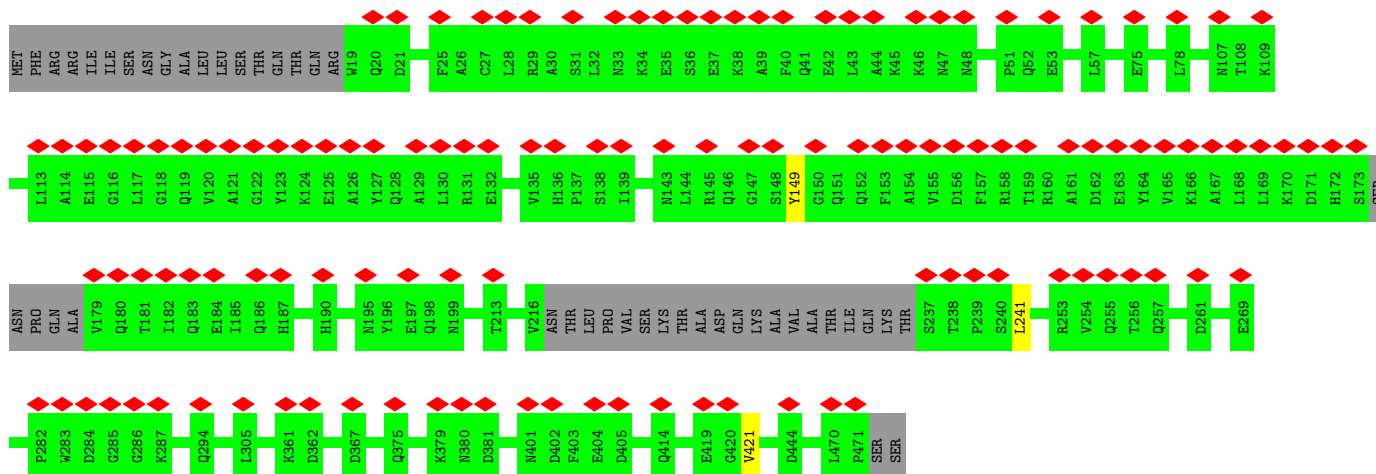
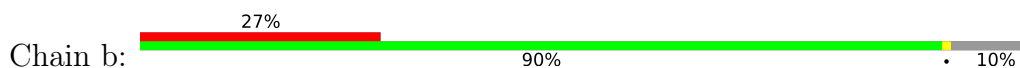
- Molecule 26: Transmembrane protein, putative



- Molecule 26: Transmembrane protein, putative



- Molecule 27: Protein phosphatase 2C, putative



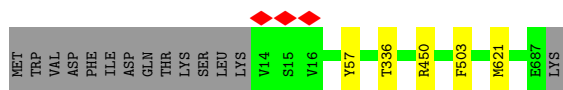
- Molecule 27: Protein phosphatase 2C, putative

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| E269 | E289 | E294 | E299 | E304 | E309 | E314 | E319 | E324 | E329 | E334 | E339 | E344 | E349 | E354 | E359 | E364 | E369 | E374 | E379 | E384 | E389 | E394 | E399 | E404 | E409 | E414 | E419 | E424 | E429 | E434 | E439 | E444 | E449 | E454 | E459 | E464 | E469 | E474 | E479 | E484 | E489 | E494 | E499 | E504 | E509 | E514 | E519 | E524 | E529 | E534 | E539 | E544 | E549 | E554 | E559 | E564 | E569 | E574 | E579 | E584 | E589 | E594 | E599 | E604 | E609 | E614 | E619 | E624 | E629 | E634 | E639 | E644 | E649 | E654 | E659 | E664 | E669 | E674 | E679 | E684 | E689 | E694 | E699 | E704 | E709 | E714 | E719 | E724 | E729 | E734 | E739 | E744 | E749 | E754 | E759 | E764 | E769 | E774 | E779 | E784 | E789 | E794 | E799 | E804 | E809 | E814 | E819 | E824 | E829 | E834 | E839 | E844 | E849 | E854 | E859 | E864 | E869 | E874 | E879 | E884 | E889 | E894 | E899 | E904 | E909 | E914 | E919 | E924 | E929 | E934 | E939 | E944 | E949 | E954 | E959 | E964 | E969 | E974 | E979 | E984 | E989 | E994 | E999 | F25 | F26 | F27 | F28 | F29 | F30 | F31 | F32 | F33 | F34 | F35 | F36 | F37 | F38 | F39 | F40 | F41 | F42 | F43 | F44 | F45 | F46 | F47 | F48 | F49 | F50 | F51 | F52 | F53 | F54 | F55 | F56 | F57 | F58 | F59 | F60 | F61 | F62 | F63 | F64 | F65 | F66 | F67 | F68 | F69 | F70 | F71 | F72 | F73 | F74 | F75 | F76 | F77 | F78 | F79 | F80 | F81 | F82 | F83 | F84 | F85 | F86 | F87 | F88 | F89 | F90 | F91 | F92 | F93 | F94 | F95 | F96 | F97 | F98 | F99 | G26 | G27 | G28 | G29 | G30 | G31 | G32 | G33 | G34 | G35 | G36 | G37 | G38 | G39 | G40 | G41 | G42 | G43 | G44 | G45 | G46 | G47 | G48 | G49 | G50 | G51 | G52 | G53 | G54 | G55 | G56 | G57 | G58 | G59 | G60 | G61 | G62 | G63 | G64 | G65 | G66 | G67 | G68 | G69 | G70 | G71 | G72 | G73 | G74 | G75 | G76 | G77 | G78 | G79 | G80 | G81 | G82 | G83 | G84 | G85 | G86 | G87 | G88 | G89 | G90 | G91 | G92 | G93 | G94 | G95 | G96 | G97 | G98 | G99 | H108 | H109 | H110 | H111 | H112 | H113 | H114 | H115 | H116 | H117 | H118 | H119 | H120 | H121 | H122 | H123 | H124 | H125 | H126 | H127 | H128 | H129 | H130 | H131 | H132 | H133 | H134 | H135 | H136 | H137 | H138 | H139 | H140 | H141 | H142 | H143 | H144 | H145 | H146 | H147 | H148 | H149 | H150 | H151 | H152 | H153 | H154 | H155 | H156 | H157 | H158 | H159 | H160 | H161 | H162 | H163 | H164 | H165 | H166 | H167 | H168 | H169 | H170 | H171 | H172 | I103 | I104 | I105 | I106 | I107 | I108 | I109 | I110 | I111 | I112 | I113 | I114 | I115 | I116 | I117 | I118 | I119 | I120 | I121 | I122 | I123 | I124 | I125 | I126 | I127 | I128 | I129 | I130 | I131 | I132 | I133 | I134 | I135 | I136 | I137 | I138 | I139 | I140 | I141 | I142 | I143 | I144 | I145 | I146 | I147 | I148 | I149 | I150 | I151 | I152 | I153 | I154 | I155 | I156 | I157 | I158 | I159 | I160 | I161 | I162 | I163 | I164 | I165 | I166 | I167 | I168 | I169 | I170 | I171 | I172 | L201 | L202 | L203 | L204 | L205 | L206 | L207 | L208 | L209 | L210 | L211 | L212 | L213 | L214 | L215 | L216 | L217 | L218 | L219 | L220 | L221 | L222 | L223 | L224 | L225 | L226 | L227 | L228 | L229 | L230 | L231 | L232 | L233 | L234 | L235 | L236 | L237 | L238 | L239 | L240 | L241 | L242 | L243 | L244 | L245 | L246 | L247 | L248 | L249 | L250 | L251 | L252 | L253 | L254 | L255 | L256 | L257 | L258 | L259 | L260 | L261 | L262 | L263 | L264 | L265 | L266 | L267 | L268 | L269 | L270 | L271 | L272 | L273 | L274 | L275 | L276 | L277 | L278 | L279 | L280 | L281 | L282 | L283 | L284 | L285 | L286 | L287 | L288 | L289 | L290 | L291 | L292 | L293 | L294 | L295 | L296 | L297 | L298 | L299 | M101 | M102 | M103 |
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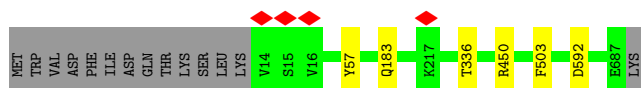
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| SER | LYS | THR | GLN | ALA | PHE | ALA | ARG | LEU | PHE | GLN | LEU | SER | SER | SER | SER | GLN | LYS | VAL | LYS | C82 | C83 | D108 | M129 | D130 | G147 | A148 | K149 | E150 | D163 | K164 | K165 | E175 | M184 | T192 | G193 | I200 | N201 | L202 | D203 | K236 | A236 | D237 | G238 | N241 | E291 | H292 | F293 | |
| MET | TYR | LEU | PHE | MET | HIS | LEU | CYS | MET | CYS | PHE | GLN | MET | ILE | SER | SER | GLN | LYS | LYS | GLU | LYS | LEU | ASN | LYS | LYS | GLY | LYS | ASN | LYS | LYS | GLU | LYS | GLN | ASN | LYS | LYS | LYS | GLU | GLU | GLU | GLU | ARG | ARG | SER | ASN | PRO | GLN | MET | ILE |

- [illegible]

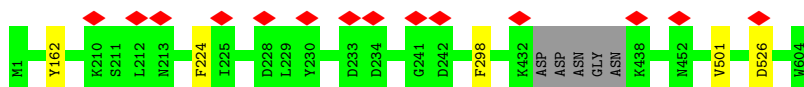
- Chain c1:  97% ...



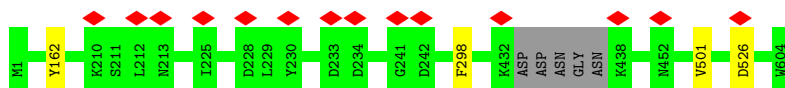
- Molecule 29: Cytochrome c oxidase subunit 1



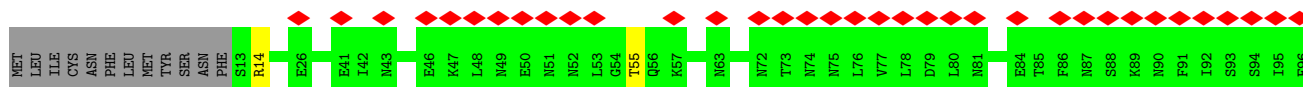
- Molecule 30: Cytochrome c oxidase subunit 2



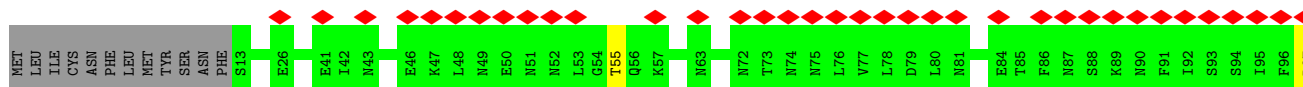
- Molecule 30: Cytochrome c oxidase subunit 2



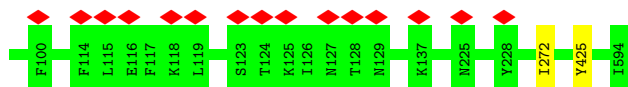
- Molecule 31: Ymf68



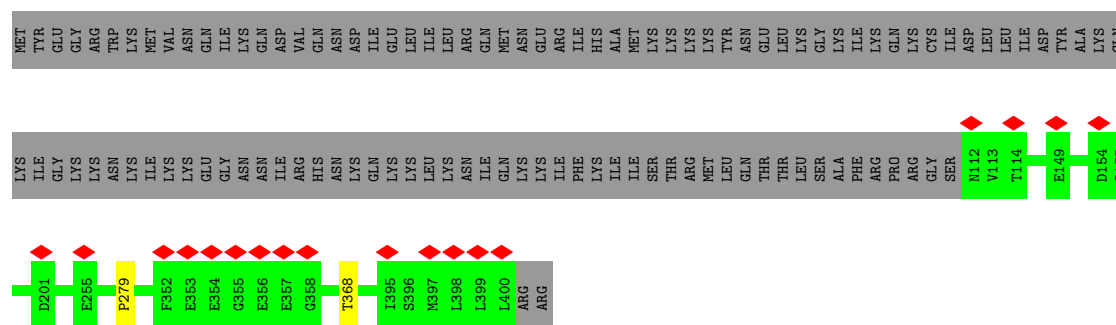
- Molecule 31: Ymf68



- Molecule 32: SURF1-like protein

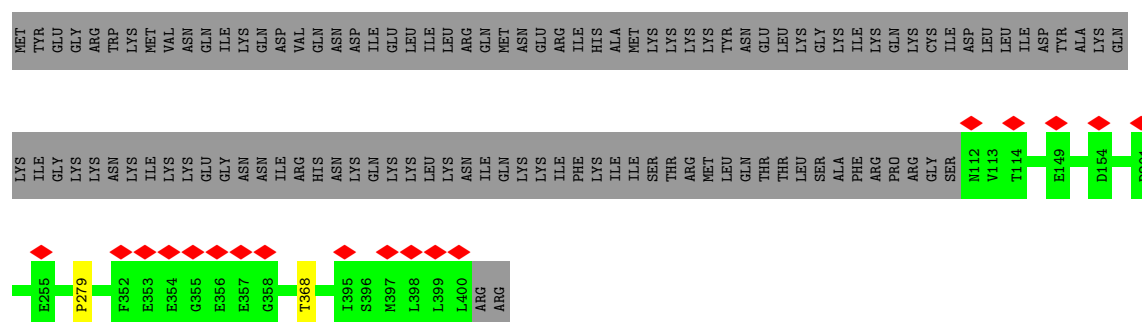


Chain d:  71% 28%



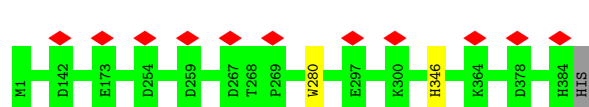
• Molecule 32: SURF1-like protein

Chain D:  71% 28%



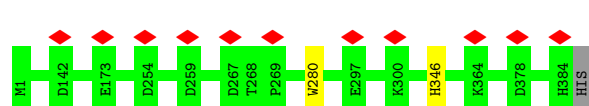
• Molecule 33: TraB family protein

Chain e:  99%



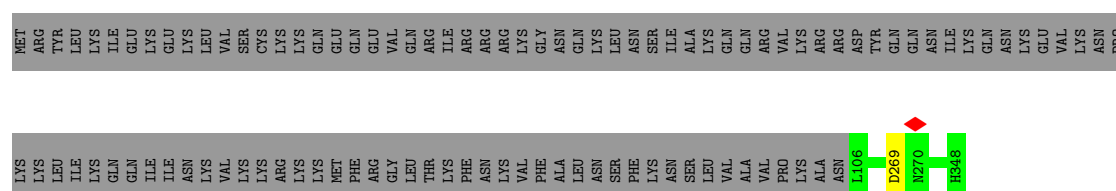
• Molecule 33: TraB family protein

Chain E:  99%

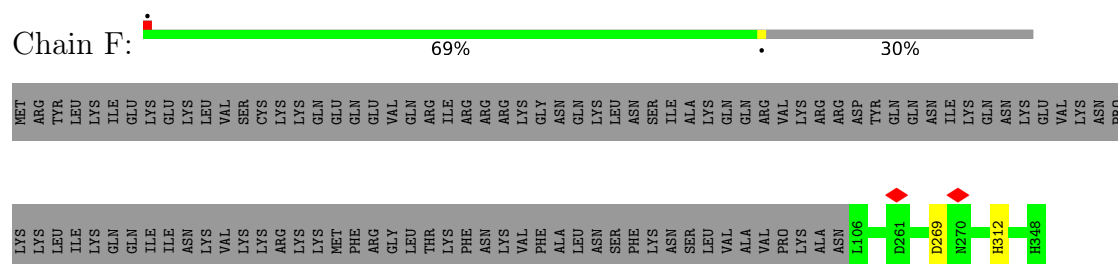


• Molecule 34: Transmembrane protein, putative

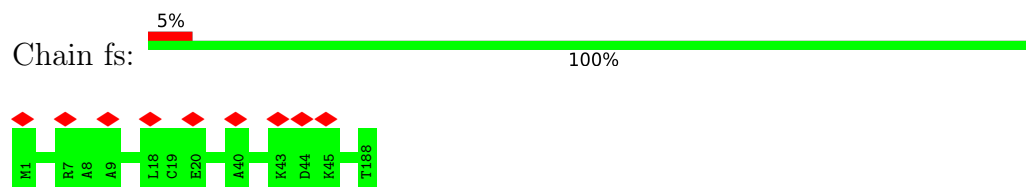
Chain f:  70% 30%



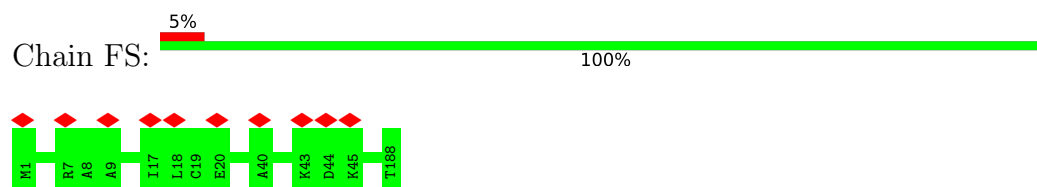
- Molecule 34: Transmembrane protein, putative



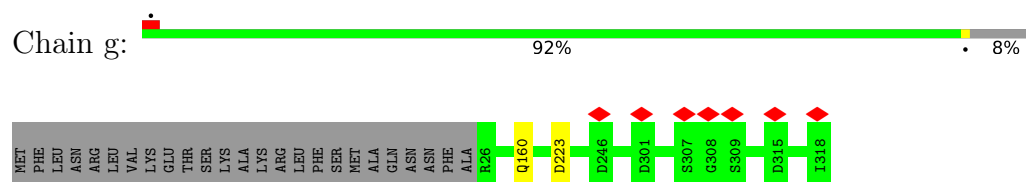
- Molecule 35: Iron-binding zinc finger CDGSH type protein



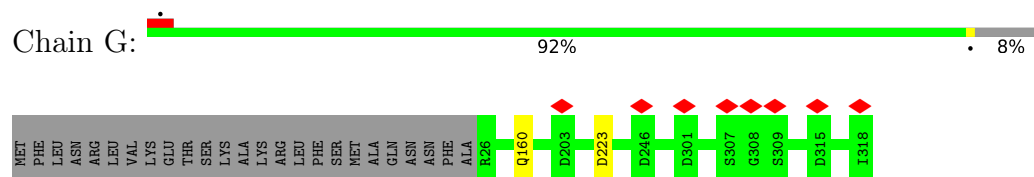
- Molecule 35: Iron-binding zinc finger CDGSH type protein



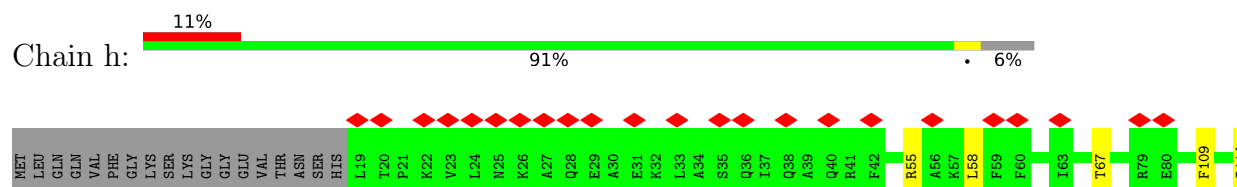
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial

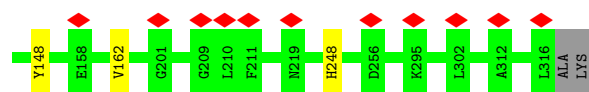


- Molecule 36: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial

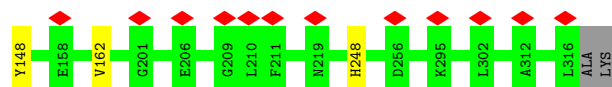
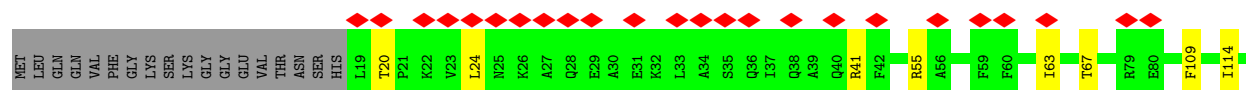
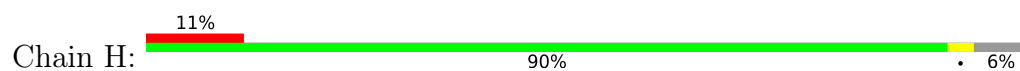


- Molecule 37: SURF1-like protein

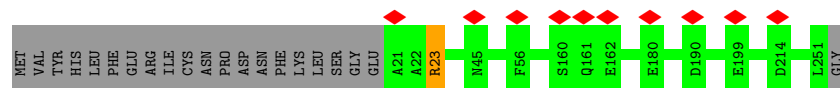




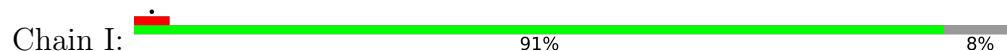
• Molecule 37: SURF1-like protein



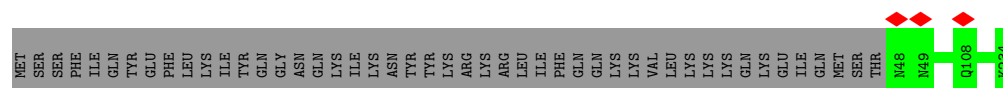
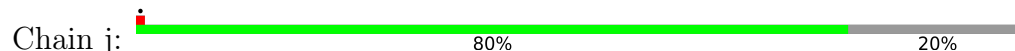
• Molecule 38: COXTT9



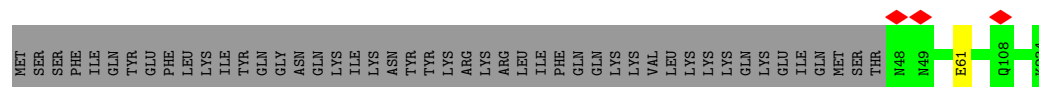
• Molecule 38: COXTT9



• Molecule 39: COXTT10

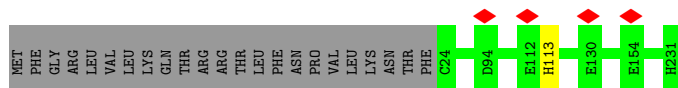


• Molecule 39: COXTT10

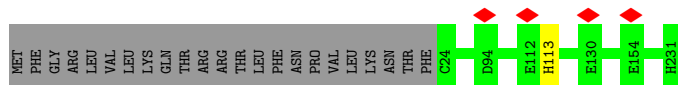
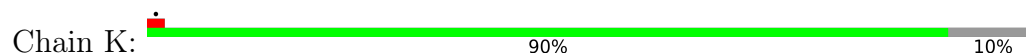


• Molecule 40: 39S ribosomal protein L9, mitochondrial

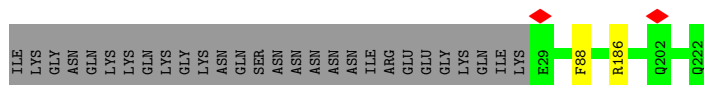
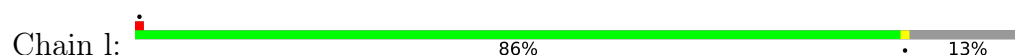




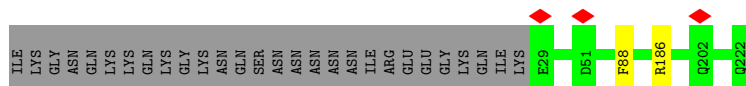
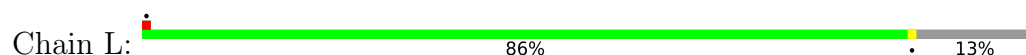
- Molecule 40: 39S ribosomal protein L9, mitochondrial



- Molecule 41: Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C



- Molecule 41: Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C



- Molecule 42: Transmembrane protein, putative



- Molecule 42: Transmembrane protein, putative



- Molecule 43: Oxoglutarate/malate translocator protein, putative



- Molecule 43: Oxoglutarate/malate translocator protein, putative

Chain M1:  100%



- Molecule 44: 2-oxoglutarate/malate carrier protein

Chain m2:  100%



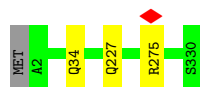
- Molecule 44: 2-oxoglutarate/malate carrier protein

Chain M2:  100%



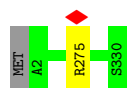
- Molecule 45: Carrier protein

Chain m3:  99%



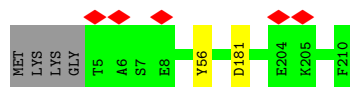
- Molecule 45: Carrier protein

Chain M3:  99%



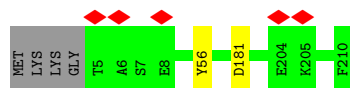
- Molecule 46: Transmembrane protein, putative

Chain n:  97%



- Molecule 46: Transmembrane protein, putative

Chain N:  97%



- Molecule 47: Mobilization protein

Chain o:  66% 33%

MET LYS GLU LYS ILE PHE ASN GLU LEU THR ARG LYS MET LYS ARG LYS ILE SER ALA LYS GLN ARG GLU ASN LYS GLN ILE LEU ILE ARG GLN ARG ASN ASN LYS TYR ILE GLN SER ILE GLN GLY ILE GLN GLN GLU ARG LYS LYS GLY LYS LEU TYR LEU VAL GLU

MET ALA THR GLN N65 D93 Y193

- Molecule 47: Mobilization protein

Chain O:  67% 33%

MET LYS GLU LYS ILE PHE ASN GLU LEU THR ARG LYS MET LYS ARG LYS ILE SER ALA LYS GLN ARG GLU ASN LYS GLN ILE LEU ILE ARG GLN ARG ASN ASN LYS TYR ILE GLN SER ILE GLN GLY ILE GLN GLN GLU ARG LYS LYS GLY LYS LEU TYR LEU VAL GLU

MET ALA THR GLN N65 Y193

- Molecule 48: YffT domain-containing protein

Chain p:  5% 99%

H1 L65 E66 G69 D72 F90 D110 D127 K128 R155 E159 H175

- Molecule 48: YffT domain-containing protein

Chain P:  5% 99%

H1 L65 E66 G69 D72 F90 D110 D127 K128 R155 E159 H175

- Molecule 49: Transmembrane protein, putative

Chain q:  99%

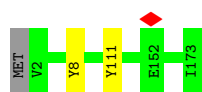
H1 D2 Y83 F173

- Molecule 49: Transmembrane protein, putative

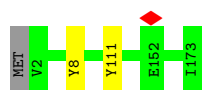
Chain Q:  100%

H1 D2 F173

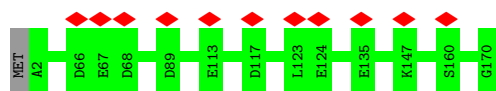
- Molecule 50: Transmembrane protein



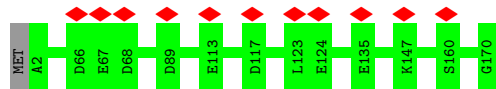
- Molecule 50: Transmembrane protein



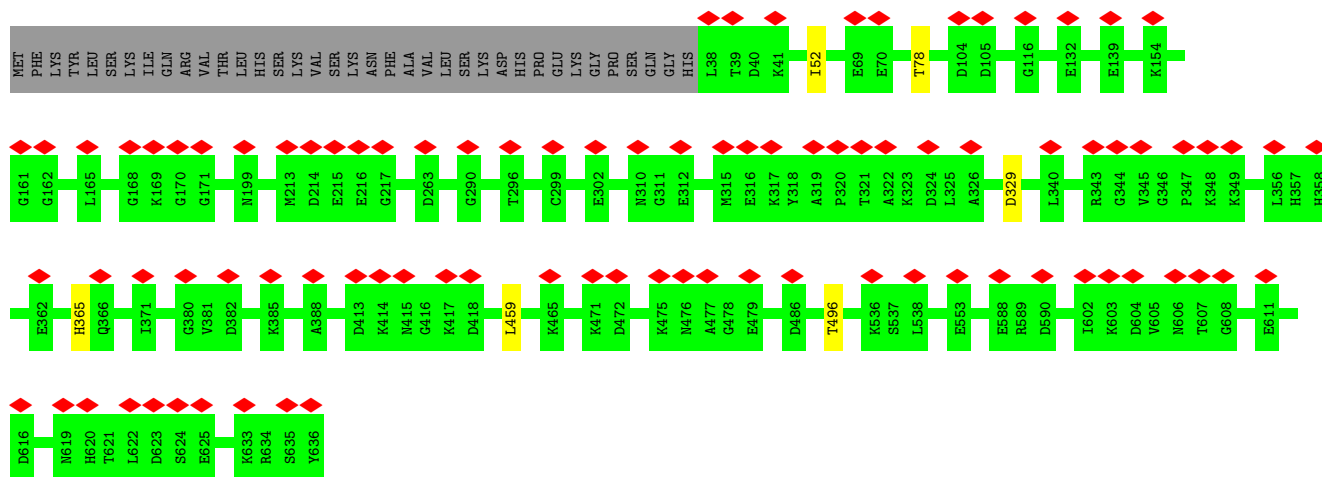
- Molecule 51: Complex III subunit VII



- Molecule 51: Complex III subunit VII

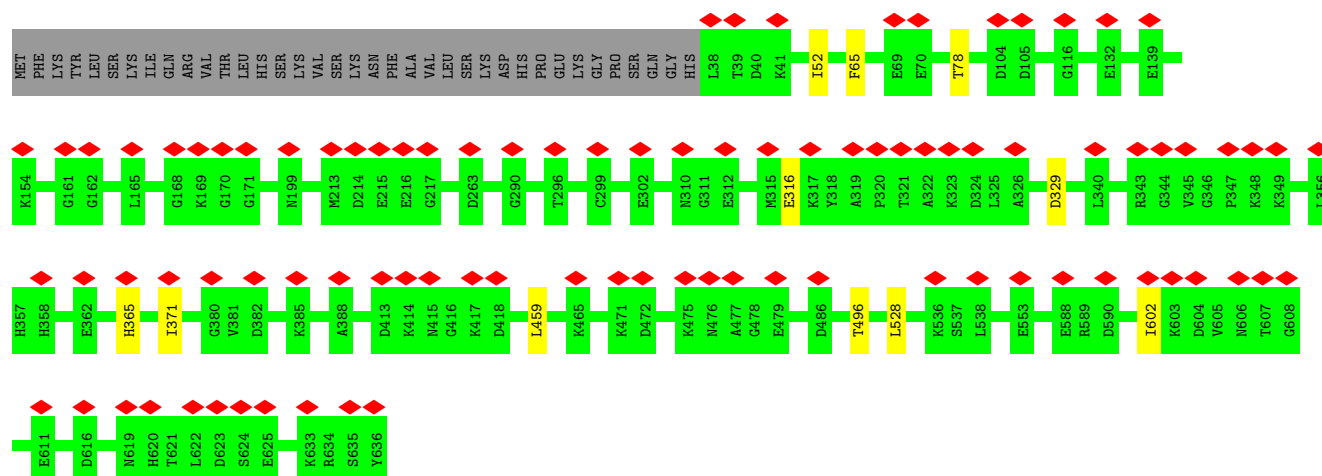


- Molecule 52: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

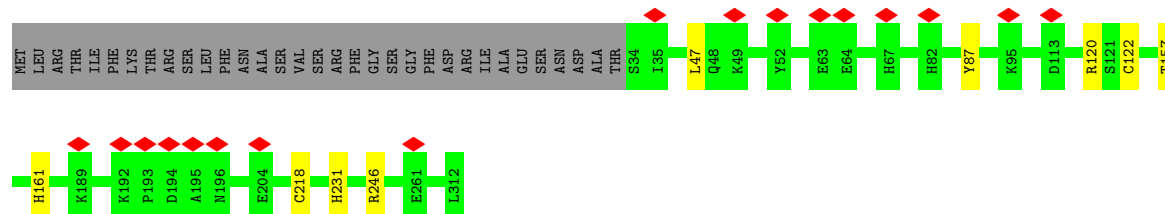
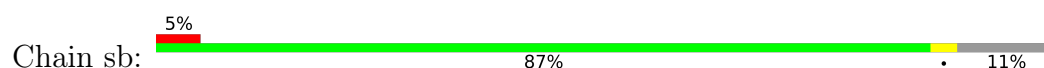


- Molecule 52: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial

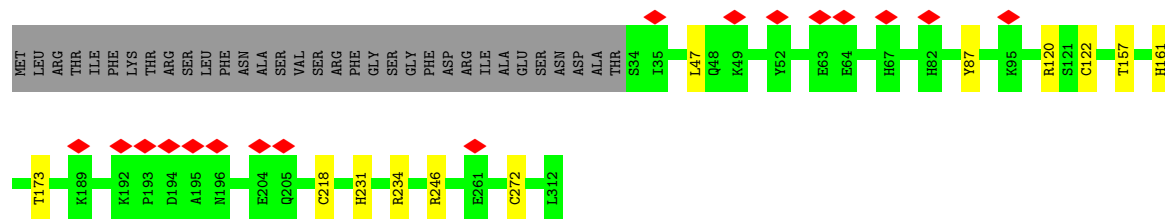
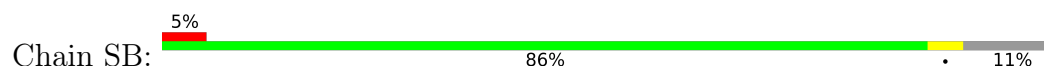




- Molecule 53: Succinate dehydrogenase (quinone)



- Molecule 53: Succinate dehydrogenase (quinone)



- Molecule 54: Cytochrome b-c1 complex subunit 8



- Molecule 54: Cytochrome b-c1 complex subunit 8



- Molecule 55: SDHD

Chain sd:  100%

There are no outlier residues recorded for this chain.

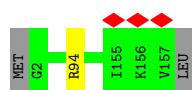
- Molecule 55: SDHD

Chain SD:  100%

There are no outlier residues recorded for this chain.

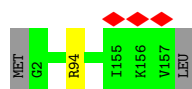
- Molecule 56: Transmembrane protein, putative

Chain t:  98% ..



- Molecule 56: Transmembrane protein, putative

Chain T:  98% ..



- Molecule 57: Transmembrane protein, putative

Chain u:  98% ..



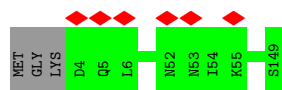
- Molecule 57: Transmembrane protein, putative

Chain U:  98% ..



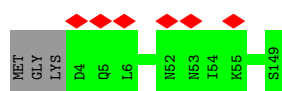
- Molecule 58: COXTT22

Chain v:  98% .



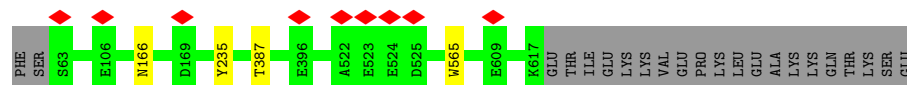
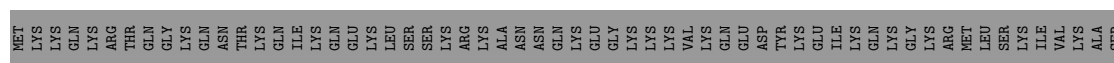
- Molecule 58: COXTT22

Chain V:  98%




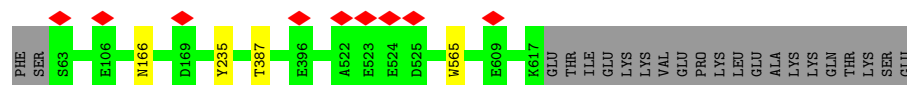
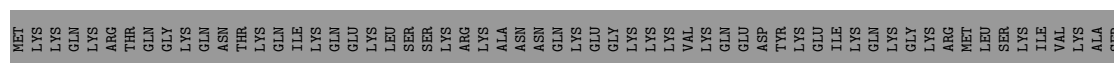
- Molecule 59: Cytochrome C oxidase subunit Vb protein

Chain vb:  86%



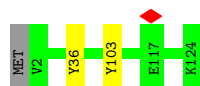
- Molecule 59: Cytochrome C oxidase subunit Vb protein

Chain VB:  86%



- Molecule 60: Transmembrane protein, putative

Chain w:  98%



- Molecule 60: Transmembrane protein, putative

Chain W:  98%



- Molecule 61: Transmembrane protein, putative

Chain x:  99%



- Molecule 61: Transmembrane protein, putative

Chain X:  99%



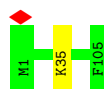
- Molecule 62: Lysozyme

Chain y:  99%



- Molecule 62: Lysozyme

Chain Y:  99%



- Molecule 63: Ymf70

Chain y0:  100%

There are no outlier residues recorded for this chain.

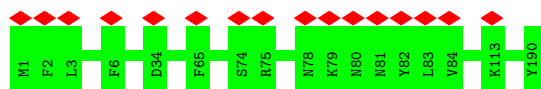
- Molecule 63: Ymf70

Chain Y0:  100%

There are no outlier residues recorded for this chain.

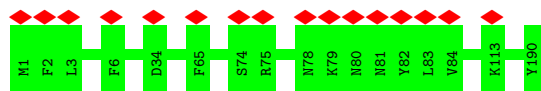
- Molecule 64: Ymf75

Chain y5:  8% 100%




- Molecule 64: Ymf75

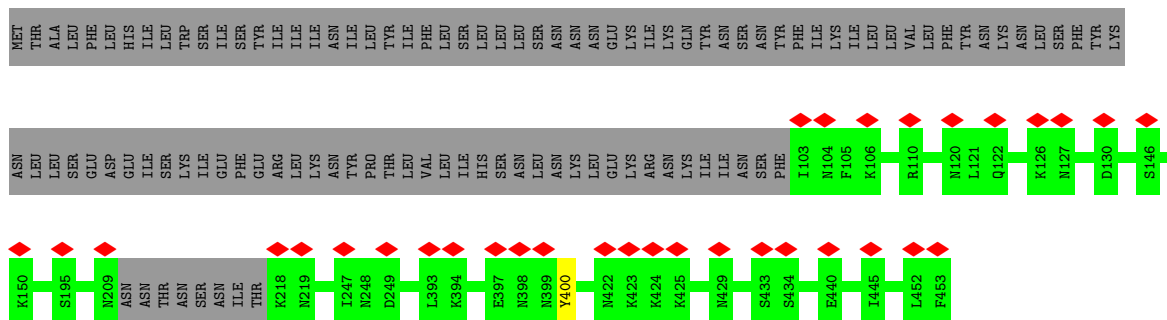
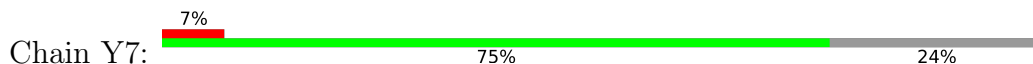
Chain Y5:  8% 100%



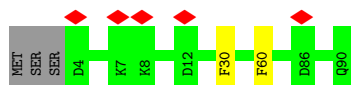
- Molecule 65: Ymf67

Chain y7:  7% 75% 24%

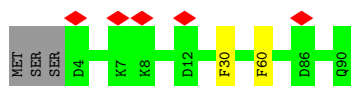
- Molecule 65: Ymf67



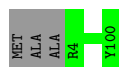
- Molecule 66: ABC transporter



- Molecule 66: ABC transporter

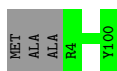


- Molecule 67: COXTT28



- Molecule 67: COXTT28





- Molecule 68: NADH dehydrogenase subunit 1

Chain 1b:  100%



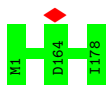
- Molecule 68: NADH dehydrogenase subunit 1

Chain 1B:  100%



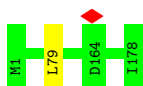
- Molecule 69: NADH dehydrogenase subunit 2

Chain 2b:  100%



- Molecule 69: NADH dehydrogenase subunit 2

Chain 2B:  99%



- Molecule 70: Ymf58

Chain 4l:  100%



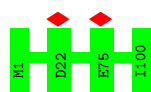
- Molecule 70: Ymf58

Chain 4L:  100%



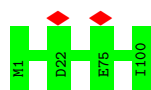
- Molecule 71: Ymf57

Chain 5b:  100%



- Molecule 71: Ymf57

Chain 5B:  100%



- Molecule 72: Transmembrane protein, putative

Chain a1:  99%



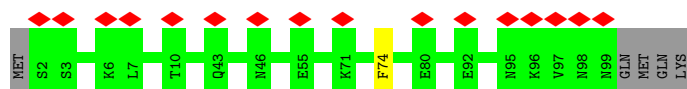
- Molecule 72: Transmembrane protein, putative

Chain A1:  99%



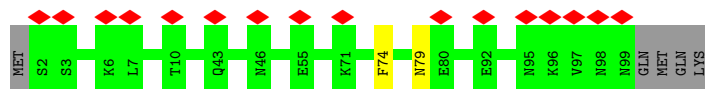
- Molecule 73: Ribosomal protein L51/S25/CI-B8 domain protein

Chain a2:  16% 94% 5%



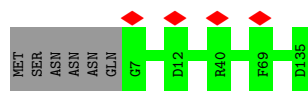
- Molecule 73: Ribosomal protein L51/S25/CI-B8 domain protein

Chain A2:  16% 93% 5%



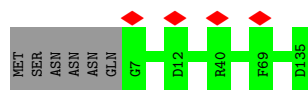
- Molecule 74: Transmembrane protein, putative

Chain a3:  96%




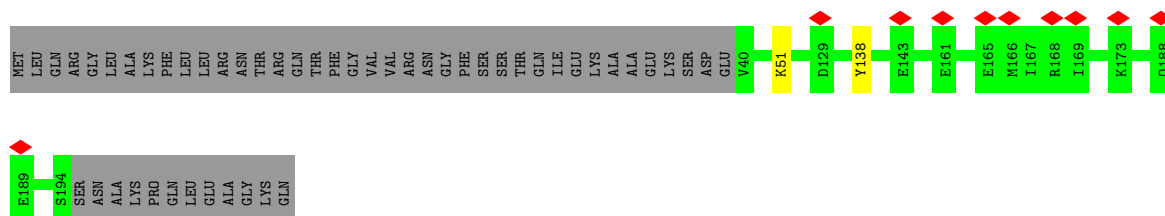
- Molecule 74: Transmembrane protein, putative

Chain A3:  96%




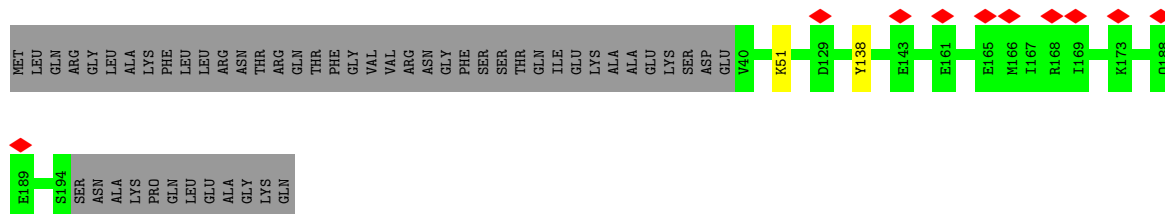
- Molecule 75: ETC complex I subunit motif protein

Chain a5:  5% 74% 25%



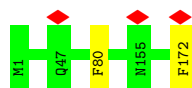
- Molecule 75: ETC complex I subunit motif protein

Chain A5:  5% 74% 25%



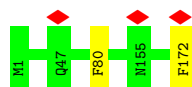
- Molecule 76: NADH dehydrogenase, putative

Chain a6:  99%



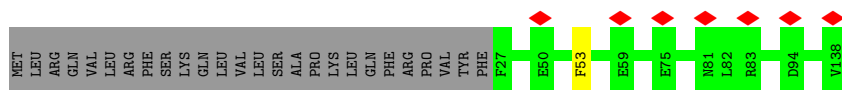
- Molecule 76: NADH dehydrogenase, putative

Chain A6:  99%

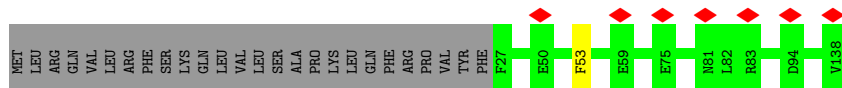
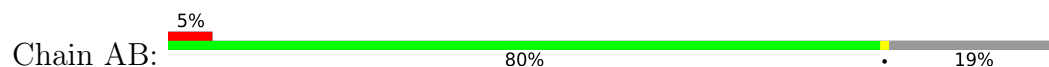


- Molecule 77: 37S ribosomal protein S25, mitochondrial

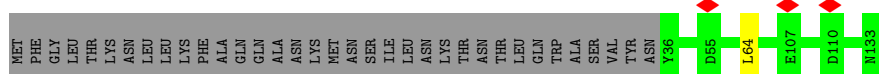
Chain a7:  9% 99%



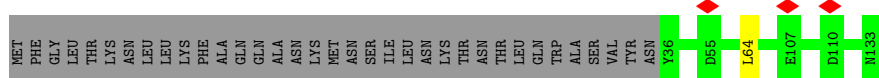
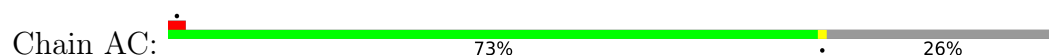
- Molecule 80: Acyl carrier protein



- Molecule 81: Acyl carrier protein



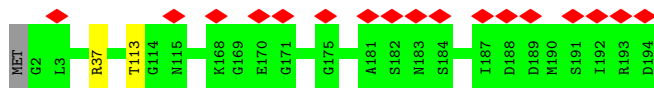
- Molecule 81: Acyl carrier protein



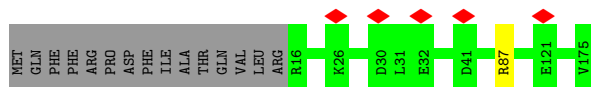
- Molecule 82: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- Molecule 82: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

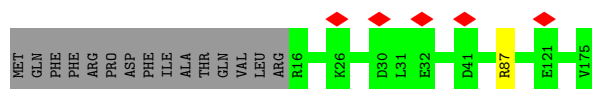


- Molecule 83: NDUA13



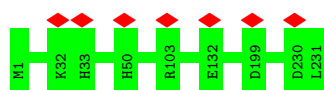
- Molecule 83: NDUA13

Chain AM:  91% 9%



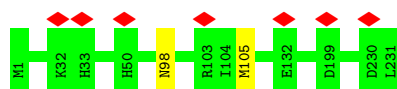
- Molecule 84: Transmembrane protein, putative

Chain an:  100%




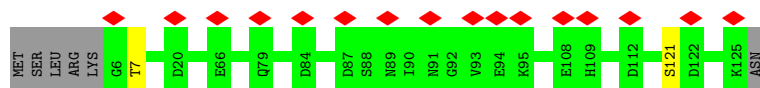
- Molecule 84: Transmembrane protein, putative

Chain AN:  99%



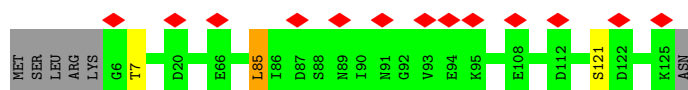
- Molecule 85: NDUB2

Chain b2:  13% 94% 5%




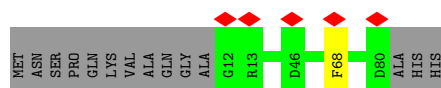
- Molecule 85: NDUB2

Chain B2:  10% 93% 5%




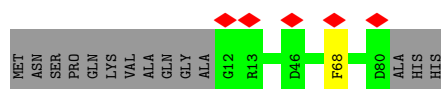
- Molecule 86: Transmembrane protein, putative

Chain b3:  6% 82% 17%




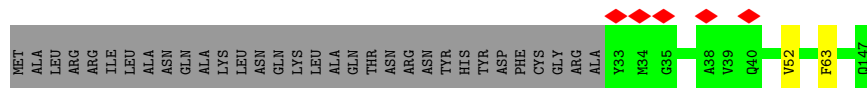
- Molecule 86: Transmembrane protein, putative

Chain B3:  6% 82% 17%




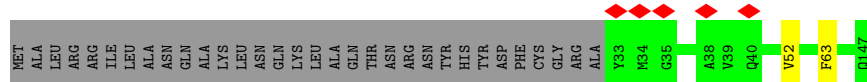
- Molecule 87: NDUB4

Chain b4: 



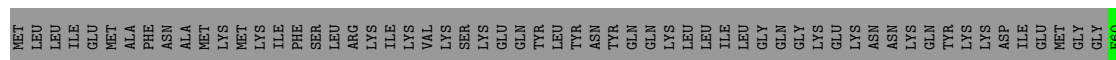
- Molecule 87: NDUB4

Chain B4: 



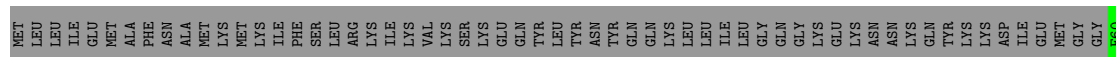
- Molecule 88: NDUB6

Chain b6: 



- Molecule 88: NDUB6

Chain B6: 



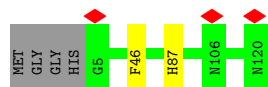
- Molecule 89: CHCH domain-containing protein

Chain b7: 

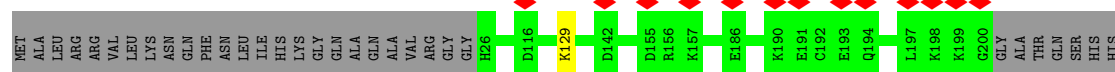
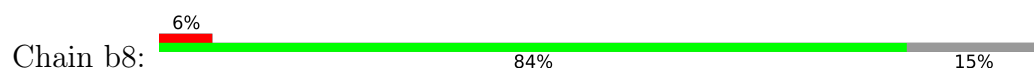


- Molecule 89: CHCH domain-containing protein

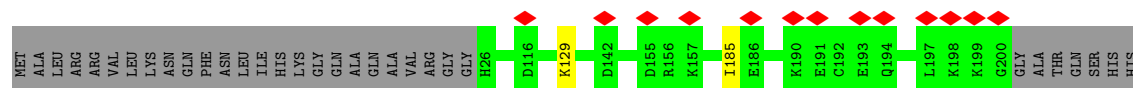
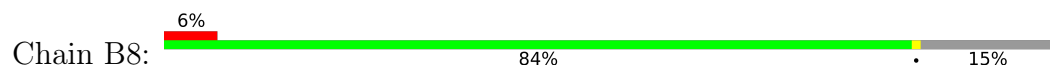
Chain B7: 



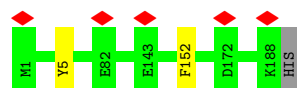
- Molecule 90: NDUB8



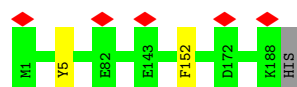
- Molecule 90: NDUB8



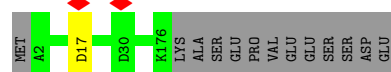
- Molecule 91: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



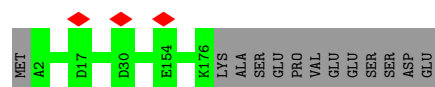
- Molecule 91: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



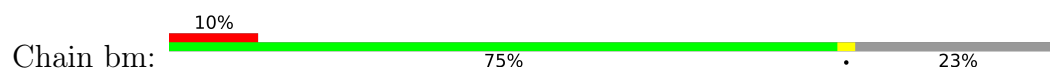
- Molecule 92: NDUB10

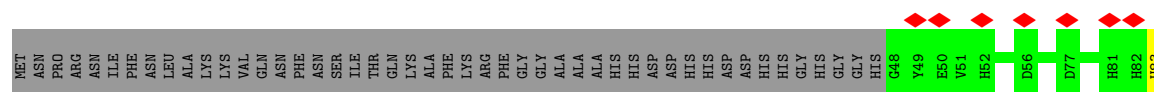


- Molecule 92: NDUB10

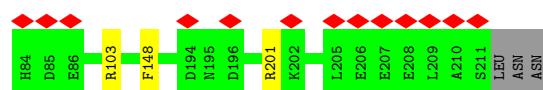
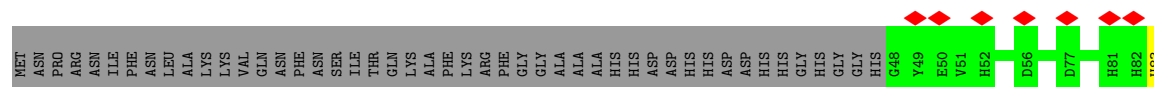
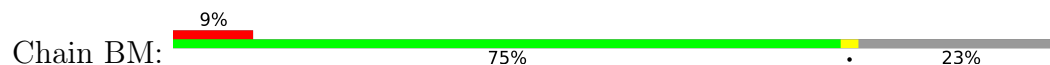


- Molecule 93: Transmembrane protein, putative





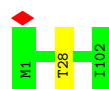
- Molecule 93: Transmembrane protein, putative



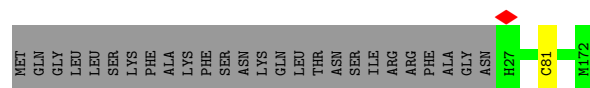
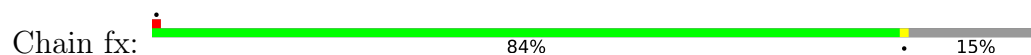
- Molecule 94: Complex I-MNLL



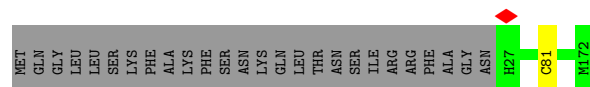
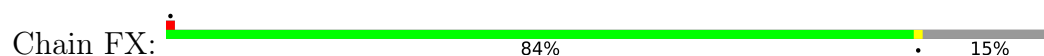
- Molecule 94: Complex I-MNLL




- Molecule 95: 2 iron, 2 sulfur cluster-binding protein

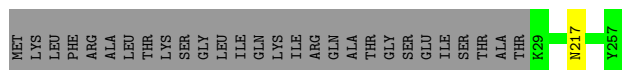


- Molecule 95: 2 iron, 2 sulfur cluster-binding protein



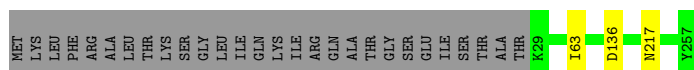
- Molecule 96: Gamma-carbonic anhydrase

Chain g1:  89% 11%



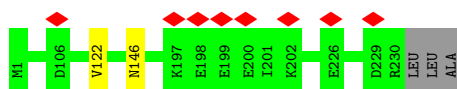
- Molecule 96: Gamma-carbonic anhydrase

Chain G1:  88% 11%



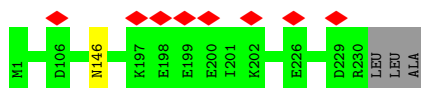
- Molecule 97: Gamma-carbonic anhydrase

Chain g2:  98% ..



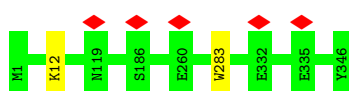
- Molecule 97: Gamma-carbonic anhydrase

Chain G2:  98% .



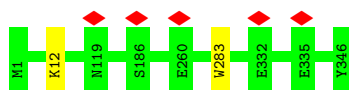
- Molecule 98: Transcription factor apf protein, putative

Chain g3:  99% .




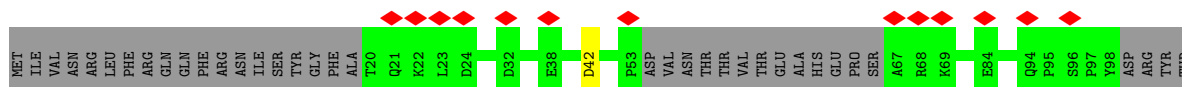
- Molecule 98: Transcription factor apf protein, putative

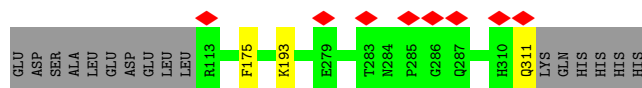
Chain G3:  99% .



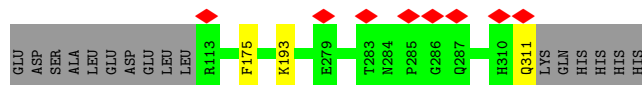
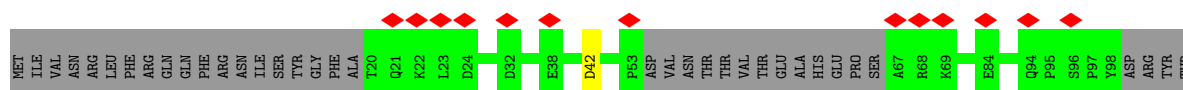
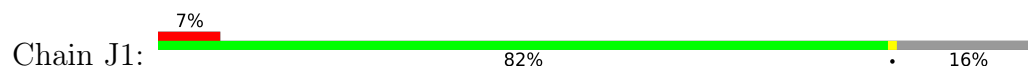
- Molecule 99: DnaJ domain protein

Chain j1:  7% 82% 16%

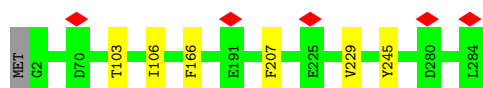




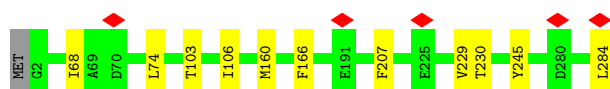
- Molecule 99: DnaJ domain protein



- Molecule 100: NADH-ubiquinone oxidoreductase chain 1



- Molecule 100: NADH-ubiquinone oxidoreductase chain 1



- Molecule 101: Ymf65

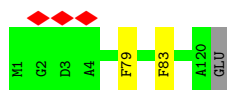


- Molecule 101: Ymf65

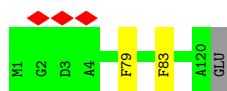


- Molecule 102: NADH-ubiquinone oxidoreductase chain 3





- Molecule 102: NADH-ubiquinone oxidoreductase chain 3



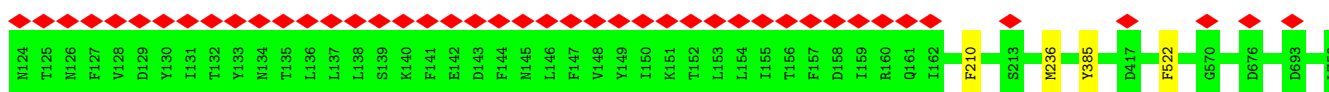
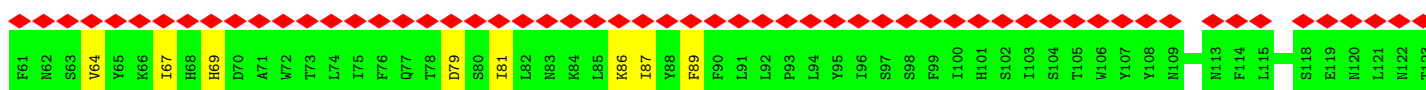
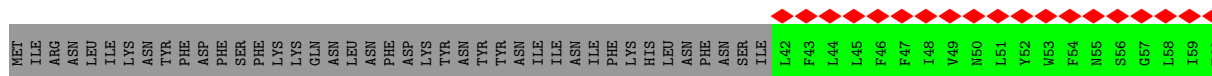
- Molecule 103: NADH-ubiquinone oxidoreductase chain 4



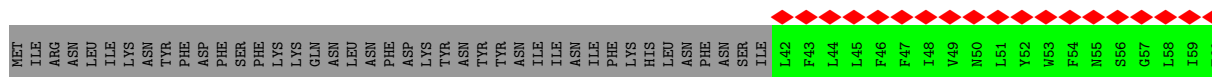
- Molecule 103: NADH-ubiquinone oxidoreductase chain 4

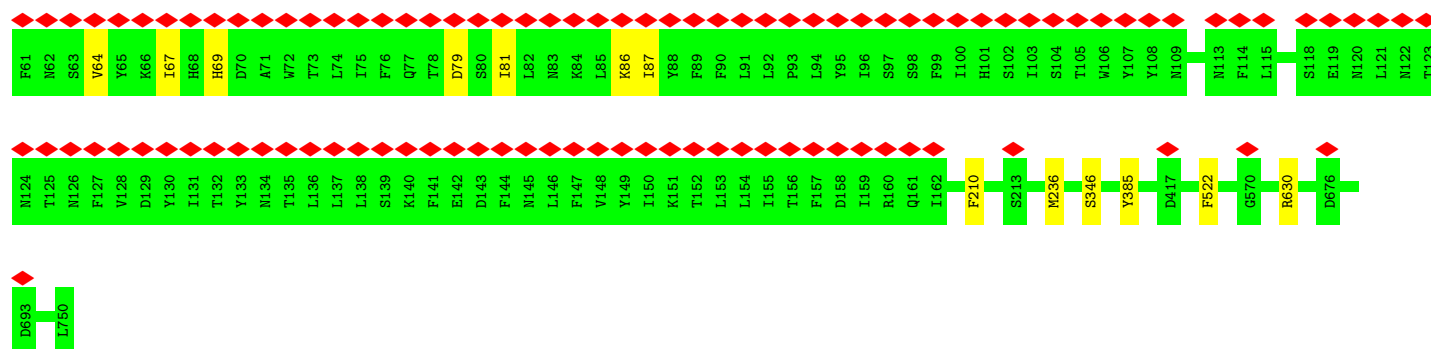


- Molecule 104: NADH dehydrogenase subunit 5

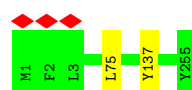


- Molecule 104: NADH dehydrogenase subunit 5

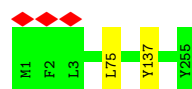




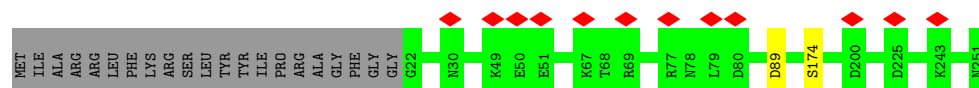
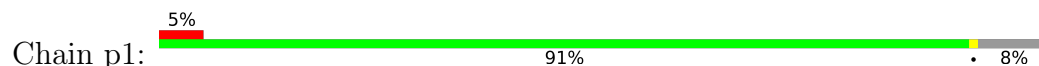
• Molecule 105: Ymf62



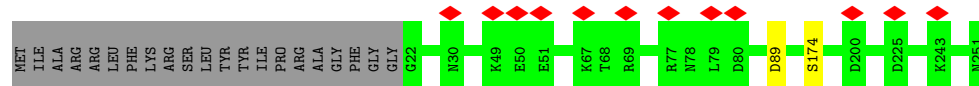
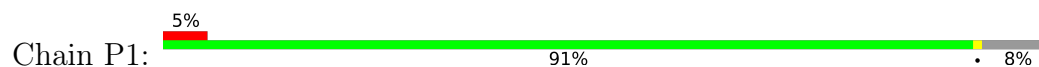
• Molecule 105: Ymf62



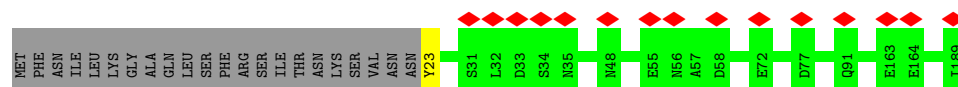
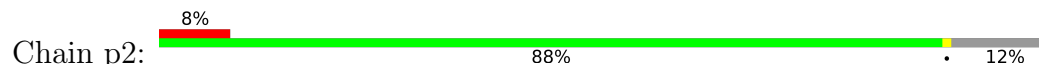
• Molecule 106: Transmembrane protein, putative



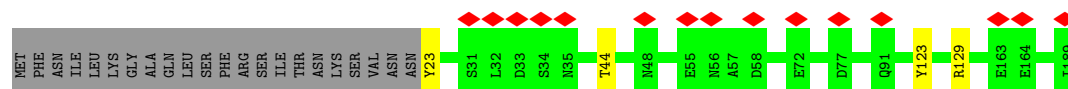
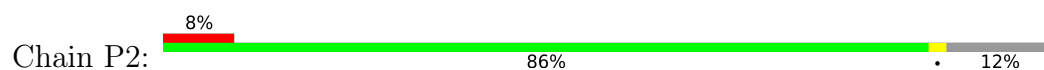
• Molecule 106: Transmembrane protein, putative



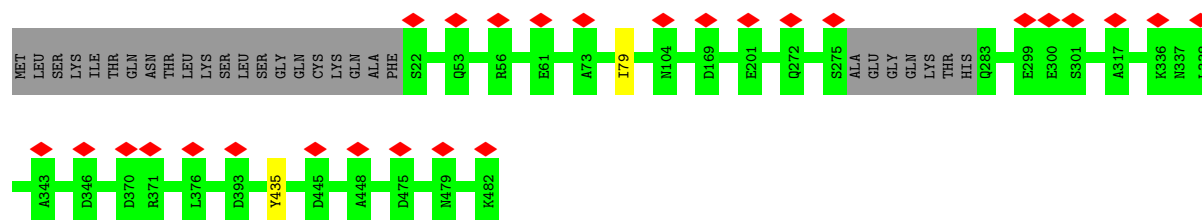
• Molecule 107: NDUPH2



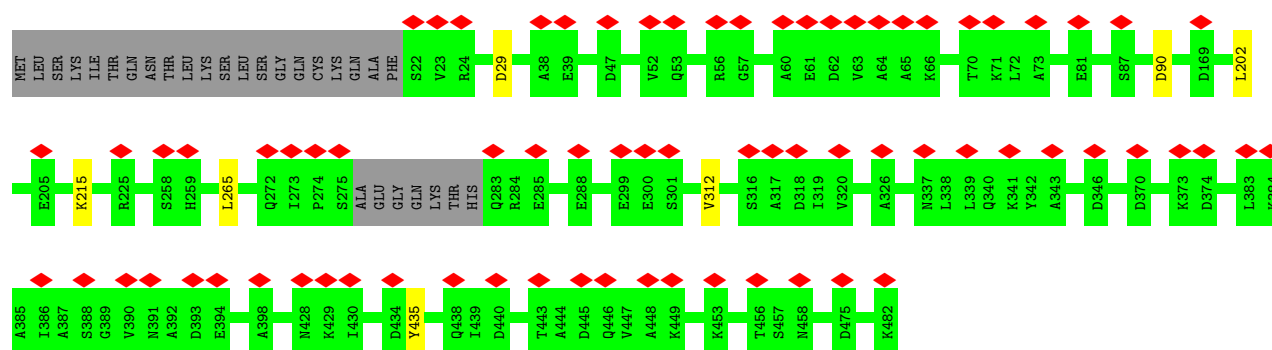
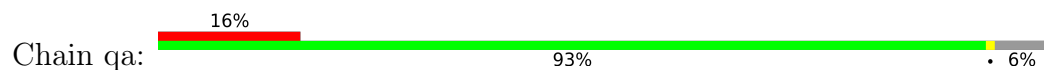
• Molecule 107: NDUPH2



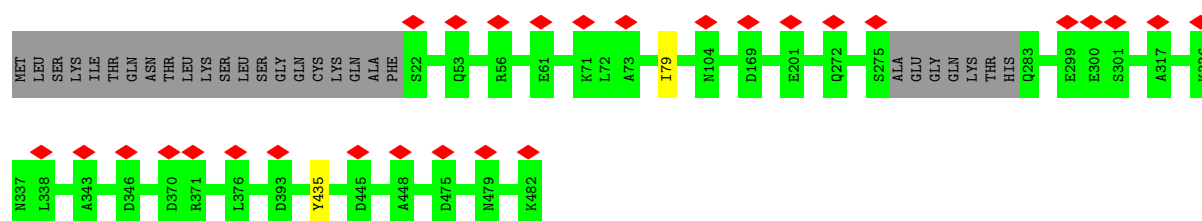
- Molecule 108: M16 family peptidase, putative



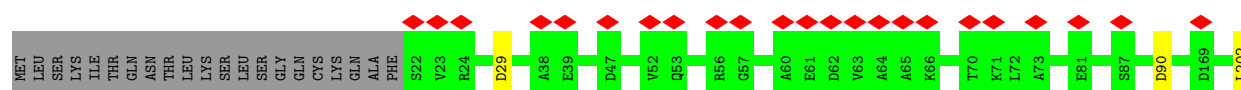
- Molecule 108: M16 family peptidase, putative

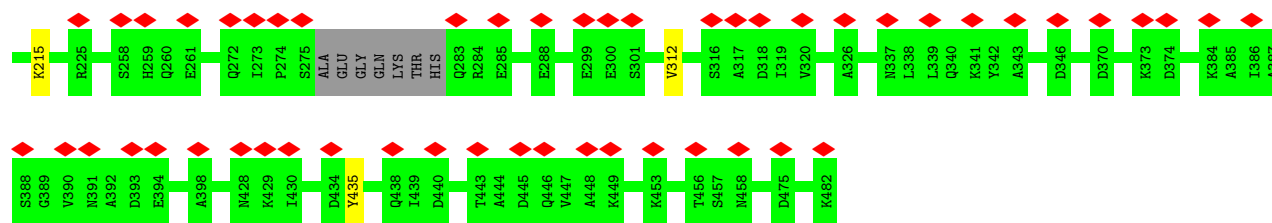


- Molecule 108: M16 family peptidase, putative



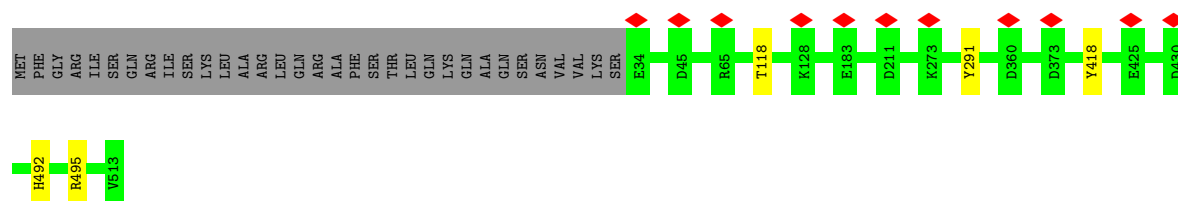
- Molecule 108: M16 family peptidase, putative





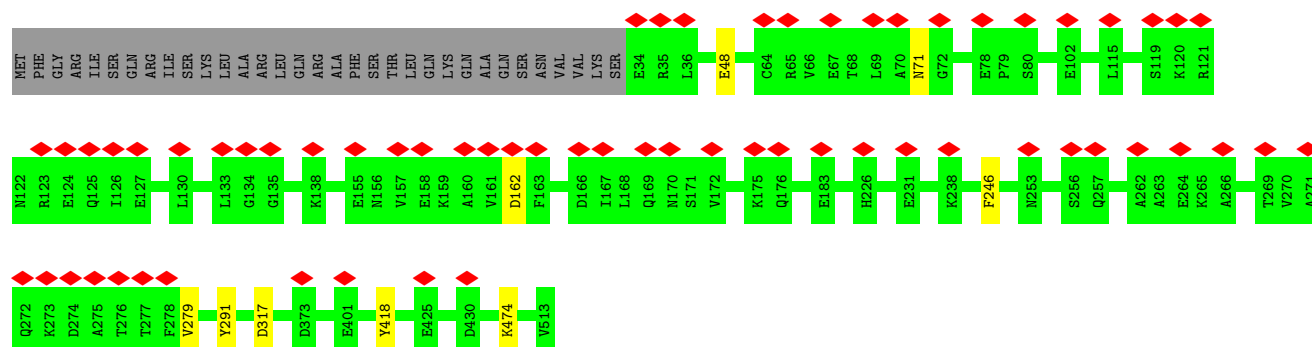
- Molecule 109: Peptidase M16 inactive domain protein

Chain qB: 93% • 6%



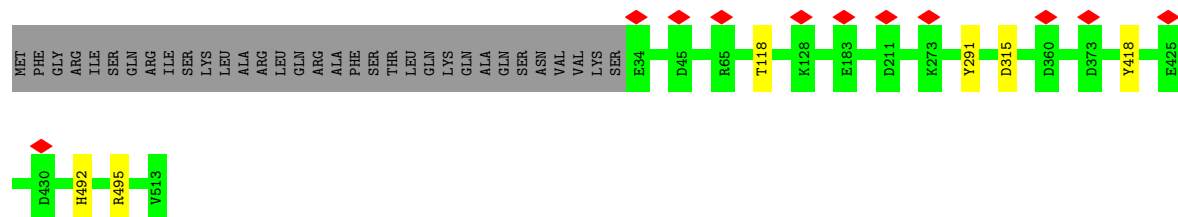
- Molecule 109: Peptidase M16 inactive domain protein

Chain qb: 12% 92% • 6%



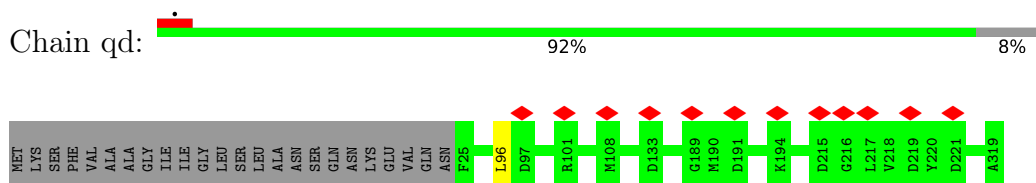
- Molecule 109: Peptidase M16 inactive domain protein

Chain QB: 12% 92% • 6%

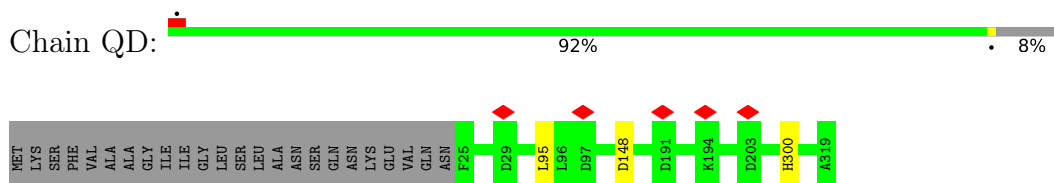


- Molecule 109: Peptidase M16 inactive domain protein

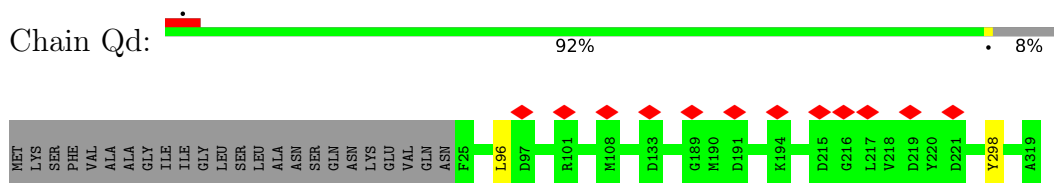
Chain Qb: 12% 92% • 6%



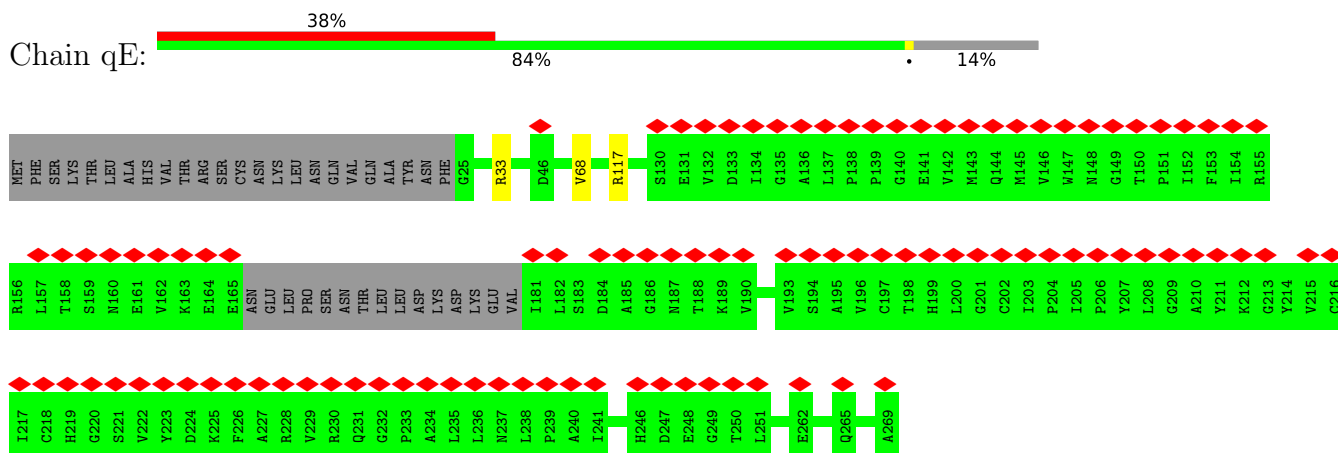
- Molecule 111: Cytochrome protein c1



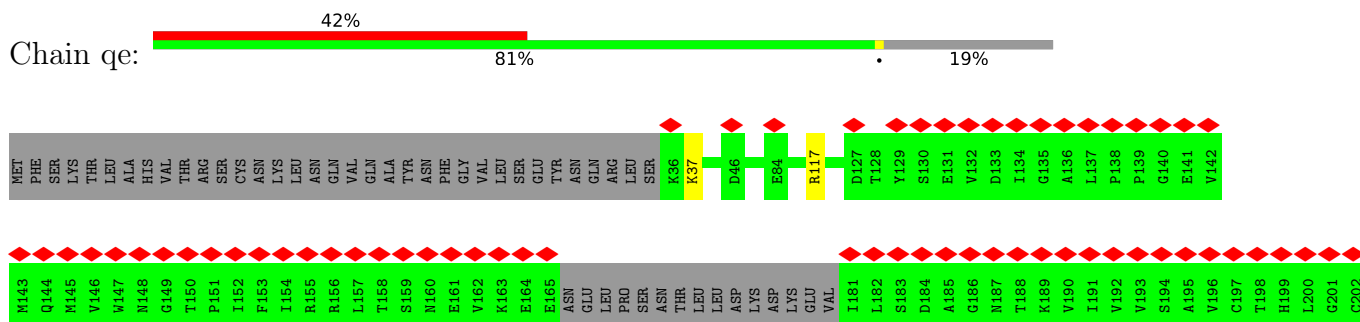
- Molecule 111: Cytochrome protein c1

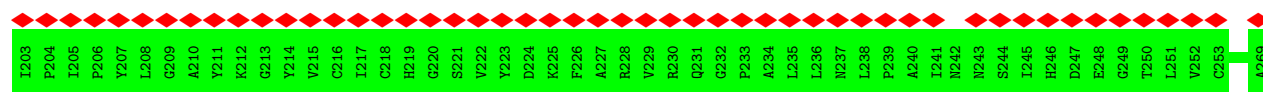


- Molecule 112: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit

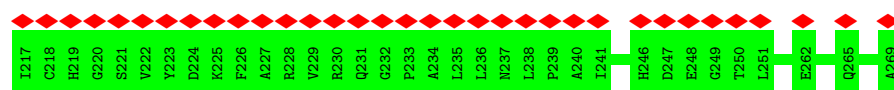
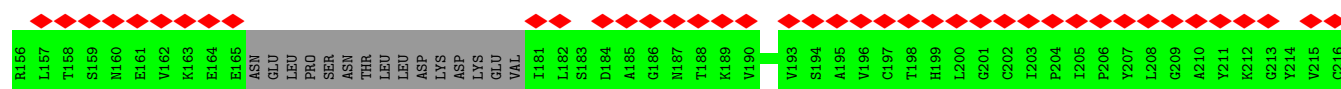
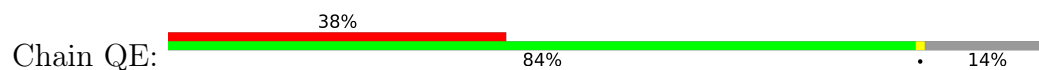


- Molecule 112: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur subunit

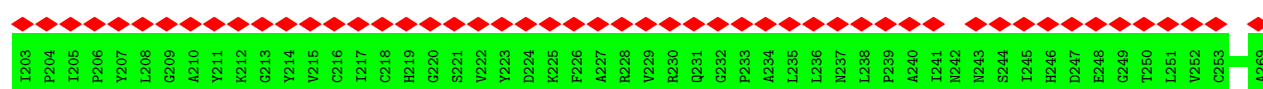
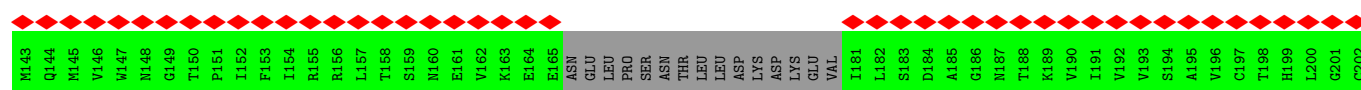
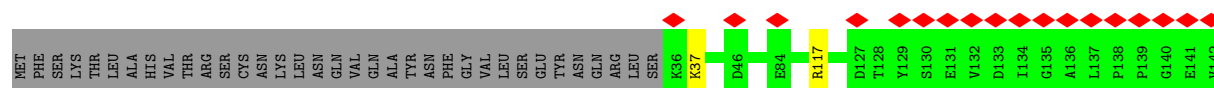
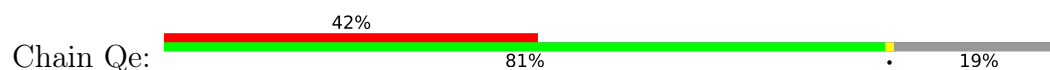




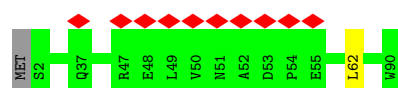
- Molecule 112: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur sub-unit



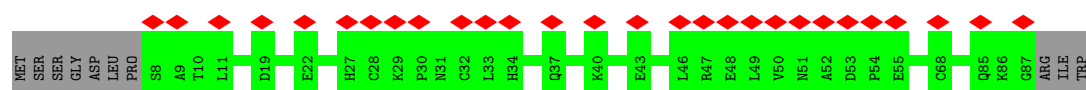
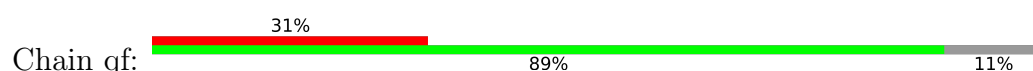
- Molecule 112: Rieske iron-sulfur protein, ubiquinol-cytochrome C reductase iron-sulfur sub-unit



- Molecule 113: Ubiquinol-cytochrome C reductase hinge protein

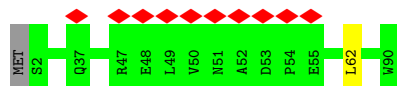


- Molecule 113: Ubiquinol-cytochrome C reductase hinge protein




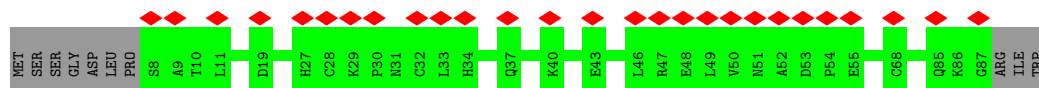
- Molecule 113: Ubiquinol-cytochrome C reductase hinge protein

Chain QF: 



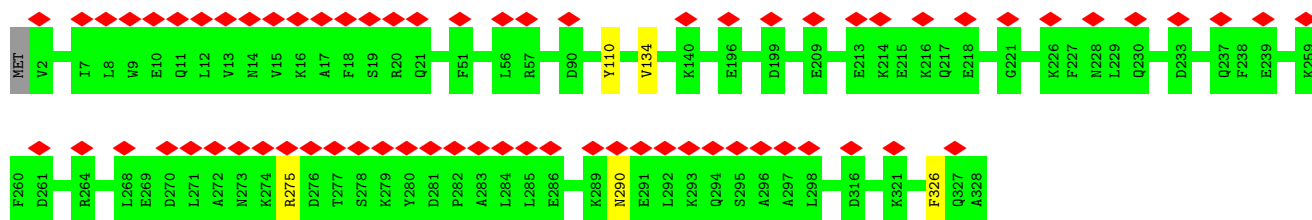
- Molecule 113: Ubiquinol-cytochrome C reductase hinge protein

Chain Qf: 



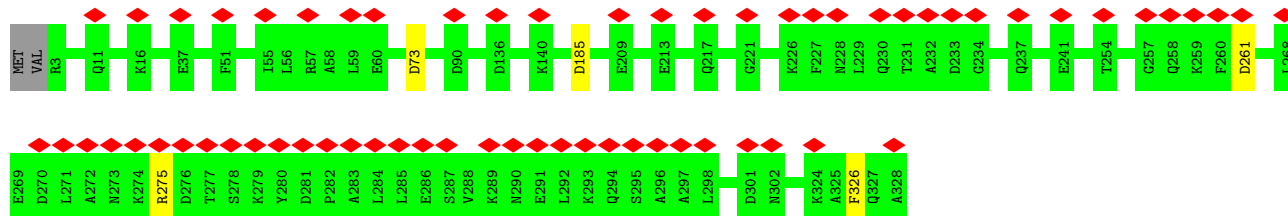
- Molecule 114: Sulphotransf domain-containing protein

Chain qG: 



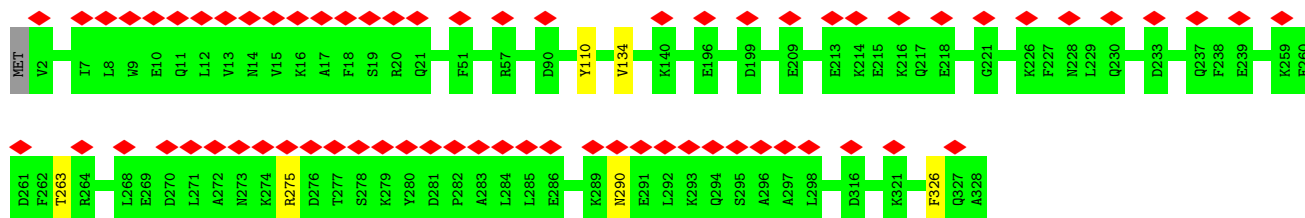
- Molecule 114: Sulphotransf domain-containing protein

Chain qg: 

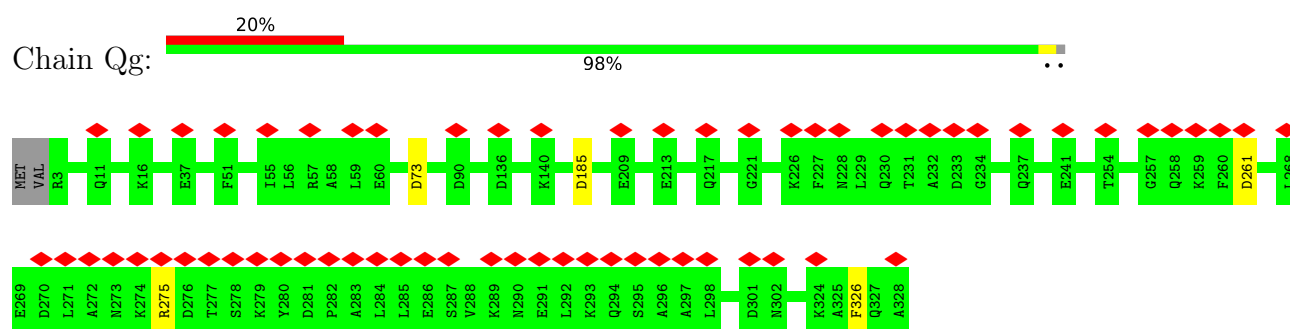


- Molecule 114: Sulphotransf domain-containing protein

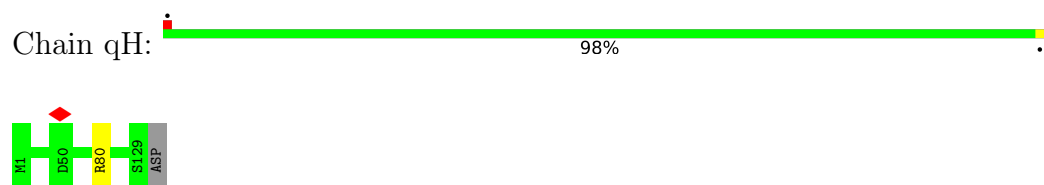
Chain QG: 



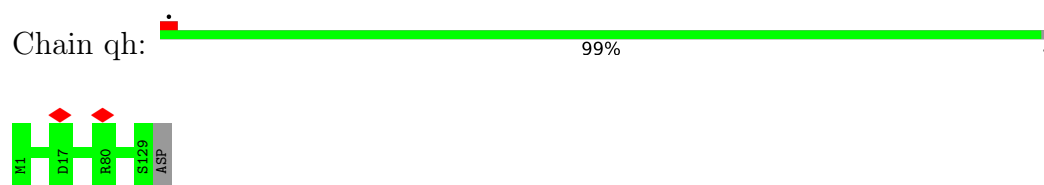
- Molecule 114: Sulphotransf domain-containing protein



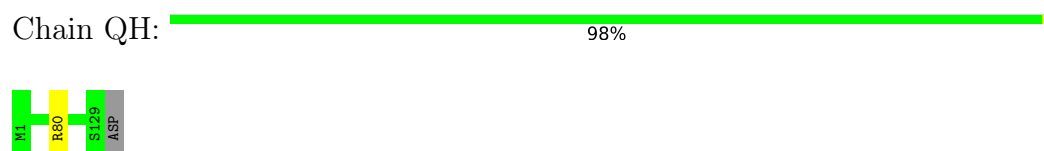
- Molecule 115: Transmembrane protein, putative



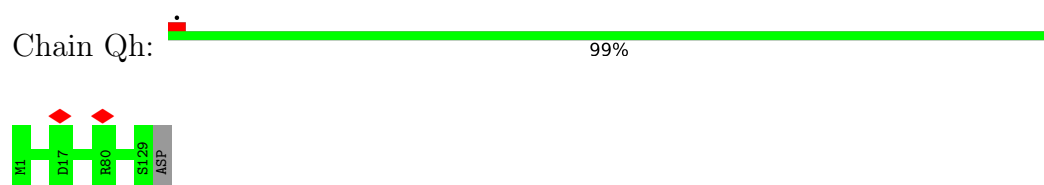
- Molecule 115: Transmembrane protein, putative



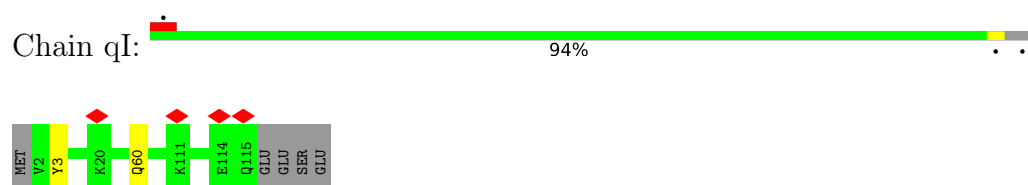
- Molecule 115: Transmembrane protein, putative



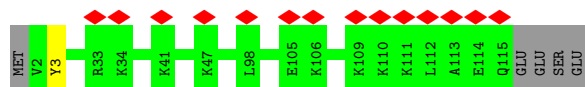
- Molecule 115: Transmembrane protein, putative



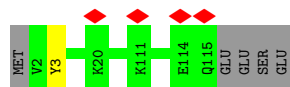
- Molecule 116: Transmembrane protein, putative



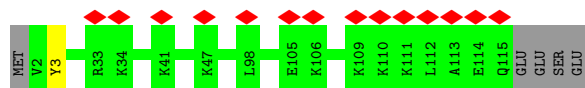
- Molecule 116: Transmembrane protein, putative



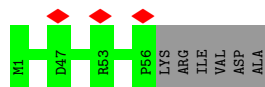
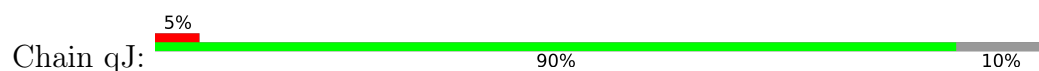
- Molecule 116: Transmembrane protein, putative



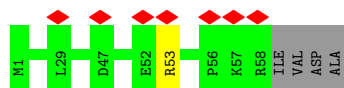
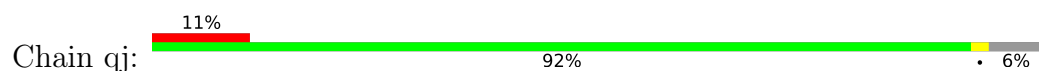
- Molecule 116: Transmembrane protein, putative



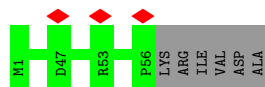
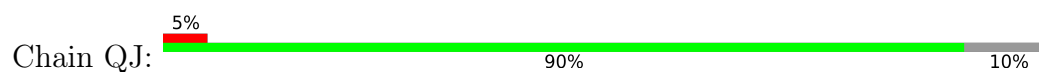
- Molecule 117: Transmembrane protein, putative



- Molecule 117: Transmembrane protein, putative



- Molecule 117: Transmembrane protein, putative

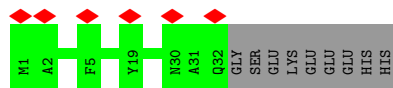
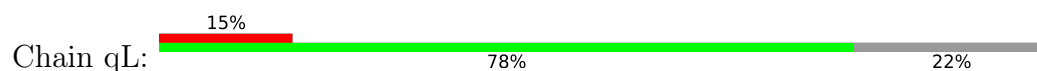


- Molecule 117: Transmembrane protein, putative

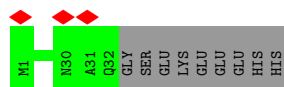
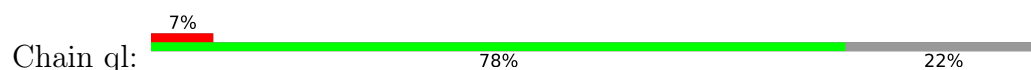




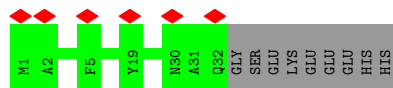
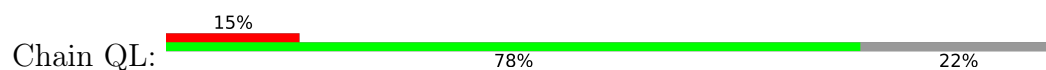
- Molecule 118: UQCRTT2



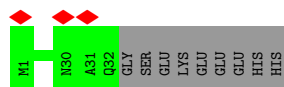
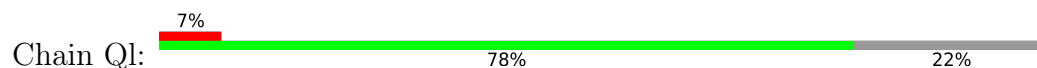
- Molecule 118: UQCRTT2



- Molecule 118: UQCRTT2



- Molecule 118: UQCRTT2



- Molecule 119: Unknown peptide



There are no outlier residues recorded for this chain.

- Molecule 119: Unknown peptide



There are no outlier residues recorded for this chain.

- Molecule 119: Unknown peptide



There are no outlier residues recorded for this chain.

- Molecule 119: Unknown peptide

Chain u2:  100%

There are no outlier residues recorded for this chain.

- Molecule 119: Unknown peptide

Chain U2:  100%

There are no outlier residues recorded for this chain.

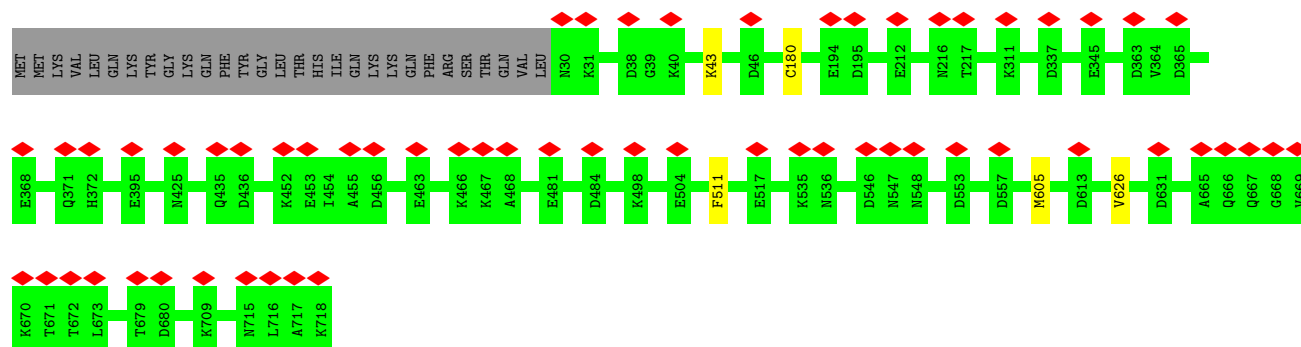
- Molecule 119: Unknown peptide

Chain QM:  100%

There are no outlier residues recorded for this chain.

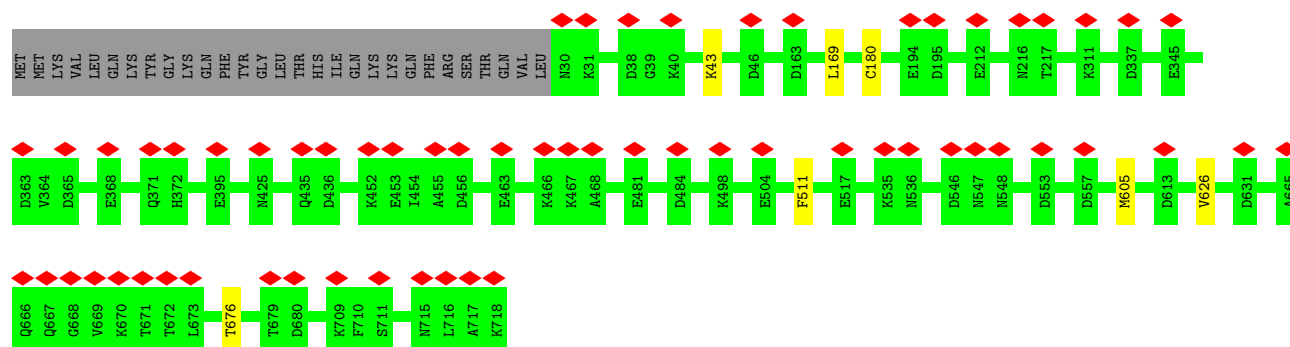
- Molecule 120: NADH-ubiquinone oxidoreductase 75 kDa subunit

Chain s1:  8% 95%



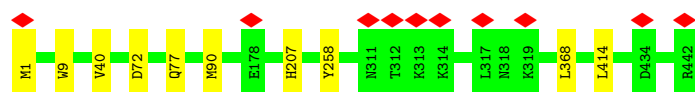
- Molecule 120: NADH-ubiquinone oxidoreductase 75 kDa subunit

Chain S1:  9% 95%

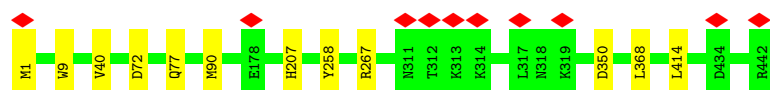


- Molecule 121: NADH dehydrogenase subunit 7

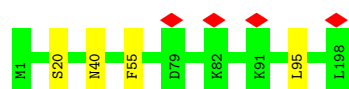
Chain s2:  98%



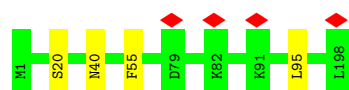
- Molecule 121: NADH dehydrogenase subunit 7



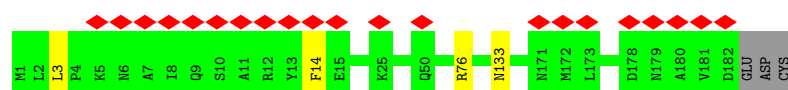
- Molecule 122: NADH dehydrogenase subunit 9



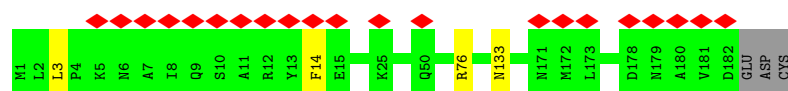
- Molecule 122: NADH dehydrogenase subunit 9



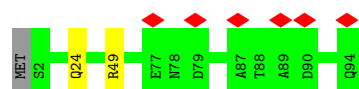
- Molecule 123: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



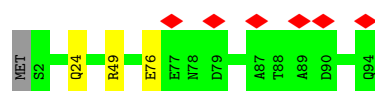
- Molecule 123: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



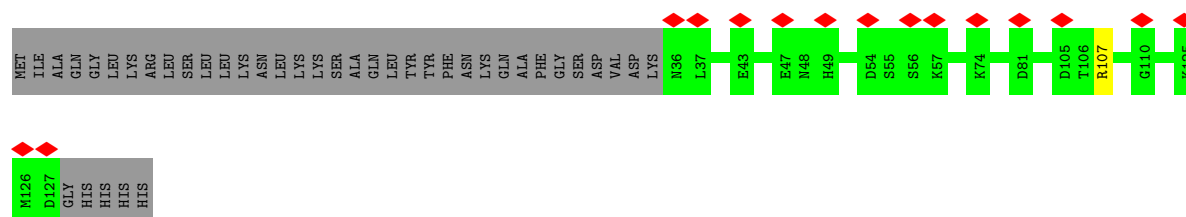
- Molecule 124: GRAM domain protein



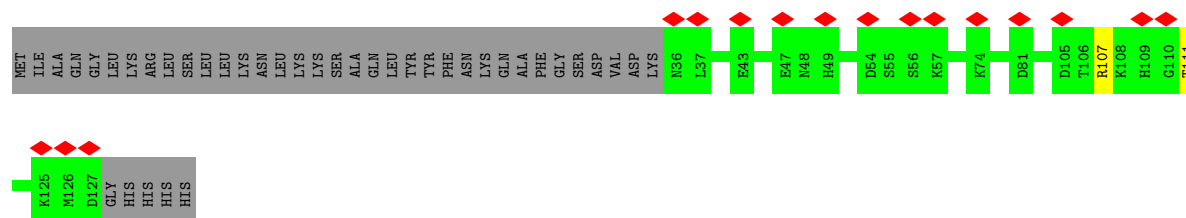
- Molecule 124: GRAM domain protein



- Molecule 125: Zinc-finger protein



- Molecule 125: Zinc-finger protein



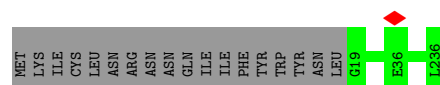
- Molecule 126: NADH dehydrogenase subunit 10



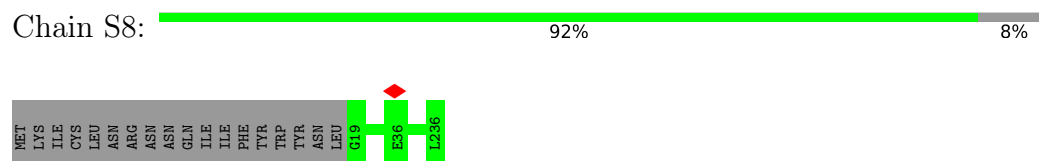
- Molecule 126: NADH dehydrogenase subunit 10



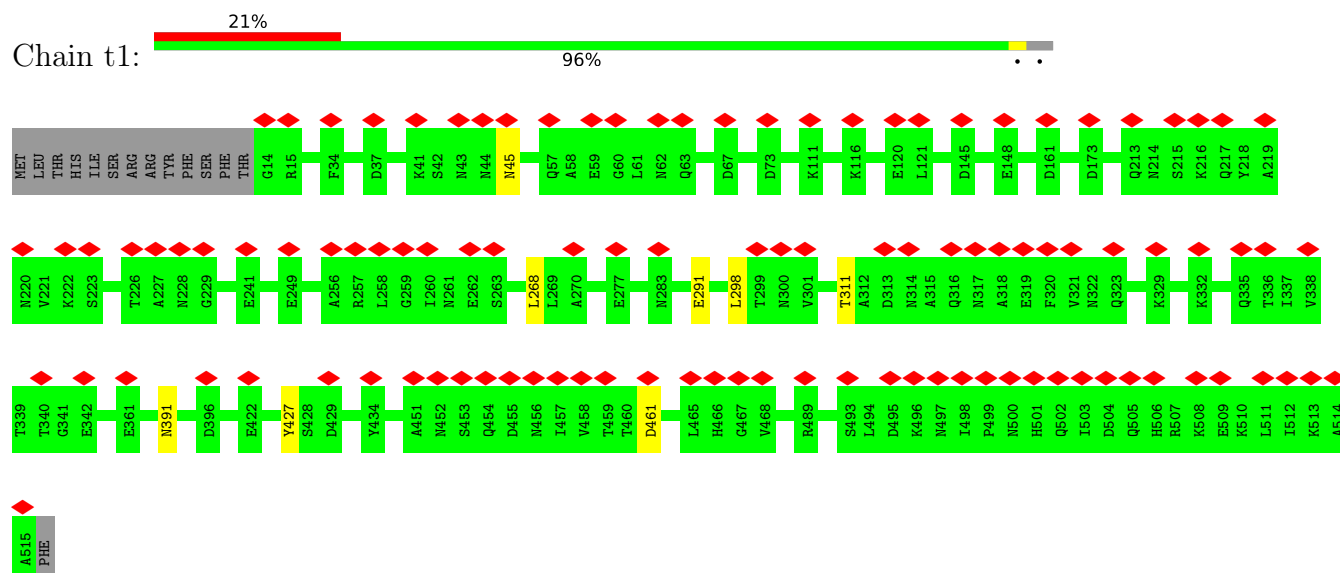
- Molecule 127: NADH-ubiquinone oxidoreductase 1, chain, putative



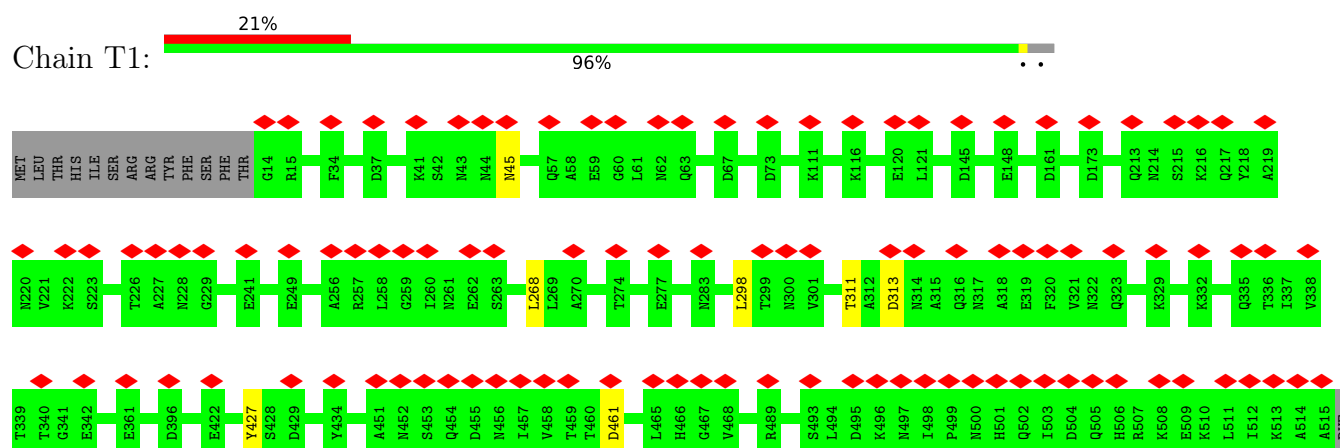
- Molecule 127: NADH-ubiquinone oxidoreductase 1, chain, putative



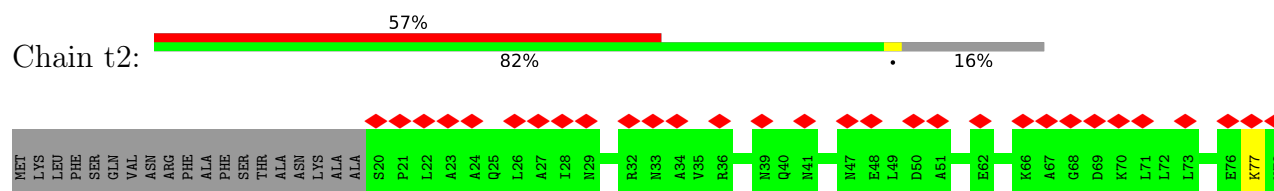
- Molecule 128: Lipid-A-disaccharide synthase

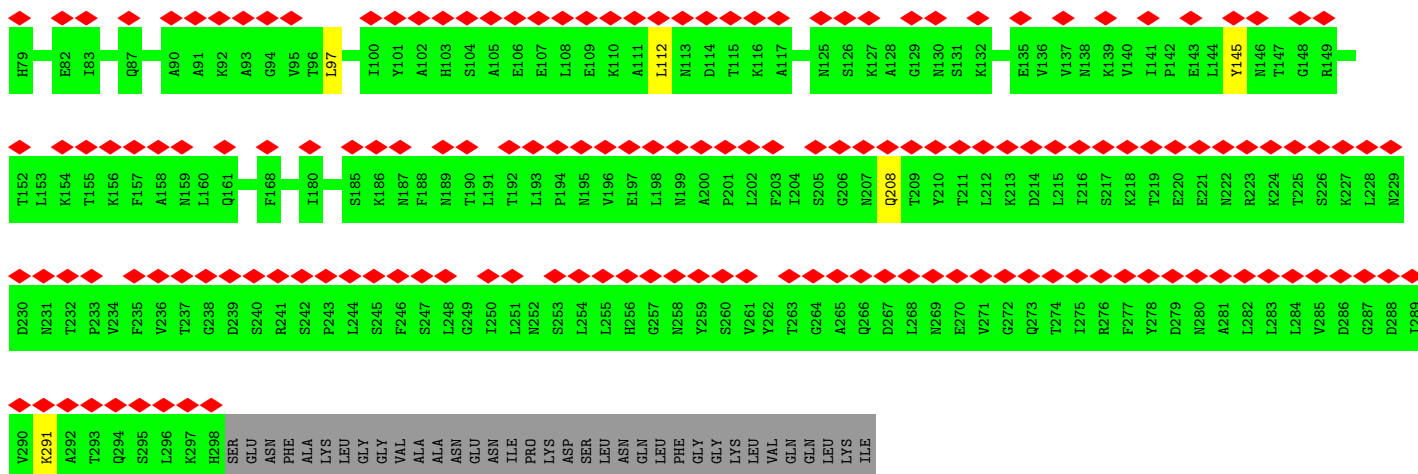


- Molecule 128: Lipid-A-disaccharide synthase



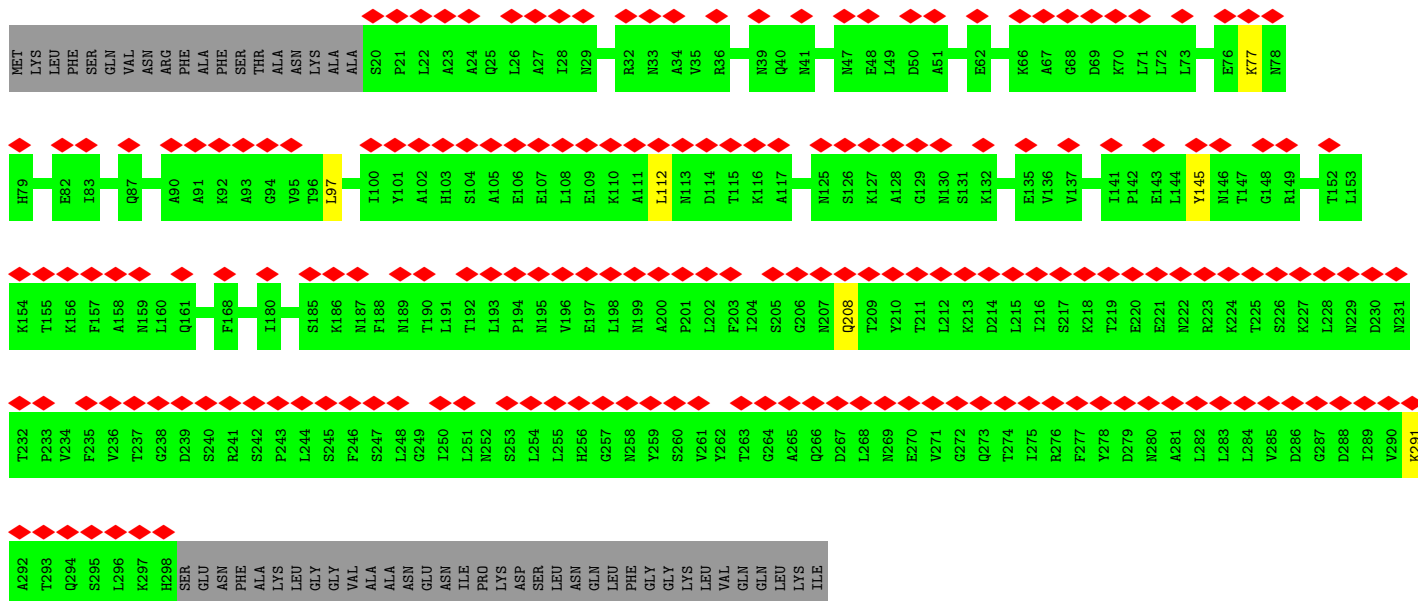
- Molecule 129: Acyl-CoA synthetase (AMP-forming)/AMP-acid ligase II





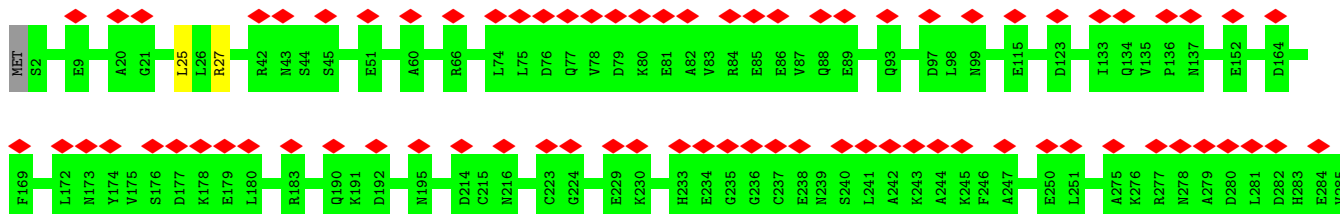
- Molecule 129: Acyl-CoA synthetase (AMP-forming)/AMP-acid ligase II

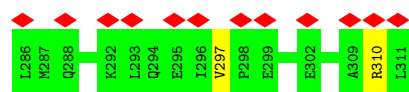
Chain T2: 57% 82% 16%



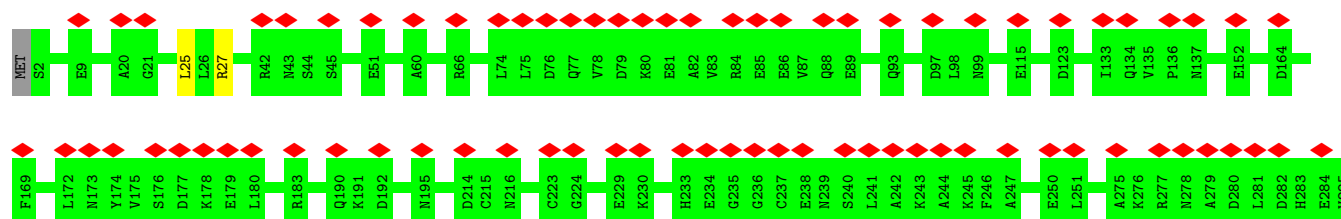
- Molecule 130: RNase III domain-containing protein

Chain t3: 28% 98%

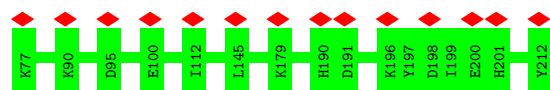
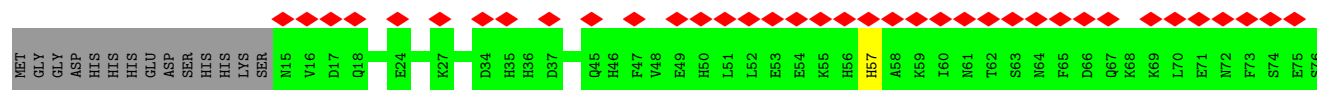




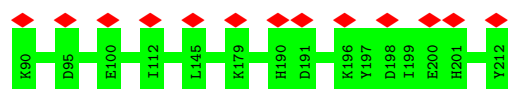
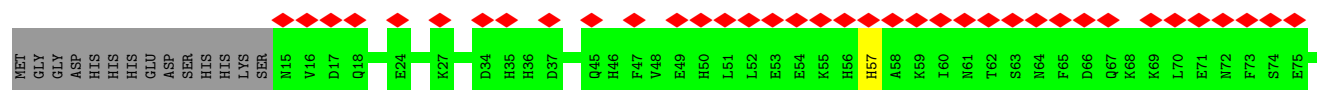
- Molecule 130: RNase III domain-containing protein



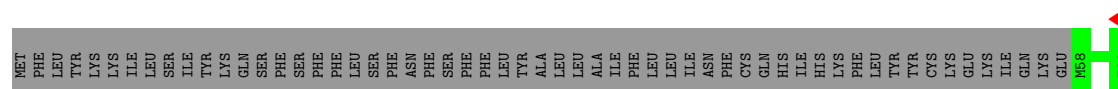
- Molecule 131: Transmembrane protein

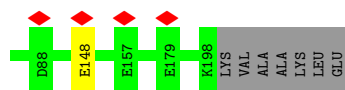


- Molecule 131: Transmembrane protein

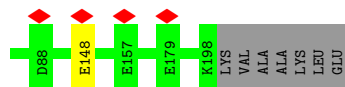
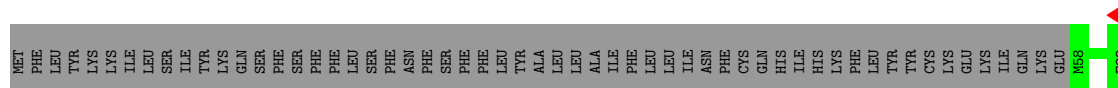


- Molecule 132: Transmembrane protein, putative

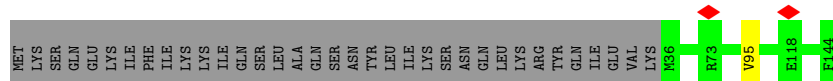
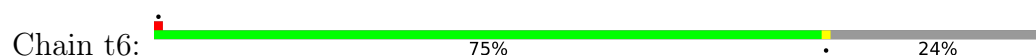




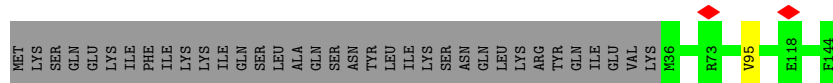
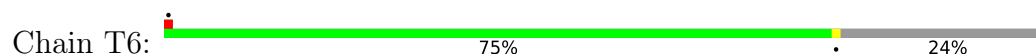
- Molecule 132: Transmembrane protein, putative



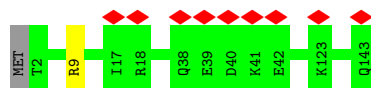
- Molecule 133: COX assembly mitochondrial protein



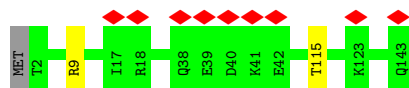
- Molecule 133: COX assembly mitochondrial protein



- Molecule 134: Transmembrane protein, putative

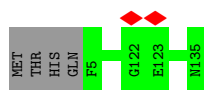


- Molecule 134: Transmembrane protein, putative

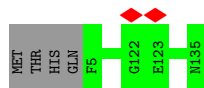


- Molecule 135: PH domain-containing protein

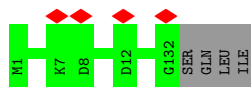




- Molecule 135: PH domain-containing protein



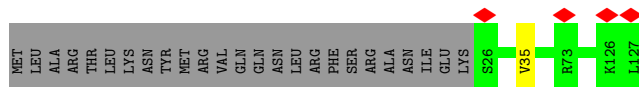
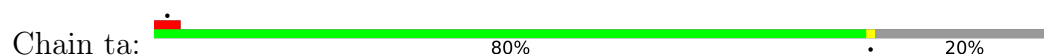
- Molecule 136: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



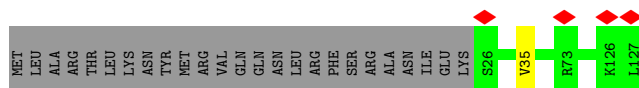
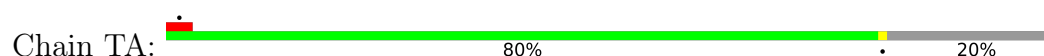
- Molecule 136: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



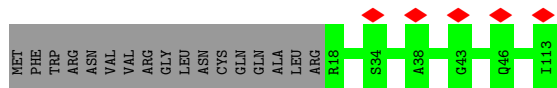
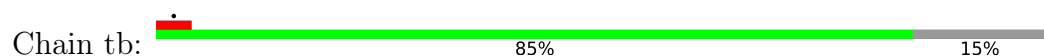
- Molecule 137: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4




- Molecule 137: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

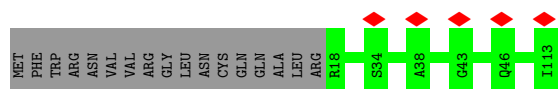


- Molecule 138: Transmembrane protein, putative



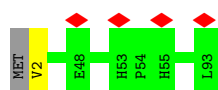
- Molecule 138: Transmembrane protein, putative

Chain TB:  85% 15%



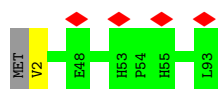
- Molecule 139: ATP synthase subunit e, mitochondrial

Chain tc:  98% ..



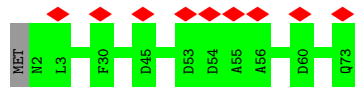
- Molecule 139: ATP synthase subunit e, mitochondrial

Chain TC:  98% ..



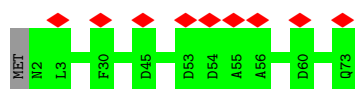
- Molecule 140: Transmembrane protein, putative

Chain td:  12% 99% .



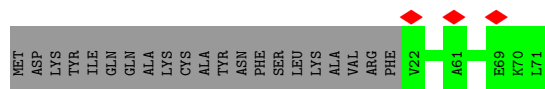
- Molecule 140: Transmembrane protein, putative

Chain TD:  12% 99% .



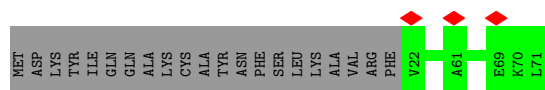
- Molecule 141: Transmembrane protein, putative

Chain te:  70% 30%

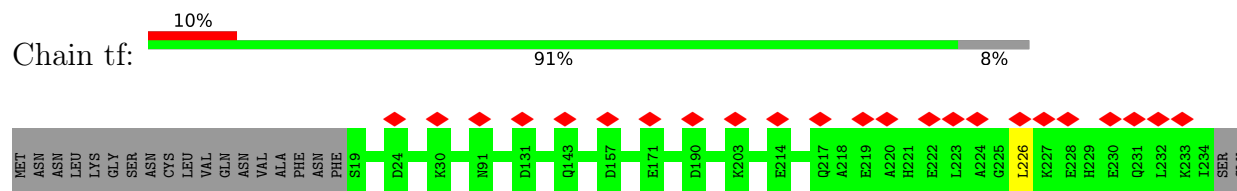


- Molecule 141: Transmembrane protein, putative

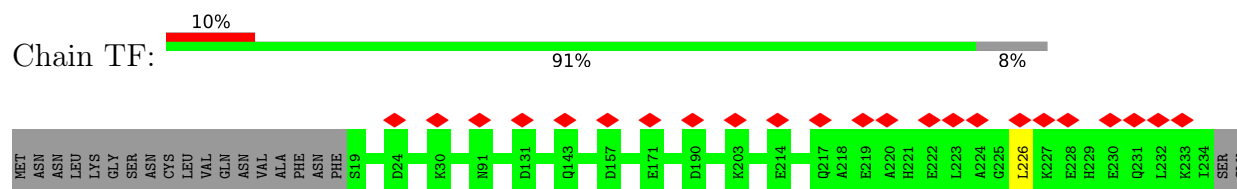
Chain TE:  70% 30%



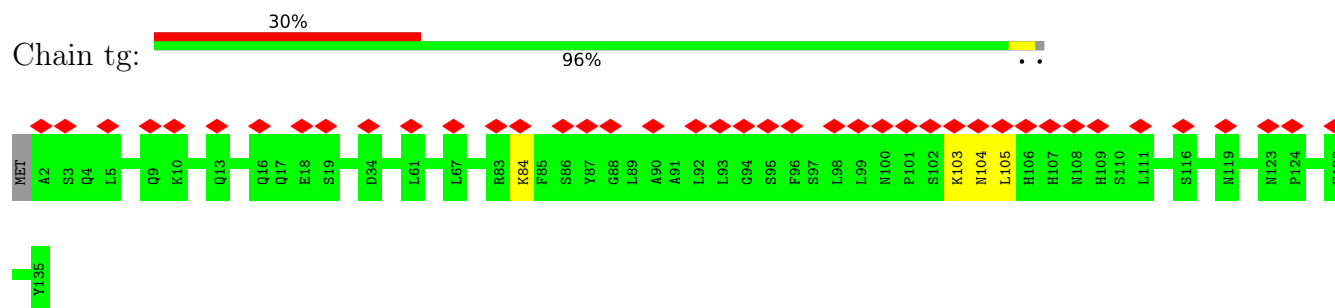
• Molecule 142: NDUTT15



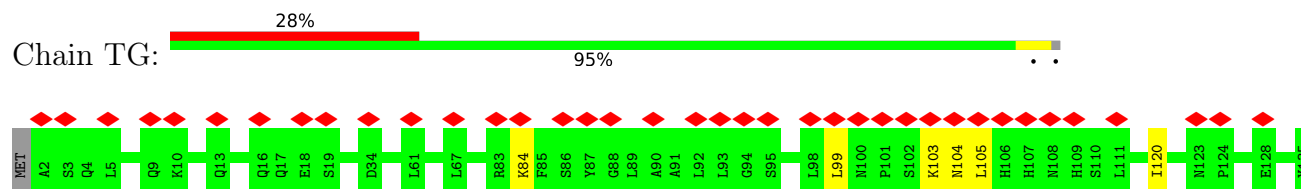
• Molecule 142: NDUTT15



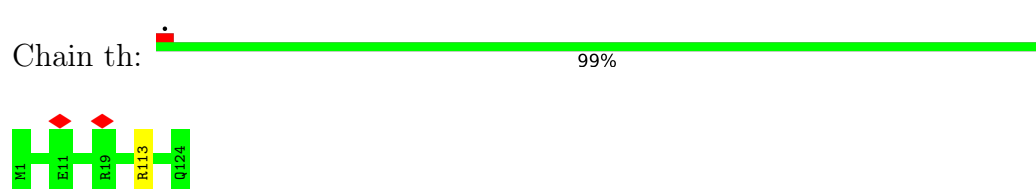
• Molecule 143: NDUTT16



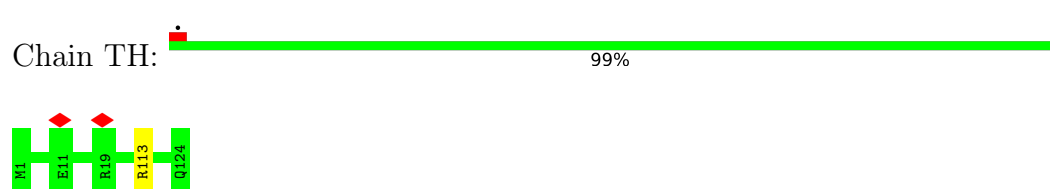
• Molecule 143: NDUTT16



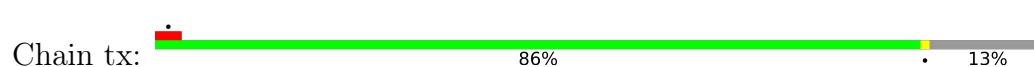
• Molecule 144: NDUTT17

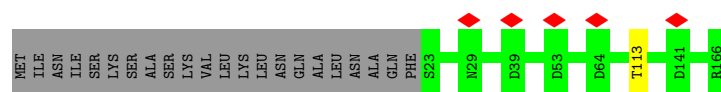


• Molecule 144: NDUTT17

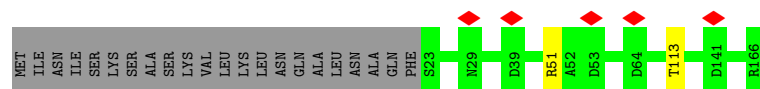


• Molecule 145: Thioredoxin

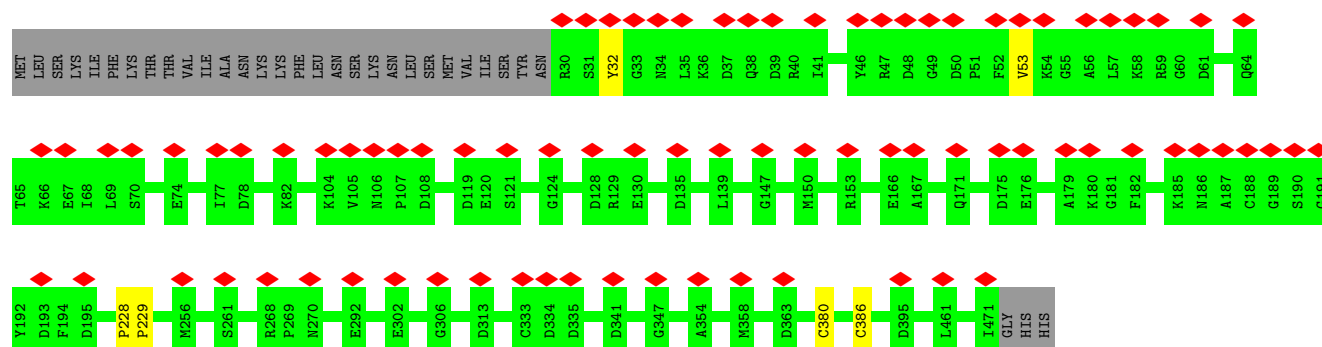




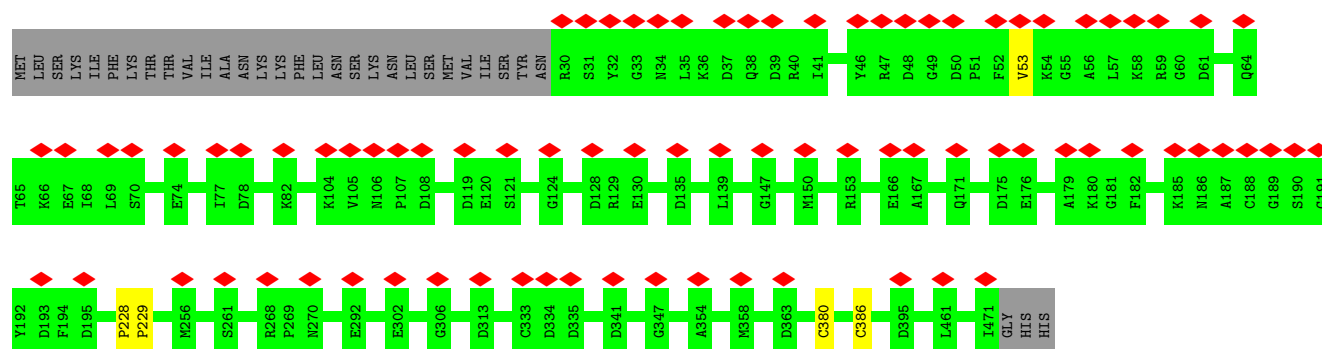
- Molecule 145: Thioredoxin



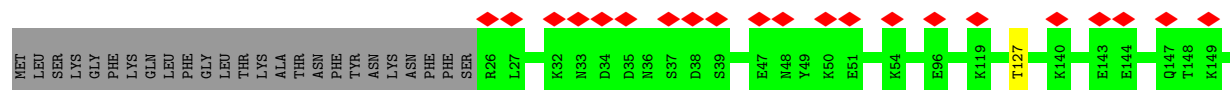
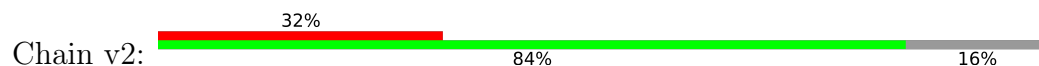
- Molecule 146: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

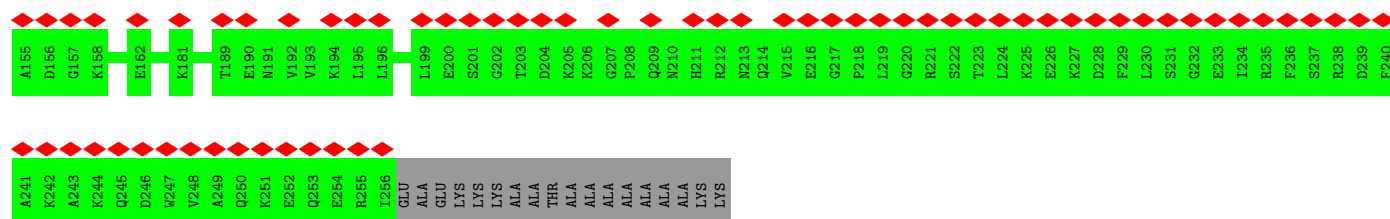


- Molecule 146: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

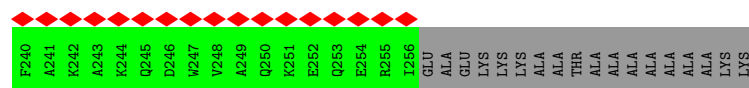
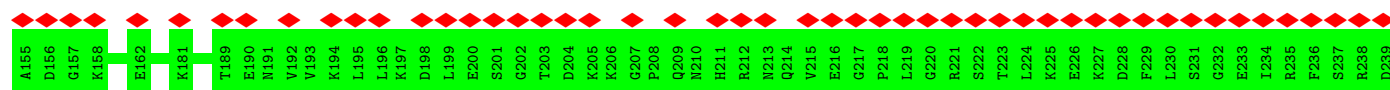
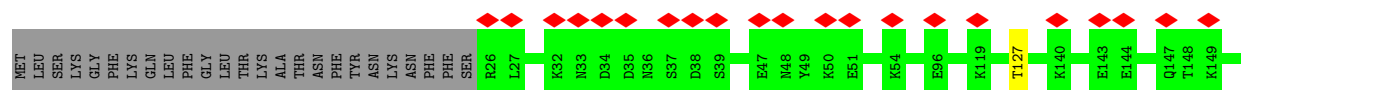
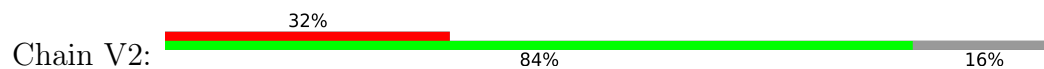


- Molecule 147: NADH-ubiquinone oxidoreductase 24 kDa subunit

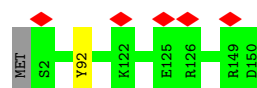




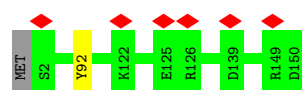
- Molecule 147: NADH-ubiquinone oxidoreductase 24 kDa subunit



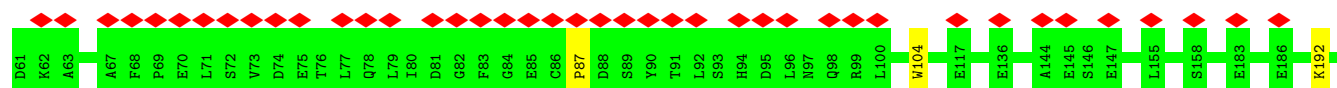
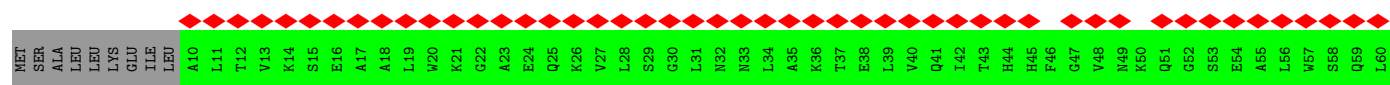
- Molecule 148: NADH-ubiquinone oxidoreductase complex I, 21 kDa subunit

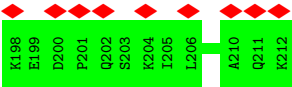


- Molecule 148: NADH-ubiquinone oxidoreductase complex I, 21 kDa subunit

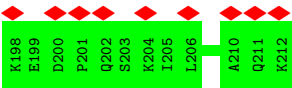
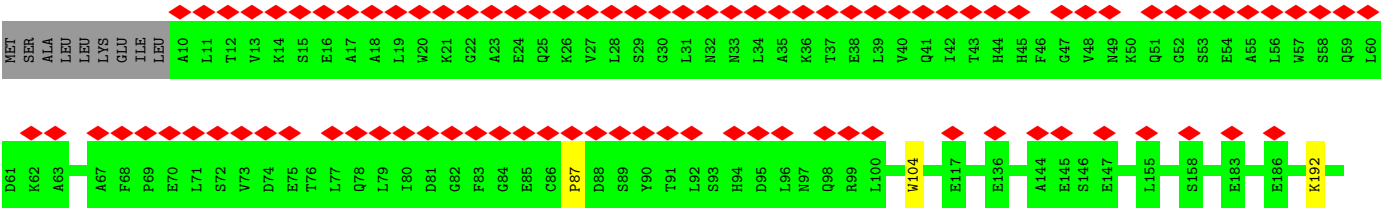
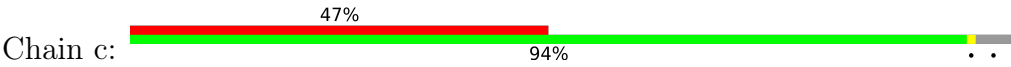


- Molecule 149: COXTT3





• Molecule 149: COXTT3



• Molecule 150: Unknown peptide



There are no outlier residues recorded for this chain.

• Molecule 150: Unknown peptide



There are no outlier residues recorded for this chain.

4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C2 | Depositor |
| Number of particles used | 97688 | 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 ($e^-/\text{\AA}^2$) | 61.5 | Depositor |
| Minimum defocus (nm) | 800 | Depositor |
| Maximum defocus (nm) | 2000 | Depositor |
| Magnification | 140000 | Depositor |
| Image detector | FEI FALCON IV (4k x 4k) | Depositor |
| Maximum map value | 60.050 | Depositor |
| Minimum map value | -23.470 | Depositor |
| Average map value | 0.005 | Depositor |
| Map value standard deviation | 1.045 | Depositor |
| Recommended contour level | 5.5 | Depositor |
| Map size (Å) | 781.2, 781.2, 781.2 | wwPDB |
| Map dimensions | 840, 840, 840 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.93, 0.93, 0.93 | Depositor |

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, ZN, FAD, HEC, HEA, 3PE, ZMP, SF4, NDP, U10, HEM, P5S, CDL, CU, TPO, FES, MG, SEP, PX2, ADP, PC1, F3S, T7X

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 | 1T | 0.25 | 0/546 | 0.39 | 0/735 |
| 1 | 1t | 0.25 | 0/546 | 0.38 | 0/735 |
| 2 | 2E | 0.25 | 0/2614 | 0.45 | 0/3553 |
| 2 | 2e | 0.25 | 0/2614 | 0.45 | 0/3553 |
| 3 | 2F | 0.27 | 0/1848 | 0.45 | 0/2500 |
| 3 | 2f | 0.27 | 0/1848 | 0.45 | 0/2500 |
| 4 | 2G | 0.26 | 0/1716 | 0.40 | 0/2317 |
| 4 | 2g | 0.26 | 0/1716 | 0.40 | 0/2317 |
| 5 | 2H | 0.25 | 0/812 | 0.42 | 0/1090 |
| 5 | 2h | 0.25 | 0/812 | 0.42 | 0/1090 |
| 6 | 2I | 0.28 | 0/930 | 0.42 | 0/1244 |
| 6 | 2i | 0.27 | 0/930 | 0.42 | 0/1244 |
| 7 | 2J | 0.27 | 0/866 | 0.39 | 0/1176 |
| 7 | 2j | 0.27 | 0/866 | 0.39 | 0/1176 |
| 8 | 2K | 0.30 | 0/821 | 0.46 | 0/1112 |
| 8 | 2k | 0.30 | 0/821 | 0.46 | 0/1112 |
| 9 | 2L | 0.27 | 0/738 | 0.43 | 0/990 |
| 9 | 2l | 0.27 | 0/738 | 0.43 | 0/990 |
| 10 | 2M | 0.25 | 0/660 | 0.48 | 0/895 |
| 10 | 2m | 0.26 | 0/660 | 0.47 | 0/895 |
| 11 | 2N | 0.28 | 0/521 | 0.49 | 0/708 |
| 11 | 2n | 0.28 | 0/521 | 0.49 | 0/708 |
| 12 | 2O | 0.28 | 0/367 | 0.45 | 0/496 |
| 12 | 2o | 0.28 | 0/367 | 0.45 | 0/496 |
| 13 | 2T | 0.24 | 0/574 | 0.43 | 0/772 |
| 13 | 2t | 0.24 | 0/574 | 0.43 | 0/772 |
| 14 | 3T | 0.25 | 0/662 | 0.42 | 0/888 |
| 14 | 3t | 0.25 | 0/662 | 0.42 | 0/888 |
| 15 | 4A | 0.25 | 0/836 | 0.47 | 0/1133 |
| 15 | 4a | 0.24 | 0/836 | 0.47 | 0/1133 |
| 16 | 4T | 0.26 | 0/491 | 0.41 | 0/662 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 16 | 4t | 0.26 | 0/491 | 0.41 | 0/662 |
| 17 | 5T | 0.26 | 0/514 | 0.41 | 0/693 |
| 17 | 5t | 0.26 | 0/514 | 0.41 | 0/693 |
| 18 | 6A | 0.26 | 0/1116 | 0.43 | 0/1512 |
| 18 | 6a | 0.26 | 0/1116 | 0.43 | 0/1512 |
| 19 | 6B | 0.26 | 0/1976 | 0.45 | 0/2673 |
| 19 | 6b | 0.26 | 0/1976 | 0.45 | 0/2673 |
| 20 | 6C | 0.28 | 0/926 | 0.48 | 0/1256 |
| 20 | 6c | 0.28 | 0/926 | 0.47 | 0/1256 |
| 21 | 6L | 0.26 | 0/649 | 0.42 | 0/871 |
| 21 | 6l | 0.25 | 0/649 | 0.42 | 0/871 |
| 22 | 6T | 0.25 | 0/573 | 0.38 | 0/770 |
| 22 | 6t | 0.25 | 0/573 | 0.39 | 0/770 |
| 23 | 7A | 0.26 | 0/1206 | 0.46 | 0/1631 |
| 23 | 7a | 0.26 | 0/1206 | 0.46 | 0/1631 |
| 24 | 7C | 0.25 | 0/1881 | 0.43 | 0/2558 |
| 24 | 7c | 0.25 | 0/1881 | 0.43 | 0/2558 |
| 25 | 7L | 0.25 | 0/1107 | 0.43 | 0/1505 |
| 25 | 7l | 0.25 | 0/1107 | 0.43 | 0/1505 |
| 26 | A | 0.26 | 0/3874 | 0.45 | 0/5273 |
| 26 | a | 0.26 | 0/3874 | 0.45 | 0/5273 |
| 27 | B | 0.24 | 0/3453 | 0.43 | 0/4671 |
| 27 | b | 0.24 | 0/3453 | 0.43 | 0/4671 |
| 28 | BP | 0.26 | 0/2988 | 0.47 | 0/4052 |
| 28 | bp | 0.26 | 0/2988 | 0.47 | 0/4052 |
| 29 | C1 | 0.27 | 0/5765 | 0.45 | 0/7819 |
| 29 | c1 | 0.27 | 0/5765 | 0.45 | 0/7819 |
| 30 | C2 | 0.25 | 0/5244 | 0.46 | 0/7107 |
| 30 | c2 | 0.25 | 0/5244 | 0.47 | 0/7107 |
| 31 | C3 | 0.27 | 0/5256 | 0.43 | 0/7142 |
| 31 | c3 | 0.27 | 0/5256 | 0.43 | 0/7142 |
| 32 | D | 0.26 | 0/2430 | 0.47 | 0/3303 |
| 32 | d | 0.26 | 0/2430 | 0.47 | 0/3303 |
| 33 | E | 0.25 | 0/3266 | 0.45 | 0/4435 |
| 33 | e | 0.25 | 0/3266 | 0.45 | 0/4435 |
| 34 | F | 0.25 | 0/2077 | 0.44 | 0/2824 |
| 34 | f | 0.25 | 0/2077 | 0.44 | 0/2824 |
| 35 | FS | 0.27 | 0/1562 | 0.46 | 0/2123 |
| 35 | fs | 0.27 | 0/1562 | 0.46 | 0/2123 |
| 36 | G | 0.26 | 0/2517 | 0.46 | 0/3433 |
| 36 | g | 0.26 | 0/2517 | 0.46 | 0/3433 |
| 37 | H | 0.26 | 0/2423 | 0.46 | 0/3279 |
| 37 | h | 0.26 | 0/2423 | 0.46 | 0/3279 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 38 | I | 0.25 | 0/2001 | 0.44 | 0/2702 |
| 38 | i | 0.25 | 0/2001 | 0.44 | 0/2702 |
| 39 | J | 0.24 | 0/1621 | 0.45 | 0/2201 |
| 39 | j | 0.24 | 0/1621 | 0.45 | 0/2201 |
| 40 | K | 0.24 | 0/1755 | 0.42 | 0/2376 |
| 40 | k | 0.24 | 0/1755 | 0.43 | 0/2376 |
| 41 | L | 0.26 | 0/1718 | 0.44 | 0/2333 |
| 41 | l | 0.26 | 0/1718 | 0.45 | 0/2333 |
| 42 | M | 0.26 | 0/1941 | 0.44 | 0/2637 |
| 42 | m | 0.26 | 0/1941 | 0.44 | 0/2637 |
| 43 | M1 | 0.26 | 0/2958 | 0.46 | 0/4013 |
| 43 | m1 | 0.26 | 0/2958 | 0.46 | 0/4013 |
| 44 | M2 | 0.25 | 0/2629 | 0.46 | 0/3564 |
| 44 | m2 | 0.25 | 0/2629 | 0.46 | 0/3564 |
| 45 | M3 | 0.26 | 0/2689 | 0.44 | 0/3657 |
| 45 | m3 | 0.26 | 0/2689 | 0.44 | 0/3657 |
| 46 | N | 0.26 | 0/1770 | 0.42 | 0/2391 |
| 46 | n | 0.26 | 0/1770 | 0.42 | 0/2391 |
| 47 | O | 0.25 | 0/1098 | 0.44 | 0/1477 |
| 47 | o | 0.25 | 0/1098 | 0.44 | 0/1477 |
| 48 | P | 0.25 | 0/1436 | 0.44 | 0/1941 |
| 48 | p | 0.25 | 0/1436 | 0.44 | 0/1941 |
| 49 | Q | 0.26 | 0/1478 | 0.46 | 0/2005 |
| 49 | q | 0.26 | 0/1478 | 0.46 | 0/2005 |
| 50 | R | 0.25 | 0/1441 | 0.43 | 0/1952 |
| 50 | r | 0.25 | 0/1441 | 0.43 | 0/1952 |
| 51 | S | 0.25 | 0/1409 | 0.44 | 0/1900 |
| 51 | s | 0.25 | 0/1409 | 0.43 | 0/1900 |
| 52 | SA | 0.25 | 0/4722 | 0.49 | 0/6385 |
| 52 | sa | 0.25 | 0/4722 | 0.49 | 0/6385 |
| 53 | SB | 0.25 | 0/2315 | 0.46 | 0/3136 |
| 53 | sb | 0.26 | 0/2315 | 0.46 | 0/3136 |
| 54 | SC | 0.27 | 0/493 | 0.47 | 0/664 |
| 54 | sc | 0.27 | 0/493 | 0.47 | 0/664 |
| 55 | SD | 0.28 | 0/404 | 0.40 | 0/542 |
| 55 | sd | 0.28 | 0/404 | 0.40 | 0/542 |
| 56 | T | 0.25 | 0/1359 | 0.44 | 0/1842 |
| 56 | t | 0.26 | 0/1359 | 0.45 | 0/1842 |
| 57 | U | 0.26 | 0/1335 | 0.45 | 0/1794 |
| 57 | u | 0.26 | 0/1335 | 0.45 | 0/1794 |
| 58 | V | 0.25 | 0/1277 | 0.46 | 0/1735 |
| 58 | v | 0.25 | 0/1277 | 0.46 | 0/1735 |
| 59 | VB | 0.26 | 0/4712 | 0.45 | 0/6357 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 59 | vb | 0.26 | 0/4712 | 0.45 | 0/6357 |
| 60 | W | 0.25 | 0/1136 | 0.45 | 0/1545 |
| 60 | w | 0.25 | 0/1136 | 0.45 | 0/1545 |
| 61 | X | 0.25 | 0/1043 | 0.43 | 0/1413 |
| 61 | x | 0.25 | 0/1043 | 0.43 | 0/1413 |
| 62 | Y | 0.27 | 0/882 | 0.45 | 0/1192 |
| 62 | y | 0.27 | 0/882 | 0.45 | 0/1192 |
| 63 | Y0 | 0.27 | 0/801 | 0.43 | 0/1087 |
| 63 | y0 | 0.27 | 0/801 | 0.43 | 0/1087 |
| 64 | Y5 | 0.27 | 0/1708 | 0.39 | 0/2306 |
| 64 | y5 | 0.27 | 0/1708 | 0.39 | 0/2306 |
| 65 | Y7 | 0.26 | 0/3012 | 0.40 | 0/4072 |
| 65 | y7 | 0.26 | 0/3012 | 0.40 | 0/4072 |
| 66 | Z | 0.25 | 0/737 | 0.45 | 0/995 |
| 66 | z | 0.25 | 0/737 | 0.44 | 0/995 |
| 67 | Z1 | 0.26 | 0/781 | 0.44 | 0/1053 |
| 67 | z1 | 0.26 | 0/781 | 0.44 | 0/1053 |
| 68 | 1B | 0.27 | 0/536 | 0.42 | 0/727 |
| 68 | 1b | 0.27 | 0/536 | 0.42 | 0/727 |
| 69 | 2B | 0.27 | 0/1520 | 0.40 | 0/2058 |
| 69 | 2b | 0.27 | 0/1520 | 0.39 | 0/2058 |
| 70 | 4L | 0.25 | 0/982 | 0.41 | 0/1335 |
| 70 | 4l | 0.25 | 0/982 | 0.41 | 0/1335 |
| 71 | 5B | 0.27 | 0/915 | 0.40 | 0/1224 |
| 71 | 5b | 0.27 | 0/915 | 0.40 | 0/1224 |
| 72 | A1 | 0.26 | 0/834 | 0.50 | 0/1132 |
| 72 | a1 | 0.26 | 0/834 | 0.50 | 0/1132 |
| 73 | A2 | 0.25 | 0/826 | 0.46 | 0/1116 |
| 73 | a2 | 0.25 | 0/826 | 0.46 | 0/1116 |
| 74 | A3 | 0.25 | 0/1115 | 0.45 | 0/1507 |
| 74 | a3 | 0.25 | 0/1115 | 0.45 | 0/1507 |
| 75 | A5 | 0.24 | 0/1336 | 0.44 | 0/1797 |
| 75 | a5 | 0.24 | 0/1336 | 0.44 | 0/1797 |
| 76 | A6 | 0.26 | 0/1459 | 0.47 | 0/1965 |
| 76 | a6 | 0.26 | 0/1459 | 0.47 | 0/1965 |
| 77 | A7 | 0.24 | 0/2408 | 0.46 | 0/3269 |
| 77 | a7 | 0.24 | 0/2408 | 0.46 | 0/3269 |
| 78 | A8 | 0.25 | 0/1099 | 0.40 | 0/1477 |
| 78 | a8 | 0.25 | 0/1099 | 0.41 | 0/1477 |
| 79 | A9 | 0.26 | 0/2807 | 0.45 | 0/3801 |
| 79 | a9 | 0.26 | 0/2807 | 0.45 | 0/3801 |
| 80 | AB | 0.24 | 0/942 | 0.42 | 0/1272 |
| 80 | ab | 0.24 | 0/942 | 0.42 | 0/1272 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 81 | AC | 0.25 | 0/822 | 0.45 | 0/1114 |
| 81 | ac | 0.25 | 0/822 | 0.45 | 0/1114 |
| 82 | AL | 0.24 | 0/1667 | 0.47 | 0/2256 |
| 82 | al | 0.24 | 0/1667 | 0.47 | 0/2256 |
| 83 | AM | 0.24 | 0/1379 | 0.48 | 0/1841 |
| 83 | am | 0.24 | 0/1379 | 0.48 | 0/1841 |
| 84 | AN | 0.25 | 0/1935 | 0.42 | 0/2616 |
| 84 | an | 0.25 | 0/1935 | 0.42 | 0/2616 |
| 85 | B2 | 0.25 | 0/991 | 0.45 | 1/1333 (0.1%) |
| 85 | b2 | 0.25 | 0/991 | 0.42 | 0/1333 |
| 86 | B3 | 0.24 | 0/621 | 0.47 | 0/840 |
| 86 | b3 | 0.25 | 0/621 | 0.47 | 0/840 |
| 87 | B4 | 0.26 | 0/1015 | 0.40 | 0/1381 |
| 87 | b4 | 0.27 | 0/1015 | 0.40 | 0/1381 |
| 88 | B6 | 0.26 | 0/623 | 0.40 | 0/850 |
| 88 | b6 | 0.26 | 0/623 | 0.40 | 0/850 |
| 89 | B7 | 0.25 | 0/968 | 0.41 | 0/1307 |
| 89 | b7 | 0.25 | 0/968 | 0.41 | 0/1307 |
| 90 | B8 | 0.25 | 0/1494 | 0.45 | 0/2016 |
| 90 | b8 | 0.25 | 0/1494 | 0.45 | 0/2016 |
| 91 | B9 | 0.26 | 0/1644 | 0.43 | 0/2224 |
| 91 | b9 | 0.26 | 0/1644 | 0.43 | 0/2224 |
| 92 | BL | 0.25 | 0/1489 | 0.47 | 0/2000 |
| 92 | bl | 0.25 | 0/1489 | 0.47 | 0/2000 |
| 93 | BM | 0.24 | 0/1351 | 0.42 | 0/1829 |
| 93 | bm | 0.24 | 0/1351 | 0.42 | 0/1829 |
| 94 | C4 | 0.27 | 0/873 | 0.45 | 0/1175 |
| 94 | c4 | 0.27 | 0/873 | 0.45 | 0/1175 |
| 95 | FX | 0.25 | 0/1186 | 0.49 | 0/1607 |
| 95 | fx | 0.25 | 0/1186 | 0.48 | 0/1607 |
| 96 | G1 | 0.25 | 0/1810 | 0.46 | 0/2465 |
| 96 | g1 | 0.26 | 0/1810 | 0.46 | 0/2465 |
| 97 | G2 | 0.25 | 0/1793 | 0.49 | 0/2438 |
| 97 | g2 | 0.25 | 0/1793 | 0.49 | 0/2438 |
| 98 | G3 | 0.26 | 0/2865 | 0.46 | 0/3877 |
| 98 | g3 | 0.26 | 0/2865 | 0.46 | 0/3877 |
| 99 | J1 | 0.25 | 0/2219 | 0.46 | 0/2988 |
| 99 | j1 | 0.25 | 0/2219 | 0.45 | 0/2988 |
| 100 | N1 | 0.26 | 0/2376 | 0.41 | 0/3234 |
| 100 | n1 | 0.26 | 0/2376 | 0.41 | 0/3234 |
| 101 | N2 | 0.27 | 0/3173 | 0.39 | 0/4312 |
| 101 | n2 | 0.27 | 0/3173 | 0.39 | 0/4312 |
| 102 | N3 | 0.27 | 0/1051 | 0.37 | 0/1429 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 102 | n3 | 0.27 | 0/1051 | 0.37 | 0/1429 |
| 103 | N4 | 0.27 | 0/4303 | 0.40 | 0/5844 |
| 103 | n4 | 0.27 | 0/4303 | 0.40 | 0/5844 |
| 104 | N5 | 0.27 | 0/6098 | 0.40 | 0/8297 |
| 104 | n5 | 0.27 | 0/6098 | 0.40 | 0/8297 |
| 105 | N6 | 0.27 | 0/2232 | 0.39 | 0/3035 |
| 105 | n6 | 0.27 | 0/2232 | 0.39 | 0/3035 |
| 106 | P1 | 0.26 | 0/1963 | 0.46 | 0/2658 |
| 106 | p1 | 0.26 | 0/1963 | 0.47 | 0/2658 |
| 107 | P2 | 0.26 | 0/1454 | 0.45 | 0/1970 |
| 107 | p2 | 0.26 | 0/1454 | 0.45 | 0/1970 |
| 108 | QA | 0.25 | 0/3569 | 0.45 | 0/4835 |
| 108 | Qa | 0.25 | 0/3569 | 0.45 | 0/4835 |
| 108 | qA | 0.25 | 0/3569 | 0.45 | 0/4835 |
| 108 | qa | 0.25 | 0/3569 | 0.45 | 0/4835 |
| 109 | QB | 0.26 | 0/3921 | 0.48 | 0/5325 |
| 109 | Qb | 0.25 | 0/3921 | 0.48 | 0/5325 |
| 109 | qB | 0.26 | 0/3921 | 0.48 | 0/5325 |
| 109 | qb | 0.26 | 0/3921 | 0.48 | 0/5325 |
| 110 | QC | 0.27 | 0/3715 | 0.42 | 0/5046 |
| 110 | Qc | 0.27 | 0/3706 | 0.41 | 0/5035 |
| 110 | qC | 0.27 | 0/3715 | 0.42 | 0/5046 |
| 110 | qc | 0.27 | 0/3706 | 0.41 | 0/5035 |
| 111 | QD | 0.27 | 0/2580 | 0.47 | 0/3491 |
| 111 | Qd | 0.27 | 0/2580 | 0.46 | 0/3491 |
| 111 | qD | 0.28 | 0/2580 | 0.47 | 0/3491 |
| 111 | qd | 0.27 | 0/2580 | 0.46 | 0/3491 |
| 112 | QE | 0.25 | 0/1588 | 0.48 | 0/2162 |
| 112 | Qe | 0.25 | 0/1499 | 0.47 | 0/2042 |
| 112 | qE | 0.25 | 0/1588 | 0.48 | 0/2162 |
| 112 | qe | 0.25 | 0/1499 | 0.47 | 0/2042 |
| 113 | QF | 0.24 | 0/716 | 0.45 | 0/969 |
| 113 | Qf | 0.24 | 0/641 | 0.44 | 0/866 |
| 113 | qF | 0.24 | 0/716 | 0.46 | 0/969 |
| 113 | qf | 0.24 | 0/641 | 0.44 | 0/866 |
| 114 | QG | 0.26 | 0/2845 | 0.47 | 0/3839 |
| 114 | Qg | 0.26 | 0/2838 | 0.46 | 0/3829 |
| 114 | qG | 0.26 | 0/2845 | 0.47 | 0/3839 |
| 114 | qg | 0.25 | 0/2838 | 0.46 | 0/3829 |
| 115 | QH | 0.26 | 0/1133 | 0.49 | 0/1524 |
| 115 | Qh | 0.26 | 0/1133 | 0.49 | 0/1524 |
| 115 | qH | 0.26 | 0/1133 | 0.49 | 0/1524 |
| 115 | qh | 0.26 | 0/1133 | 0.48 | 0/1524 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 116 | QI | 0.25 | 0/1005 | 0.40 | 0/1365 |
| 116 | Qi | 0.26 | 0/1005 | 0.40 | 0/1365 |
| 116 | qI | 0.25 | 0/1005 | 0.40 | 0/1365 |
| 116 | qi | 0.25 | 0/1005 | 0.40 | 0/1365 |
| 117 | QJ | 0.26 | 0/502 | 0.41 | 0/687 |
| 117 | Qj | 0.26 | 0/522 | 0.44 | 0/712 |
| 117 | qJ | 0.26 | 0/502 | 0.41 | 0/687 |
| 117 | qj | 0.26 | 0/522 | 0.44 | 0/712 |
| 118 | QL | 0.25 | 0/273 | 0.38 | 0/371 |
| 118 | Ql | 0.26 | 0/273 | 0.37 | 0/371 |
| 118 | qL | 0.25 | 0/273 | 0.39 | 0/371 |
| 118 | ql | 0.26 | 0/273 | 0.37 | 0/371 |
| 120 | S1 | 0.25 | 0/5518 | 0.47 | 0/7476 |
| 120 | s1 | 0.25 | 0/5518 | 0.47 | 0/7476 |
| 121 | S2 | 0.26 | 0/3680 | 0.47 | 0/4969 |
| 121 | s2 | 0.26 | 0/3680 | 0.47 | 0/4969 |
| 122 | S3 | 0.26 | 0/1718 | 0.44 | 0/2319 |
| 122 | s3 | 0.26 | 0/1718 | 0.44 | 0/2319 |
| 123 | S4 | 0.25 | 0/1543 | 0.48 | 0/2088 |
| 123 | s4 | 0.25 | 0/1543 | 0.48 | 0/2088 |
| 124 | S5 | 0.25 | 0/775 | 0.43 | 0/1048 |
| 124 | s5 | 0.26 | 0/775 | 0.43 | 0/1048 |
| 125 | S6 | 0.25 | 0/755 | 0.45 | 0/1022 |
| 125 | s6 | 0.25 | 0/755 | 0.44 | 0/1022 |
| 126 | S7 | 0.26 | 0/1311 | 0.50 | 0/1779 |
| 126 | s7 | 0.26 | 0/1311 | 0.50 | 0/1779 |
| 127 | S8 | 0.26 | 0/1867 | 0.47 | 0/2538 |
| 127 | s8 | 0.26 | 0/1867 | 0.47 | 0/2538 |
| 128 | T1 | 0.26 | 0/4153 | 0.44 | 0/5618 |
| 128 | t1 | 0.26 | 0/4153 | 0.44 | 0/5618 |
| 129 | T2 | 0.24 | 0/2224 | 0.44 | 0/3022 |
| 129 | t2 | 0.24 | 0/2224 | 0.44 | 0/3022 |
| 130 | T3 | 0.24 | 0/2527 | 0.43 | 0/3423 |
| 130 | t3 | 0.24 | 0/2527 | 0.43 | 0/3423 |
| 131 | T4 | 0.25 | 0/1689 | 0.41 | 0/2284 |
| 131 | t4 | 0.25 | 0/1689 | 0.41 | 0/2284 |
| 132 | T5 | 0.24 | 0/1163 | 0.46 | 0/1574 |
| 132 | t5 | 0.25 | 0/1163 | 0.46 | 0/1574 |
| 133 | T6 | 0.25 | 0/923 | 0.43 | 0/1239 |
| 133 | t6 | 0.25 | 0/923 | 0.43 | 0/1239 |
| 134 | T7 | 0.26 | 0/1223 | 0.45 | 0/1648 |
| 134 | t7 | 0.26 | 0/1223 | 0.45 | 0/1648 |
| 135 | T8 | 0.24 | 0/1112 | 0.44 | 0/1507 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 135 | t8 | 0.24 | 0/1112 | 0.44 | 0/1507 |
| 136 | T9 | 0.25 | 0/1088 | 0.46 | 0/1458 |
| 136 | t9 | 0.26 | 0/1088 | 0.46 | 0/1458 |
| 137 | TA | 0.26 | 0/877 | 0.42 | 0/1181 |
| 137 | ta | 0.26 | 0/877 | 0.42 | 0/1181 |
| 138 | TB | 0.27 | 0/825 | 0.44 | 0/1115 |
| 138 | tb | 0.27 | 0/825 | 0.44 | 0/1115 |
| 139 | TC | 0.26 | 0/811 | 0.44 | 0/1093 |
| 139 | tc | 0.26 | 0/811 | 0.44 | 0/1093 |
| 140 | TD | 0.24 | 0/634 | 0.45 | 0/855 |
| 140 | td | 0.24 | 0/634 | 0.45 | 0/855 |
| 141 | TE | 0.27 | 0/432 | 0.41 | 0/583 |
| 141 | te | 0.27 | 0/432 | 0.42 | 0/583 |
| 142 | TF | 0.24 | 0/1828 | 0.43 | 0/2472 |
| 142 | tf | 0.24 | 0/1828 | 0.43 | 0/2472 |
| 143 | TG | 0.24 | 0/1101 | 0.45 | 0/1486 |
| 143 | tg | 0.24 | 0/1101 | 0.44 | 0/1486 |
| 144 | TH | 0.25 | 0/1015 | 0.47 | 0/1366 |
| 144 | th | 0.25 | 0/1015 | 0.46 | 0/1366 |
| 145 | TX | 0.25 | 0/1235 | 0.45 | 0/1662 |
| 145 | tx | 0.25 | 0/1235 | 0.45 | 0/1662 |
| 146 | V1 | 0.25 | 0/3485 | 0.49 | 1/4713 (0.0%) |
| 146 | v1 | 0.25 | 0/3485 | 0.49 | 1/4713 (0.0%) |
| 147 | V2 | 0.24 | 0/1895 | 0.44 | 0/2559 |
| 147 | v2 | 0.24 | 0/1895 | 0.44 | 0/2559 |
| 148 | X1 | 0.26 | 0/1261 | 0.47 | 0/1698 |
| 148 | x1 | 0.26 | 0/1261 | 0.47 | 0/1698 |
| 149 | C | 0.24 | 0/1383 | 0.40 | 0/1880 |
| 149 | c | 0.24 | 0/1383 | 0.40 | 0/1880 |
| All | All | 0.26 | 0/556450 | 0.45 | 3/753536 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 146 | V1 | 0 | 1 |
| 146 | v1 | 0 | 1 |
| All | All | 0 | 2 |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 85 | B2 | 85 | LEU | CA-CB-CG | 6.86 | 131.08 | 115.30 |
| 146 | v1 | 229 | PRO | C-N-CA | -5.59 | 107.72 | 121.70 |
| 146 | V1 | 229 | PRO | C-N-CA | -5.52 | 107.91 | 121.70 |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 146 | V1 | 228 | PRO | Peptide |
| 146 | v1 | 228 | PRO | Peptide |

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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 | 1T | 68/72 (94%) | 68 (100%) | 0 | 0 | 100 | 100 |
| 1 | 1t | 68/72 (94%) | 68 (100%) | 0 | 0 | 100 | 100 |
| 2 | 2E | 319/322 (99%) | 300 (94%) | 19 (6%) | 0 | 100 | 100 |
| 2 | 2e | 319/322 (99%) | 300 (94%) | 19 (6%) | 0 | 100 | 100 |
| 3 | 2F | 215/296 (73%) | 206 (96%) | 9 (4%) | 0 | 100 | 100 |
| 3 | 2f | 215/296 (73%) | 206 (96%) | 9 (4%) | 0 | 100 | 100 |
| 4 | 2G | 196/198 (99%) | 189 (96%) | 7 (4%) | 0 | 100 | 100 |
| 4 | 2g | 196/198 (99%) | 189 (96%) | 7 (4%) | 0 | 100 | 100 |
| 5 | 2H | 98/195 (50%) | 92 (94%) | 6 (6%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 5 | 2h | 98/195 (50%) | 92 (94%) | 6 (6%) | 0 | 100 | 100 |
| 6 | 2I | 112/114 (98%) | 109 (97%) | 3 (3%) | 0 | 100 | 100 |
| 6 | 2i | 112/114 (98%) | 109 (97%) | 3 (3%) | 0 | 100 | 100 |
| 7 | 2J | 100/103 (97%) | 96 (96%) | 4 (4%) | 0 | 100 | 100 |
| 7 | 2j | 100/103 (97%) | 96 (96%) | 4 (4%) | 0 | 100 | 100 |
| 8 | 2K | 91/93 (98%) | 87 (96%) | 4 (4%) | 0 | 100 | 100 |
| 8 | 2k | 91/93 (98%) | 87 (96%) | 4 (4%) | 0 | 100 | 100 |
| 9 | 2L | 81/89 (91%) | 80 (99%) | 1 (1%) | 0 | 100 | 100 |
| 9 | 2l | 81/89 (91%) | 80 (99%) | 1 (1%) | 0 | 100 | 100 |
| 10 | 2M | 73/76 (96%) | 68 (93%) | 5 (7%) | 0 | 100 | 100 |
| 10 | 2m | 73/76 (96%) | 68 (93%) | 5 (7%) | 0 | 100 | 100 |
| 11 | 2N | 59/62 (95%) | 52 (88%) | 7 (12%) | 0 | 100 | 100 |
| 11 | 2n | 59/62 (95%) | 52 (88%) | 7 (12%) | 0 | 100 | 100 |
| 12 | 2O | 40/46 (87%) | 38 (95%) | 2 (5%) | 0 | 100 | 100 |
| 12 | 2o | 40/46 (87%) | 38 (95%) | 2 (5%) | 0 | 100 | 100 |
| 13 | 2T | 68/72 (94%) | 67 (98%) | 1 (2%) | 0 | 100 | 100 |
| 13 | 2t | 68/72 (94%) | 67 (98%) | 1 (2%) | 0 | 100 | 100 |
| 14 | 3T | 81/93 (87%) | 79 (98%) | 2 (2%) | 0 | 100 | 100 |
| 14 | 3t | 81/93 (87%) | 79 (98%) | 2 (2%) | 0 | 100 | 100 |
| 15 | 4A | 98/127 (77%) | 97 (99%) | 1 (1%) | 0 | 100 | 100 |
| 15 | 4a | 98/127 (77%) | 97 (99%) | 1 (1%) | 0 | 100 | 100 |
| 16 | 4T | 55/68 (81%) | 54 (98%) | 1 (2%) | 0 | 100 | 100 |
| 16 | 4t | 55/68 (81%) | 54 (98%) | 1 (2%) | 0 | 100 | 100 |
| 17 | 5T | 60/81 (74%) | 59 (98%) | 1 (2%) | 0 | 100 | 100 |
| 17 | 5t | 60/81 (74%) | 59 (98%) | 1 (2%) | 0 | 100 | 100 |
| 18 | 6A | 124/130 (95%) | 119 (96%) | 5 (4%) | 0 | 100 | 100 |
| 18 | 6a | 124/130 (95%) | 119 (96%) | 5 (4%) | 0 | 100 | 100 |
| 19 | 6B | 220/230 (96%) | 215 (98%) | 5 (2%) | 0 | 100 | 100 |
| 19 | 6b | 220/230 (96%) | 216 (98%) | 4 (2%) | 0 | 100 | 100 |
| 20 | 6C | 99/103 (96%) | 94 (95%) | 5 (5%) | 0 | 100 | 100 |
| 20 | 6c | 99/103 (96%) | 94 (95%) | 5 (5%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 21 | 6L | 75/88 (85%) | 74 (99%) | 1 (1%) | 0 | 100 | 100 |
| 21 | 6l | 75/88 (85%) | 74 (99%) | 1 (1%) | 0 | 100 | 100 |
| 22 | 6T | 68/72 (94%) | 67 (98%) | 1 (2%) | 0 | 100 | 100 |
| 22 | 6t | 68/72 (94%) | 67 (98%) | 1 (2%) | 0 | 100 | 100 |
| 23 | 7A | 131/133 (98%) | 128 (98%) | 3 (2%) | 0 | 100 | 100 |
| 23 | 7a | 131/133 (98%) | 128 (98%) | 3 (2%) | 0 | 100 | 100 |
| 24 | 7C | 208/236 (88%) | 199 (96%) | 9 (4%) | 0 | 100 | 100 |
| 24 | 7c | 208/236 (88%) | 199 (96%) | 9 (4%) | 0 | 100 | 100 |
| 25 | 7L | 129/990 (13%) | 116 (90%) | 13 (10%) | 0 | 100 | 100 |
| 25 | 7l | 129/990 (13%) | 116 (90%) | 13 (10%) | 0 | 100 | 100 |
| 26 | A | 447/490 (91%) | 429 (96%) | 18 (4%) | 0 | 100 | 100 |
| 26 | a | 447/490 (91%) | 431 (96%) | 16 (4%) | 0 | 100 | 100 |
| 27 | B | 422/473 (89%) | 411 (97%) | 10 (2%) | 1 (0%) | 44 | 67 |
| 27 | b | 422/473 (89%) | 408 (97%) | 14 (3%) | 0 | 100 | 100 |
| 28 | BP | 379/462 (82%) | 348 (92%) | 31 (8%) | 0 | 100 | 100 |
| 28 | bp | 379/462 (82%) | 349 (92%) | 30 (8%) | 0 | 100 | 100 |
| 29 | C1 | 672/688 (98%) | 648 (96%) | 24 (4%) | 0 | 100 | 100 |
| 29 | c1 | 672/688 (98%) | 648 (96%) | 24 (4%) | 0 | 100 | 100 |
| 30 | C2 | 595/604 (98%) | 572 (96%) | 23 (4%) | 0 | 100 | 100 |
| 30 | c2 | 595/604 (98%) | 573 (96%) | 22 (4%) | 0 | 100 | 100 |
| 31 | C3 | 580/594 (98%) | 557 (96%) | 23 (4%) | 0 | 100 | 100 |
| 31 | c3 | 580/594 (98%) | 558 (96%) | 22 (4%) | 0 | 100 | 100 |
| 32 | D | 287/402 (71%) | 278 (97%) | 9 (3%) | 0 | 100 | 100 |
| 32 | d | 287/402 (71%) | 279 (97%) | 8 (3%) | 0 | 100 | 100 |
| 33 | E | 382/385 (99%) | 362 (95%) | 20 (5%) | 0 | 100 | 100 |
| 33 | e | 382/385 (99%) | 365 (96%) | 17 (4%) | 0 | 100 | 100 |
| 34 | F | 241/348 (69%) | 239 (99%) | 2 (1%) | 0 | 100 | 100 |
| 34 | f | 241/348 (69%) | 239 (99%) | 2 (1%) | 0 | 100 | 100 |
| 35 | FS | 186/188 (99%) | 177 (95%) | 9 (5%) | 0 | 100 | 100 |
| 35 | fs | 186/188 (99%) | 177 (95%) | 9 (5%) | 0 | 100 | 100 |
| 36 | G | 291/318 (92%) | 282 (97%) | 9 (3%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 36 | g | 291/318 (92%) | 282 (97%) | 9 (3%) | 0 | 100 | 100 |
| 37 | H | 296/318 (93%) | 286 (97%) | 10 (3%) | 0 | 100 | 100 |
| 37 | h | 296/318 (93%) | 289 (98%) | 7 (2%) | 0 | 100 | 100 |
| 38 | I | 229/252 (91%) | 220 (96%) | 9 (4%) | 0 | 100 | 100 |
| 38 | i | 229/252 (91%) | 222 (97%) | 6 (3%) | 1 (0%) | 30 | 54 |
| 39 | J | 185/234 (79%) | 183 (99%) | 2 (1%) | 0 | 100 | 100 |
| 39 | j | 185/234 (79%) | 183 (99%) | 2 (1%) | 0 | 100 | 100 |
| 40 | K | 206/231 (89%) | 198 (96%) | 8 (4%) | 0 | 100 | 100 |
| 40 | k | 206/231 (89%) | 198 (96%) | 8 (4%) | 0 | 100 | 100 |
| 41 | L | 192/222 (86%) | 186 (97%) | 6 (3%) | 0 | 100 | 100 |
| 41 | l | 192/222 (86%) | 186 (97%) | 6 (3%) | 0 | 100 | 100 |
| 42 | M | 217/220 (99%) | 209 (96%) | 8 (4%) | 0 | 100 | 100 |
| 42 | m | 217/220 (99%) | 207 (95%) | 10 (5%) | 0 | 100 | 100 |
| 43 | M1 | 344/346 (99%) | 329 (96%) | 15 (4%) | 0 | 100 | 100 |
| 43 | m1 | 344/346 (99%) | 331 (96%) | 13 (4%) | 0 | 100 | 100 |
| 44 | M2 | 316/318 (99%) | 310 (98%) | 6 (2%) | 0 | 100 | 100 |
| 44 | m2 | 316/318 (99%) | 310 (98%) | 6 (2%) | 0 | 100 | 100 |
| 45 | M3 | 327/330 (99%) | 317 (97%) | 10 (3%) | 0 | 100 | 100 |
| 45 | m3 | 327/330 (99%) | 317 (97%) | 10 (3%) | 0 | 100 | 100 |
| 46 | N | 204/210 (97%) | 199 (98%) | 5 (2%) | 0 | 100 | 100 |
| 46 | n | 204/210 (97%) | 200 (98%) | 4 (2%) | 0 | 100 | 100 |
| 47 | O | 127/193 (66%) | 126 (99%) | 1 (1%) | 0 | 100 | 100 |
| 47 | o | 127/193 (66%) | 126 (99%) | 1 (1%) | 0 | 100 | 100 |
| 48 | P | 173/175 (99%) | 167 (96%) | 6 (4%) | 0 | 100 | 100 |
| 48 | p | 173/175 (99%) | 168 (97%) | 5 (3%) | 0 | 100 | 100 |
| 49 | Q | 171/173 (99%) | 169 (99%) | 2 (1%) | 0 | 100 | 100 |
| 49 | q | 171/173 (99%) | 169 (99%) | 2 (1%) | 0 | 100 | 100 |
| 50 | R | 170/173 (98%) | 167 (98%) | 3 (2%) | 0 | 100 | 100 |
| 50 | r | 170/173 (98%) | 167 (98%) | 3 (2%) | 0 | 100 | 100 |
| 51 | S | 167/170 (98%) | 163 (98%) | 4 (2%) | 0 | 100 | 100 |
| 51 | s | 167/170 (98%) | 163 (98%) | 4 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 52 | SA | 597/636 (94%) | 563 (94%) | 34 (6%) | 0 | 100 | 100 |
| 52 | sa | 597/636 (94%) | 565 (95%) | 32 (5%) | 0 | 100 | 100 |
| 53 | SB | 277/312 (89%) | 256 (92%) | 21 (8%) | 0 | 100 | 100 |
| 53 | sb | 277/312 (89%) | 256 (92%) | 21 (8%) | 0 | 100 | 100 |
| 54 | SC | 56/60 (93%) | 55 (98%) | 1 (2%) | 0 | 100 | 100 |
| 54 | sc | 56/60 (93%) | 55 (98%) | 1 (2%) | 0 | 100 | 100 |
| 55 | SD | 42/44 (96%) | 42 (100%) | 0 | 0 | 100 | 100 |
| 55 | sd | 42/44 (96%) | 42 (100%) | 0 | 0 | 100 | 100 |
| 56 | T | 154/158 (98%) | 150 (97%) | 4 (3%) | 0 | 100 | 100 |
| 56 | t | 154/158 (98%) | 150 (97%) | 4 (3%) | 0 | 100 | 100 |
| 57 | U | 151/154 (98%) | 148 (98%) | 3 (2%) | 0 | 100 | 100 |
| 57 | u | 151/154 (98%) | 148 (98%) | 3 (2%) | 0 | 100 | 100 |
| 58 | V | 144/149 (97%) | 138 (96%) | 6 (4%) | 0 | 100 | 100 |
| 58 | v | 144/149 (97%) | 138 (96%) | 6 (4%) | 0 | 100 | 100 |
| 59 | VB | 551/637 (86%) | 542 (98%) | 9 (2%) | 0 | 100 | 100 |
| 59 | vb | 551/637 (86%) | 542 (98%) | 9 (2%) | 0 | 100 | 100 |
| 60 | W | 121/124 (98%) | 116 (96%) | 5 (4%) | 0 | 100 | 100 |
| 60 | w | 121/124 (98%) | 116 (96%) | 5 (4%) | 0 | 100 | 100 |
| 61 | X | 120/122 (98%) | 120 (100%) | 0 | 0 | 100 | 100 |
| 61 | x | 120/122 (98%) | 120 (100%) | 0 | 0 | 100 | 100 |
| 62 | Y | 103/105 (98%) | 103 (100%) | 0 | 0 | 100 | 100 |
| 62 | y | 103/105 (98%) | 103 (100%) | 0 | 0 | 100 | 100 |
| 63 | Y0 | 87/89 (98%) | 86 (99%) | 1 (1%) | 0 | 100 | 100 |
| 63 | y0 | 87/89 (98%) | 86 (99%) | 1 (1%) | 0 | 100 | 100 |
| 64 | Y5 | 188/190 (99%) | 181 (96%) | 7 (4%) | 0 | 100 | 100 |
| 64 | y5 | 188/190 (99%) | 181 (96%) | 7 (4%) | 0 | 100 | 100 |
| 65 | Y7 | 339/453 (75%) | 326 (96%) | 13 (4%) | 0 | 100 | 100 |
| 65 | y7 | 339/453 (75%) | 325 (96%) | 14 (4%) | 0 | 100 | 100 |
| 66 | Z | 85/90 (94%) | 84 (99%) | 1 (1%) | 0 | 100 | 100 |
| 66 | z | 85/90 (94%) | 84 (99%) | 1 (1%) | 0 | 100 | 100 |
| 67 | Z1 | 95/100 (95%) | 95 (100%) | 0 | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 67 | z1 | 95/100 (95%) | 95 (100%) | 0 | 0 | 100 | 100 |
| 68 | 1B | 57/59 (97%) | 54 (95%) | 3 (5%) | 0 | 100 | 100 |
| 68 | 1b | 57/59 (97%) | 54 (95%) | 3 (5%) | 0 | 100 | 100 |
| 69 | 2B | 176/178 (99%) | 172 (98%) | 4 (2%) | 0 | 100 | 100 |
| 69 | 2b | 176/178 (99%) | 172 (98%) | 4 (2%) | 0 | 100 | 100 |
| 70 | 4L | 114/116 (98%) | 112 (98%) | 2 (2%) | 0 | 100 | 100 |
| 70 | 4l | 114/116 (98%) | 112 (98%) | 2 (2%) | 0 | 100 | 100 |
| 71 | 5B | 98/100 (98%) | 94 (96%) | 4 (4%) | 0 | 100 | 100 |
| 71 | 5b | 98/100 (98%) | 94 (96%) | 4 (4%) | 0 | 100 | 100 |
| 72 | A1 | 91/94 (97%) | 87 (96%) | 4 (4%) | 0 | 100 | 100 |
| 72 | a1 | 91/94 (97%) | 86 (94%) | 5 (6%) | 0 | 100 | 100 |
| 73 | A2 | 96/103 (93%) | 94 (98%) | 2 (2%) | 0 | 100 | 100 |
| 73 | a2 | 96/103 (93%) | 94 (98%) | 2 (2%) | 0 | 100 | 100 |
| 74 | A3 | 127/135 (94%) | 124 (98%) | 3 (2%) | 0 | 100 | 100 |
| 74 | a3 | 127/135 (94%) | 123 (97%) | 4 (3%) | 0 | 100 | 100 |
| 75 | A5 | 153/206 (74%) | 150 (98%) | 3 (2%) | 0 | 100 | 100 |
| 75 | a5 | 153/206 (74%) | 150 (98%) | 3 (2%) | 0 | 100 | 100 |
| 76 | A6 | 170/172 (99%) | 168 (99%) | 2 (1%) | 0 | 100 | 100 |
| 76 | a6 | 170/172 (99%) | 168 (99%) | 2 (1%) | 0 | 100 | 100 |
| 77 | A7 | 280/282 (99%) | 274 (98%) | 6 (2%) | 0 | 100 | 100 |
| 77 | a7 | 280/282 (99%) | 274 (98%) | 6 (2%) | 0 | 100 | 100 |
| 78 | A8 | 130/238 (55%) | 130 (100%) | 0 | 0 | 100 | 100 |
| 78 | a8 | 130/238 (55%) | 130 (100%) | 0 | 0 | 100 | 100 |
| 79 | A9 | 338/362 (93%) | 321 (95%) | 17 (5%) | 0 | 100 | 100 |
| 79 | a9 | 338/362 (93%) | 321 (95%) | 17 (5%) | 0 | 100 | 100 |
| 80 | AB | 110/138 (80%) | 109 (99%) | 1 (1%) | 0 | 100 | 100 |
| 80 | ab | 110/138 (80%) | 109 (99%) | 1 (1%) | 0 | 100 | 100 |
| 81 | AC | 96/133 (72%) | 93 (97%) | 3 (3%) | 0 | 100 | 100 |
| 81 | ac | 96/133 (72%) | 93 (97%) | 3 (3%) | 0 | 100 | 100 |
| 82 | AL | 191/194 (98%) | 181 (95%) | 10 (5%) | 0 | 100 | 100 |
| 82 | al | 191/194 (98%) | 182 (95%) | 9 (5%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 83 | AM | 158/175 (90%) | 155 (98%) | 3 (2%) | 0 | 100 | 100 |
| 83 | am | 158/175 (90%) | 155 (98%) | 3 (2%) | 0 | 100 | 100 |
| 84 | AN | 229/231 (99%) | 223 (97%) | 6 (3%) | 0 | 100 | 100 |
| 84 | an | 229/231 (99%) | 223 (97%) | 6 (3%) | 0 | 100 | 100 |
| 85 | B2 | 118/126 (94%) | 117 (99%) | 1 (1%) | 0 | 100 | 100 |
| 85 | b2 | 118/126 (94%) | 117 (99%) | 1 (1%) | 0 | 100 | 100 |
| 86 | B3 | 67/83 (81%) | 66 (98%) | 1 (2%) | 0 | 100 | 100 |
| 86 | b3 | 67/83 (81%) | 66 (98%) | 1 (2%) | 0 | 100 | 100 |
| 87 | B4 | 113/147 (77%) | 112 (99%) | 1 (1%) | 0 | 100 | 100 |
| 87 | b4 | 113/147 (77%) | 112 (99%) | 1 (1%) | 0 | 100 | 100 |
| 88 | B6 | 68/129 (53%) | 68 (100%) | 0 | 0 | 100 | 100 |
| 88 | b6 | 68/129 (53%) | 68 (100%) | 0 | 0 | 100 | 100 |
| 89 | B7 | 114/120 (95%) | 114 (100%) | 0 | 0 | 100 | 100 |
| 89 | b7 | 114/120 (95%) | 114 (100%) | 0 | 0 | 100 | 100 |
| 90 | B8 | 173/207 (84%) | 171 (99%) | 2 (1%) | 0 | 100 | 100 |
| 90 | b8 | 173/207 (84%) | 171 (99%) | 2 (1%) | 0 | 100 | 100 |
| 91 | B9 | 186/189 (98%) | 180 (97%) | 6 (3%) | 0 | 100 | 100 |
| 91 | b9 | 186/189 (98%) | 180 (97%) | 6 (3%) | 0 | 100 | 100 |
| 92 | BL | 173/188 (92%) | 167 (96%) | 6 (4%) | 0 | 100 | 100 |
| 92 | bl | 173/188 (92%) | 167 (96%) | 6 (4%) | 0 | 100 | 100 |
| 93 | BM | 162/214 (76%) | 156 (96%) | 6 (4%) | 0 | 100 | 100 |
| 93 | bm | 162/214 (76%) | 156 (96%) | 6 (4%) | 0 | 100 | 100 |
| 94 | C4 | 100/102 (98%) | 98 (98%) | 2 (2%) | 0 | 100 | 100 |
| 94 | c4 | 100/102 (98%) | 99 (99%) | 1 (1%) | 0 | 100 | 100 |
| 95 | FX | 144/172 (84%) | 139 (96%) | 5 (4%) | 0 | 100 | 100 |
| 95 | fx | 144/172 (84%) | 139 (96%) | 5 (4%) | 0 | 100 | 100 |
| 96 | G1 | 227/257 (88%) | 222 (98%) | 5 (2%) | 0 | 100 | 100 |
| 96 | g1 | 227/257 (88%) | 222 (98%) | 5 (2%) | 0 | 100 | 100 |
| 97 | G2 | 228/233 (98%) | 223 (98%) | 5 (2%) | 0 | 100 | 100 |
| 97 | g2 | 228/233 (98%) | 223 (98%) | 5 (2%) | 0 | 100 | 100 |
| 98 | G3 | 344/346 (99%) | 335 (97%) | 9 (3%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 98 | g3 | 344/346 (99%) | 335 (97%) | 9 (3%) | 0 | 100 | 100 |
| 99 | J1 | 259/317 (82%) | 255 (98%) | 4 (2%) | 0 | 100 | 100 |
| 99 | j1 | 259/317 (82%) | 255 (98%) | 4 (2%) | 0 | 100 | 100 |
| 100 | N1 | 281/284 (99%) | 269 (96%) | 11 (4%) | 1 (0%) | 30 | 54 |
| 100 | n1 | 281/284 (99%) | 268 (95%) | 12 (4%) | 1 (0%) | 30 | 54 |
| 101 | N2 | 358/360 (99%) | 348 (97%) | 10 (3%) | 0 | 100 | 100 |
| 101 | n2 | 358/360 (99%) | 350 (98%) | 8 (2%) | 0 | 100 | 100 |
| 102 | N3 | 118/121 (98%) | 114 (97%) | 4 (3%) | 0 | 100 | 100 |
| 102 | n3 | 118/121 (98%) | 113 (96%) | 5 (4%) | 0 | 100 | 100 |
| 103 | N4 | 503/505 (100%) | 495 (98%) | 8 (2%) | 0 | 100 | 100 |
| 103 | n4 | 503/505 (100%) | 496 (99%) | 7 (1%) | 0 | 100 | 100 |
| 104 | N5 | 707/750 (94%) | 677 (96%) | 30 (4%) | 0 | 100 | 100 |
| 104 | n5 | 707/750 (94%) | 678 (96%) | 29 (4%) | 0 | 100 | 100 |
| 105 | N6 | 253/255 (99%) | 245 (97%) | 8 (3%) | 0 | 100 | 100 |
| 105 | n6 | 253/255 (99%) | 245 (97%) | 8 (3%) | 0 | 100 | 100 |
| 106 | P1 | 228/251 (91%) | 218 (96%) | 10 (4%) | 0 | 100 | 100 |
| 106 | p1 | 228/251 (91%) | 219 (96%) | 9 (4%) | 0 | 100 | 100 |
| 107 | P2 | 165/189 (87%) | 160 (97%) | 5 (3%) | 0 | 100 | 100 |
| 107 | p2 | 165/189 (87%) | 160 (97%) | 5 (3%) | 0 | 100 | 100 |
| 108 | QA | 450/482 (93%) | 437 (97%) | 13 (3%) | 0 | 100 | 100 |
| 108 | Qa | 450/482 (93%) | 434 (96%) | 16 (4%) | 0 | 100 | 100 |
| 108 | qA | 450/482 (93%) | 438 (97%) | 12 (3%) | 0 | 100 | 100 |
| 108 | qa | 450/482 (93%) | 433 (96%) | 17 (4%) | 0 | 100 | 100 |
| 109 | QB | 478/513 (93%) | 463 (97%) | 15 (3%) | 0 | 100 | 100 |
| 109 | Qb | 478/513 (93%) | 454 (95%) | 24 (5%) | 0 | 100 | 100 |
| 109 | qB | 478/513 (93%) | 463 (97%) | 15 (3%) | 0 | 100 | 100 |
| 109 | qb | 478/513 (93%) | 453 (95%) | 25 (5%) | 0 | 100 | 100 |
| 110 | QC | 424/426 (100%) | 404 (95%) | 20 (5%) | 0 | 100 | 100 |
| 110 | Qc | 423/426 (99%) | 405 (96%) | 18 (4%) | 0 | 100 | 100 |
| 110 | qC | 424/426 (100%) | 405 (96%) | 19 (4%) | 0 | 100 | 100 |
| 110 | qc | 423/426 (99%) | 405 (96%) | 18 (4%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 111 | QD | 293/319 (92%) | 279 (95%) | 14 (5%) | 0 | 100 | 100 |
| 111 | Qd | 293/319 (92%) | 276 (94%) | 17 (6%) | 0 | 100 | 100 |
| 111 | qD | 293/319 (92%) | 282 (96%) | 11 (4%) | 0 | 100 | 100 |
| 111 | qd | 293/319 (92%) | 275 (94%) | 18 (6%) | 0 | 100 | 100 |
| 112 | QE | 226/269 (84%) | 216 (96%) | 10 (4%) | 0 | 100 | 100 |
| 112 | Qe | 215/269 (80%) | 204 (95%) | 11 (5%) | 0 | 100 | 100 |
| 112 | qE | 226/269 (84%) | 216 (96%) | 10 (4%) | 0 | 100 | 100 |
| 112 | qe | 215/269 (80%) | 205 (95%) | 10 (5%) | 0 | 100 | 100 |
| 113 | QF | 87/90 (97%) | 87 (100%) | 0 | 0 | 100 | 100 |
| 113 | Qf | 78/90 (87%) | 76 (97%) | 2 (3%) | 0 | 100 | 100 |
| 113 | qF | 87/90 (97%) | 87 (100%) | 0 | 0 | 100 | 100 |
| 113 | qf | 78/90 (87%) | 76 (97%) | 2 (3%) | 0 | 100 | 100 |
| 114 | QG | 325/328 (99%) | 313 (96%) | 12 (4%) | 0 | 100 | 100 |
| 114 | Qg | 324/328 (99%) | 316 (98%) | 8 (2%) | 0 | 100 | 100 |
| 114 | qG | 325/328 (99%) | 312 (96%) | 13 (4%) | 0 | 100 | 100 |
| 114 | qg | 324/328 (99%) | 316 (98%) | 8 (2%) | 0 | 100 | 100 |
| 115 | QH | 127/130 (98%) | 124 (98%) | 3 (2%) | 0 | 100 | 100 |
| 115 | Qh | 127/130 (98%) | 120 (94%) | 7 (6%) | 0 | 100 | 100 |
| 115 | qH | 127/130 (98%) | 123 (97%) | 4 (3%) | 0 | 100 | 100 |
| 115 | qh | 127/130 (98%) | 120 (94%) | 7 (6%) | 0 | 100 | 100 |
| 116 | QI | 112/119 (94%) | 108 (96%) | 4 (4%) | 0 | 100 | 100 |
| 116 | Qi | 112/119 (94%) | 111 (99%) | 1 (1%) | 0 | 100 | 100 |
| 116 | qI | 112/119 (94%) | 108 (96%) | 4 (4%) | 0 | 100 | 100 |
| 116 | qi | 112/119 (94%) | 110 (98%) | 2 (2%) | 0 | 100 | 100 |
| 117 | QJ | 54/62 (87%) | 54 (100%) | 0 | 0 | 100 | 100 |
| 117 | Qj | 56/62 (90%) | 53 (95%) | 3 (5%) | 0 | 100 | 100 |
| 117 | qJ | 54/62 (87%) | 54 (100%) | 0 | 0 | 100 | 100 |
| 117 | qj | 56/62 (90%) | 54 (96%) | 2 (4%) | 0 | 100 | 100 |
| 118 | QL | 30/41 (73%) | 30 (100%) | 0 | 0 | 100 | 100 |
| 118 | Ql | 30/41 (73%) | 30 (100%) | 0 | 0 | 100 | 100 |
| 118 | qL | 30/41 (73%) | 30 (100%) | 0 | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 118 | ql | 30/41 (73%) | 30 (100%) | 0 | 0 | 100 | 100 |
| 120 | S1 | 687/718 (96%) | 661 (96%) | 26 (4%) | 0 | 100 | 100 |
| 120 | s1 | 687/718 (96%) | 662 (96%) | 25 (4%) | 0 | 100 | 100 |
| 121 | S2 | 440/442 (100%) | 424 (96%) | 16 (4%) | 0 | 100 | 100 |
| 121 | s2 | 440/442 (100%) | 423 (96%) | 17 (4%) | 0 | 100 | 100 |
| 122 | S3 | 196/198 (99%) | 193 (98%) | 3 (2%) | 0 | 100 | 100 |
| 122 | s3 | 196/198 (99%) | 193 (98%) | 3 (2%) | 0 | 100 | 100 |
| 123 | S4 | 180/185 (97%) | 172 (96%) | 8 (4%) | 0 | 100 | 100 |
| 123 | s4 | 180/185 (97%) | 172 (96%) | 8 (4%) | 0 | 100 | 100 |
| 124 | S5 | 91/94 (97%) | 87 (96%) | 4 (4%) | 0 | 100 | 100 |
| 124 | s5 | 91/94 (97%) | 86 (94%) | 5 (6%) | 0 | 100 | 100 |
| 125 | S6 | 90/132 (68%) | 84 (93%) | 6 (7%) | 0 | 100 | 100 |
| 125 | s6 | 90/132 (68%) | 85 (94%) | 5 (6%) | 0 | 100 | 100 |
| 126 | S7 | 159/162 (98%) | 152 (96%) | 7 (4%) | 0 | 100 | 100 |
| 126 | s7 | 159/162 (98%) | 151 (95%) | 8 (5%) | 0 | 100 | 100 |
| 127 | S8 | 216/236 (92%) | 214 (99%) | 2 (1%) | 0 | 100 | 100 |
| 127 | s8 | 216/236 (92%) | 214 (99%) | 2 (1%) | 0 | 100 | 100 |
| 128 | T1 | 500/516 (97%) | 482 (96%) | 18 (4%) | 0 | 100 | 100 |
| 128 | t1 | 500/516 (97%) | 481 (96%) | 19 (4%) | 0 | 100 | 100 |
| 129 | T2 | 277/333 (83%) | 268 (97%) | 8 (3%) | 1 (0%) | 30 | 54 |
| 129 | t2 | 277/333 (83%) | 267 (96%) | 9 (3%) | 1 (0%) | 30 | 54 |
| 130 | T3 | 308/311 (99%) | 304 (99%) | 4 (1%) | 0 | 100 | 100 |
| 130 | t3 | 308/311 (99%) | 304 (99%) | 4 (1%) | 0 | 100 | 100 |
| 131 | T4 | 196/212 (92%) | 194 (99%) | 2 (1%) | 0 | 100 | 100 |
| 131 | t4 | 196/212 (92%) | 194 (99%) | 2 (1%) | 0 | 100 | 100 |
| 132 | T5 | 139/205 (68%) | 136 (98%) | 3 (2%) | 0 | 100 | 100 |
| 132 | t5 | 139/205 (68%) | 136 (98%) | 3 (2%) | 0 | 100 | 100 |
| 133 | T6 | 107/144 (74%) | 103 (96%) | 4 (4%) | 0 | 100 | 100 |
| 133 | t6 | 107/144 (74%) | 103 (96%) | 4 (4%) | 0 | 100 | 100 |
| 134 | T7 | 140/143 (98%) | 138 (99%) | 2 (1%) | 0 | 100 | 100 |
| 134 | t7 | 140/143 (98%) | 138 (99%) | 2 (1%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|-----------|----------|-------------|-----|
| 135 | T8 | 129/135 (96%) | 128 (99%) | 1 (1%) | 0 | 100 | 100 |
| 135 | t8 | 129/135 (96%) | 128 (99%) | 1 (1%) | 0 | 100 | 100 |
| 136 | T9 | 130/136 (96%) | 128 (98%) | 2 (2%) | 0 | 100 | 100 |
| 136 | t9 | 130/136 (96%) | 128 (98%) | 2 (2%) | 0 | 100 | 100 |
| 137 | TA | 100/127 (79%) | 96 (96%) | 4 (4%) | 0 | 100 | 100 |
| 137 | ta | 100/127 (79%) | 95 (95%) | 5 (5%) | 0 | 100 | 100 |
| 138 | TB | 94/113 (83%) | 94 (100%) | 0 | 0 | 100 | 100 |
| 138 | tb | 94/113 (83%) | 94 (100%) | 0 | 0 | 100 | 100 |
| 139 | TC | 90/93 (97%) | 89 (99%) | 1 (1%) | 0 | 100 | 100 |
| 139 | tc | 90/93 (97%) | 89 (99%) | 1 (1%) | 0 | 100 | 100 |
| 140 | TD | 70/73 (96%) | 70 (100%) | 0 | 0 | 100 | 100 |
| 140 | td | 70/73 (96%) | 70 (100%) | 0 | 0 | 100 | 100 |
| 141 | TE | 48/71 (68%) | 43 (90%) | 5 (10%) | 0 | 100 | 100 |
| 141 | te | 48/71 (68%) | 43 (90%) | 5 (10%) | 0 | 100 | 100 |
| 142 | TF | 214/236 (91%) | 212 (99%) | 2 (1%) | 0 | 100 | 100 |
| 142 | tf | 214/236 (91%) | 212 (99%) | 2 (1%) | 0 | 100 | 100 |
| 143 | TG | 132/135 (98%) | 130 (98%) | 2 (2%) | 0 | 100 | 100 |
| 143 | tg | 132/135 (98%) | 132 (100%) | 0 | 0 | 100 | 100 |
| 144 | TH | 122/124 (98%) | 120 (98%) | 2 (2%) | 0 | 100 | 100 |
| 144 | th | 122/124 (98%) | 120 (98%) | 2 (2%) | 0 | 100 | 100 |
| 145 | TX | 142/166 (86%) | 141 (99%) | 1 (1%) | 0 | 100 | 100 |
| 145 | tx | 142/166 (86%) | 141 (99%) | 1 (1%) | 0 | 100 | 100 |
| 146 | V1 | 440/474 (93%) | 424 (96%) | 16 (4%) | 0 | 100 | 100 |
| 146 | v1 | 440/474 (93%) | 424 (96%) | 16 (4%) | 0 | 100 | 100 |
| 147 | V2 | 229/274 (84%) | 219 (96%) | 10 (4%) | 0 | 100 | 100 |
| 147 | v2 | 229/274 (84%) | 220 (96%) | 9 (4%) | 0 | 100 | 100 |
| 148 | X1 | 147/150 (98%) | 145 (99%) | 2 (1%) | 0 | 100 | 100 |
| 148 | x1 | 147/150 (98%) | 145 (99%) | 2 (1%) | 0 | 100 | 100 |
| 149 | C | 201/212 (95%) | 192 (96%) | 8 (4%) | 1 (0%) | 25 | 50 |
| 149 | c | 201/212 (95%) | 192 (96%) | 8 (4%) | 1 (0%) | 25 | 50 |
| All | All | 65386/73196 (89%) | 63252 (97%) | 2126 (3%) | 8 (0%) | 100 | 100 |

5 of 8 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 129 | t2 | 77 | LYS |
| 129 | T2 | 77 | LYS |
| 149 | C | 87 | PRO |
| 149 | c | 87 | PRO |
| 100 | n1 | 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 | 1T | 61/63 (97%) | 60 (98%) | 1 (2%) | 58 | 77 |
| 1 | 1t | 61/63 (97%) | 60 (98%) | 1 (2%) | 58 | 77 |
| 2 | 2E | 286/287 (100%) | 280 (98%) | 6 (2%) | 48 | 70 |
| 2 | 2e | 286/287 (100%) | 280 (98%) | 6 (2%) | 48 | 70 |
| 3 | 2F | 193/268 (72%) | 189 (98%) | 4 (2%) | 48 | 70 |
| 3 | 2f | 193/268 (72%) | 189 (98%) | 4 (2%) | 48 | 70 |
| 4 | 2G | 181/181 (100%) | 179 (99%) | 2 (1%) | 70 | 83 |
| 4 | 2g | 181/181 (100%) | 179 (99%) | 2 (1%) | 70 | 83 |
| 5 | 2H | 93/184 (50%) | 92 (99%) | 1 (1%) | 70 | 83 |
| 5 | 2h | 93/184 (50%) | 92 (99%) | 1 (1%) | 70 | 83 |
| 6 | 2I | 97/97 (100%) | 95 (98%) | 2 (2%) | 48 | 70 |
| 6 | 2i | 97/97 (100%) | 94 (97%) | 3 (3%) | 35 | 59 |
| 7 | 2J | 85/86 (99%) | 84 (99%) | 1 (1%) | 67 | 82 |
| 7 | 2j | 85/86 (99%) | 84 (99%) | 1 (1%) | 67 | 82 |
| 8 | 2K | 85/85 (100%) | 83 (98%) | 2 (2%) | 44 | 68 |
| 8 | 2k | 85/85 (100%) | 83 (98%) | 2 (2%) | 44 | 68 |
| 9 | 2L | 77/83 (93%) | 75 (97%) | 2 (3%) | 41 | 65 |
| 9 | 2l | 77/83 (93%) | 76 (99%) | 1 (1%) | 65 | 80 |
| 10 | 2M | 66/67 (98%) | 65 (98%) | 1 (2%) | 60 | 78 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 10 | 2m | 66/67 (98%) | 65 (98%) | 1 (2%) | 60 | 78 |
| 11 | 2N | 55/56 (98%) | 53 (96%) | 2 (4%) | 30 | 55 |
| 11 | 2n | 55/56 (98%) | 54 (98%) | 1 (2%) | 54 | 75 |
| 12 | 2O | 37/40 (92%) | 36 (97%) | 1 (3%) | 40 | 64 |
| 12 | 2o | 37/40 (92%) | 36 (97%) | 1 (3%) | 40 | 64 |
| 13 | 2T | 65/67 (97%) | 65 (100%) | 0 | 100 | 100 |
| 13 | 2t | 65/67 (97%) | 65 (100%) | 0 | 100 | 100 |
| 14 | 3T | 76/83 (92%) | 74 (97%) | 2 (3%) | 41 | 65 |
| 14 | 3t | 76/83 (92%) | 74 (97%) | 2 (3%) | 41 | 65 |
| 15 | 4A | 87/113 (77%) | 85 (98%) | 2 (2%) | 45 | 69 |
| 15 | 4a | 87/113 (77%) | 85 (98%) | 2 (2%) | 45 | 69 |
| 16 | 4T | 54/63 (86%) | 52 (96%) | 2 (4%) | 29 | 54 |
| 16 | 4t | 54/63 (86%) | 52 (96%) | 2 (4%) | 29 | 54 |
| 17 | 5T | 56/66 (85%) | 56 (100%) | 0 | 100 | 100 |
| 17 | 5t | 56/66 (85%) | 56 (100%) | 0 | 100 | 100 |
| 18 | 6A | 114/116 (98%) | 113 (99%) | 1 (1%) | 75 | 86 |
| 18 | 6a | 114/116 (98%) | 113 (99%) | 1 (1%) | 75 | 86 |
| 19 | 6B | 200/207 (97%) | 199 (100%) | 1 (0%) | 86 | 93 |
| 19 | 6b | 200/207 (97%) | 199 (100%) | 1 (0%) | 86 | 93 |
| 20 | 6C | 86/88 (98%) | 85 (99%) | 1 (1%) | 67 | 82 |
| 20 | 6c | 86/88 (98%) | 85 (99%) | 1 (1%) | 67 | 82 |
| 21 | 6L | 72/81 (89%) | 72 (100%) | 0 | 100 | 100 |
| 21 | 6l | 72/81 (89%) | 72 (100%) | 0 | 100 | 100 |
| 22 | 6T | 62/63 (98%) | 62 (100%) | 0 | 100 | 100 |
| 22 | 6t | 62/63 (98%) | 62 (100%) | 0 | 100 | 100 |
| 23 | 7A | 120/120 (100%) | 119 (99%) | 1 (1%) | 79 | 88 |
| 23 | 7a | 120/120 (100%) | 119 (99%) | 1 (1%) | 79 | 88 |
| 24 | 7C | 198/218 (91%) | 196 (99%) | 2 (1%) | 73 | 85 |
| 24 | 7c | 198/218 (91%) | 196 (99%) | 2 (1%) | 73 | 85 |
| 25 | 7L | 122/943 (13%) | 121 (99%) | 1 (1%) | 79 | 88 |
| 25 | 7l | 122/943 (13%) | 121 (99%) | 1 (1%) | 79 | 88 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 26 | A | 410/447 (92%) | 410 (100%) | 0 | 100 | 100 |
| 26 | a | 410/447 (92%) | 410 (100%) | 0 | 100 | 100 |
| 27 | B | 374/413 (91%) | 370 (99%) | 4 (1%) | 70 | 83 |
| 27 | b | 374/413 (91%) | 371 (99%) | 3 (1%) | 79 | 88 |
| 28 | BP | 308/386 (80%) | 308 (100%) | 0 | 100 | 100 |
| 28 | bp | 308/386 (80%) | 308 (100%) | 0 | 100 | 100 |
| 29 | C1 | 599/613 (98%) | 593 (99%) | 6 (1%) | 73 | 85 |
| 29 | c1 | 599/613 (98%) | 594 (99%) | 5 (1%) | 79 | 88 |
| 30 | C2 | 565/569 (99%) | 561 (99%) | 4 (1%) | 81 | 90 |
| 30 | c2 | 565/569 (99%) | 560 (99%) | 5 (1%) | 75 | 86 |
| 31 | C3 | 553/565 (98%) | 549 (99%) | 4 (1%) | 81 | 90 |
| 31 | c3 | 553/565 (98%) | 549 (99%) | 4 (1%) | 81 | 90 |
| 32 | D | 253/358 (71%) | 251 (99%) | 2 (1%) | 79 | 88 |
| 32 | d | 253/358 (71%) | 250 (99%) | 3 (1%) | 67 | 82 |
| 33 | E | 342/343 (100%) | 340 (99%) | 2 (1%) | 84 | 91 |
| 33 | e | 342/343 (100%) | 340 (99%) | 2 (1%) | 84 | 91 |
| 34 | F | 219/318 (69%) | 217 (99%) | 2 (1%) | 75 | 86 |
| 34 | f | 219/318 (69%) | 218 (100%) | 1 (0%) | 86 | 93 |
| 35 | FS | 164/164 (100%) | 164 (100%) | 0 | 100 | 100 |
| 35 | fs | 164/164 (100%) | 164 (100%) | 0 | 100 | 100 |
| 36 | G | 267/289 (92%) | 265 (99%) | 2 (1%) | 81 | 90 |
| 36 | g | 267/289 (92%) | 265 (99%) | 2 (1%) | 81 | 90 |
| 37 | H | 256/272 (94%) | 245 (96%) | 11 (4%) | 25 | 49 |
| 37 | h | 256/272 (94%) | 248 (97%) | 8 (3%) | 35 | 59 |
| 38 | I | 200/219 (91%) | 199 (100%) | 1 (0%) | 86 | 93 |
| 38 | i | 200/219 (91%) | 199 (100%) | 1 (0%) | 86 | 93 |
| 39 | J | 170/216 (79%) | 169 (99%) | 1 (1%) | 84 | 91 |
| 39 | j | 170/216 (79%) | 170 (100%) | 0 | 100 | 100 |
| 40 | K | 191/213 (90%) | 190 (100%) | 1 (0%) | 86 | 93 |
| 40 | k | 191/213 (90%) | 190 (100%) | 1 (0%) | 86 | 93 |
| 41 | L | 181/206 (88%) | 179 (99%) | 2 (1%) | 70 | 83 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 41 | l | 181/206 (88%) | 179 (99%) | 2 (1%) | 70 | 83 |
| 42 | M | 198/199 (100%) | 197 (100%) | 1 (0%) | 86 | 93 |
| 42 | m | 198/199 (100%) | 197 (100%) | 1 (0%) | 86 | 93 |
| 43 | M1 | 294/294 (100%) | 293 (100%) | 1 (0%) | 91 | 96 |
| 43 | m1 | 294/294 (100%) | 293 (100%) | 1 (0%) | 91 | 96 |
| 44 | M2 | 260/260 (100%) | 259 (100%) | 1 (0%) | 89 | 95 |
| 44 | m2 | 260/260 (100%) | 259 (100%) | 1 (0%) | 89 | 95 |
| 45 | M3 | 275/276 (100%) | 274 (100%) | 1 (0%) | 89 | 95 |
| 45 | m3 | 275/276 (100%) | 272 (99%) | 3 (1%) | 70 | 83 |
| 46 | N | 178/181 (98%) | 176 (99%) | 2 (1%) | 70 | 83 |
| 46 | n | 178/181 (98%) | 176 (99%) | 2 (1%) | 70 | 83 |
| 47 | O | 120/180 (67%) | 120 (100%) | 0 | 100 | 100 |
| 47 | o | 120/180 (67%) | 119 (99%) | 1 (1%) | 79 | 88 |
| 48 | P | 157/157 (100%) | 155 (99%) | 2 (1%) | 65 | 80 |
| 48 | p | 157/157 (100%) | 155 (99%) | 2 (1%) | 65 | 80 |
| 49 | Q | 157/157 (100%) | 157 (100%) | 0 | 100 | 100 |
| 49 | q | 157/157 (100%) | 156 (99%) | 1 (1%) | 84 | 91 |
| 50 | R | 156/157 (99%) | 154 (99%) | 2 (1%) | 65 | 80 |
| 50 | r | 156/157 (99%) | 154 (99%) | 2 (1%) | 65 | 80 |
| 51 | S | 153/154 (99%) | 153 (100%) | 0 | 100 | 100 |
| 51 | s | 153/154 (99%) | 153 (100%) | 0 | 100 | 100 |
| 52 | SA | 481/515 (93%) | 470 (98%) | 11 (2%) | 45 | 69 |
| 52 | sa | 481/515 (93%) | 475 (99%) | 6 (1%) | 67 | 82 |
| 53 | SB | 255/283 (90%) | 243 (95%) | 12 (5%) | 22 | 46 |
| 53 | sb | 255/283 (90%) | 246 (96%) | 9 (4%) | 31 | 56 |
| 54 | SC | 49/51 (96%) | 47 (96%) | 2 (4%) | 26 | 51 |
| 54 | sc | 49/51 (96%) | 47 (96%) | 2 (4%) | 26 | 51 |
| 55 | SD | 43/43 (100%) | 43 (100%) | 0 | 100 | 100 |
| 55 | sd | 43/43 (100%) | 43 (100%) | 0 | 100 | 100 |
| 56 | T | 137/139 (99%) | 136 (99%) | 1 (1%) | 81 | 90 |
| 56 | t | 137/139 (99%) | 136 (99%) | 1 (1%) | 81 | 90 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 57 | U | 137/138 (99%) | 135 (98%) | 2 (2%) | 60 | 78 |
| 57 | u | 137/138 (99%) | 135 (98%) | 2 (2%) | 60 | 78 |
| 58 | V | 133/135 (98%) | 133 (100%) | 0 | 100 | 100 |
| 58 | v | 133/135 (98%) | 133 (100%) | 0 | 100 | 100 |
| 59 | VB | 503/579 (87%) | 500 (99%) | 3 (1%) | 84 | 91 |
| 59 | vb | 503/579 (87%) | 500 (99%) | 3 (1%) | 84 | 91 |
| 60 | W | 112/113 (99%) | 110 (98%) | 2 (2%) | 54 | 75 |
| 60 | w | 112/113 (99%) | 110 (98%) | 2 (2%) | 54 | 75 |
| 61 | X | 105/105 (100%) | 104 (99%) | 1 (1%) | 73 | 85 |
| 61 | x | 105/105 (100%) | 104 (99%) | 1 (1%) | 73 | 85 |
| 62 | Y | 88/88 (100%) | 87 (99%) | 1 (1%) | 70 | 83 |
| 62 | y | 88/88 (100%) | 87 (99%) | 1 (1%) | 70 | 83 |
| 63 | Y0 | 84/84 (100%) | 84 (100%) | 0 | 100 | 100 |
| 63 | y0 | 84/84 (100%) | 84 (100%) | 0 | 100 | 100 |
| 64 | Y5 | 185/185 (100%) | 185 (100%) | 0 | 100 | 100 |
| 64 | y5 | 185/185 (100%) | 185 (100%) | 0 | 100 | 100 |
| 65 | Y7 | 333/442 (75%) | 332 (100%) | 1 (0%) | 91 | 96 |
| 65 | y7 | 333/442 (75%) | 332 (100%) | 1 (0%) | 91 | 96 |
| 66 | Z | 77/80 (96%) | 75 (97%) | 2 (3%) | 41 | 65 |
| 66 | z | 77/80 (96%) | 75 (97%) | 2 (3%) | 41 | 65 |
| 67 | Z1 | 77/78 (99%) | 77 (100%) | 0 | 100 | 100 |
| 67 | z1 | 77/78 (99%) | 77 (100%) | 0 | 100 | 100 |
| 68 | 1B | 55/55 (100%) | 55 (100%) | 0 | 100 | 100 |
| 68 | 1b | 55/55 (100%) | 55 (100%) | 0 | 100 | 100 |
| 69 | 2B | 170/170 (100%) | 169 (99%) | 1 (1%) | 84 | 91 |
| 69 | 2b | 170/170 (100%) | 170 (100%) | 0 | 100 | 100 |
| 70 | 4L | 108/108 (100%) | 108 (100%) | 0 | 100 | 100 |
| 70 | 4l | 108/108 (100%) | 108 (100%) | 0 | 100 | 100 |
| 71 | 5B | 98/98 (100%) | 98 (100%) | 0 | 100 | 100 |
| 71 | 5b | 98/98 (100%) | 98 (100%) | 0 | 100 | 100 |
| 72 | A1 | 88/89 (99%) | 88 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 72 | a1 | 88/89 (99%) | 88 (100%) | 0 | 100 | 100 |
| 73 | A2 | 88/93 (95%) | 86 (98%) | 2 (2%) | 45 | 69 |
| 73 | a2 | 88/93 (95%) | 87 (99%) | 1 (1%) | 70 | 83 |
| 74 | A3 | 108/114 (95%) | 108 (100%) | 0 | 100 | 100 |
| 74 | a3 | 108/114 (95%) | 108 (100%) | 0 | 100 | 100 |
| 75 | A5 | 144/186 (77%) | 142 (99%) | 2 (1%) | 62 | 79 |
| 75 | a5 | 144/186 (77%) | 142 (99%) | 2 (1%) | 62 | 79 |
| 76 | A6 | 154/154 (100%) | 152 (99%) | 2 (1%) | 65 | 80 |
| 76 | a6 | 154/154 (100%) | 152 (99%) | 2 (1%) | 65 | 80 |
| 77 | A7 | 257/257 (100%) | 255 (99%) | 2 (1%) | 79 | 88 |
| 77 | a7 | 257/257 (100%) | 255 (99%) | 2 (1%) | 79 | 88 |
| 78 | A8 | 121/224 (54%) | 121 (100%) | 0 | 100 | 100 |
| 78 | a8 | 121/224 (54%) | 121 (100%) | 0 | 100 | 100 |
| 79 | A9 | 290/311 (93%) | 290 (100%) | 0 | 100 | 100 |
| 79 | a9 | 290/311 (93%) | 290 (100%) | 0 | 100 | 100 |
| 80 | AB | 104/129 (81%) | 103 (99%) | 1 (1%) | 73 | 85 |
| 80 | ab | 104/129 (81%) | 103 (99%) | 1 (1%) | 73 | 85 |
| 81 | AC | 88/119 (74%) | 87 (99%) | 1 (1%) | 70 | 83 |
| 81 | ac | 88/119 (74%) | 87 (99%) | 1 (1%) | 70 | 83 |
| 82 | AL | 169/170 (99%) | 167 (99%) | 2 (1%) | 67 | 82 |
| 82 | al | 169/170 (99%) | 168 (99%) | 1 (1%) | 84 | 91 |
| 83 | AM | 142/156 (91%) | 141 (99%) | 1 (1%) | 81 | 90 |
| 83 | am | 142/156 (91%) | 141 (99%) | 1 (1%) | 81 | 90 |
| 84 | AN | 199/199 (100%) | 197 (99%) | 2 (1%) | 73 | 85 |
| 84 | an | 199/199 (100%) | 199 (100%) | 0 | 100 | 100 |
| 85 | B2 | 103/109 (94%) | 100 (97%) | 3 (3%) | 37 | 61 |
| 85 | b2 | 103/109 (94%) | 101 (98%) | 2 (2%) | 52 | 73 |
| 86 | B3 | 64/74 (86%) | 63 (98%) | 1 (2%) | 58 | 77 |
| 86 | b3 | 64/74 (86%) | 63 (98%) | 1 (2%) | 58 | 77 |
| 87 | B4 | 102/128 (80%) | 100 (98%) | 2 (2%) | 50 | 72 |
| 87 | b4 | 102/128 (80%) | 100 (98%) | 2 (2%) | 50 | 72 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 88 | B6 | 64/117 (55%) | 64 (100%) | 0 | 100 | 100 |
| 88 | b6 | 64/117 (55%) | 64 (100%) | 0 | 100 | 100 |
| 89 | B7 | 97/99 (98%) | 95 (98%) | 2 (2%) | 48 | 70 |
| 89 | b7 | 97/99 (98%) | 95 (98%) | 2 (2%) | 48 | 70 |
| 90 | B8 | 156/180 (87%) | 154 (99%) | 2 (1%) | 65 | 80 |
| 90 | b8 | 156/180 (87%) | 155 (99%) | 1 (1%) | 84 | 91 |
| 91 | B9 | 171/172 (99%) | 169 (99%) | 2 (1%) | 67 | 82 |
| 91 | b9 | 171/172 (99%) | 169 (99%) | 2 (1%) | 67 | 82 |
| 92 | BL | 160/172 (93%) | 160 (100%) | 0 | 100 | 100 |
| 92 | bl | 160/172 (93%) | 159 (99%) | 1 (1%) | 84 | 91 |
| 93 | BM | 142/182 (78%) | 138 (97%) | 4 (3%) | 38 | 63 |
| 93 | bm | 142/182 (78%) | 138 (97%) | 4 (3%) | 38 | 63 |
| 94 | C4 | 89/89 (100%) | 88 (99%) | 1 (1%) | 70 | 83 |
| 94 | c4 | 89/89 (100%) | 89 (100%) | 0 | 100 | 100 |
| 95 | FX | 130/152 (86%) | 129 (99%) | 1 (1%) | 79 | 88 |
| 95 | fx | 130/152 (86%) | 129 (99%) | 1 (1%) | 79 | 88 |
| 96 | G1 | 195/218 (89%) | 192 (98%) | 3 (2%) | 60 | 78 |
| 96 | g1 | 195/218 (89%) | 194 (100%) | 1 (0%) | 86 | 93 |
| 97 | G2 | 195/197 (99%) | 194 (100%) | 1 (0%) | 86 | 93 |
| 97 | g2 | 195/197 (99%) | 193 (99%) | 2 (1%) | 73 | 85 |
| 98 | G3 | 309/309 (100%) | 307 (99%) | 2 (1%) | 84 | 91 |
| 98 | g3 | 309/309 (100%) | 307 (99%) | 2 (1%) | 84 | 91 |
| 99 | J1 | 222/270 (82%) | 218 (98%) | 4 (2%) | 54 | 75 |
| 99 | j1 | 222/270 (82%) | 218 (98%) | 4 (2%) | 54 | 75 |
| 100 | N1 | 249/250 (100%) | 239 (96%) | 10 (4%) | 27 | 51 |
| 100 | n1 | 249/250 (100%) | 244 (98%) | 5 (2%) | 50 | 72 |
| 101 | N2 | 346/346 (100%) | 338 (98%) | 8 (2%) | 45 | 69 |
| 101 | n2 | 346/346 (100%) | 341 (99%) | 5 (1%) | 62 | 79 |
| 102 | N3 | 111/112 (99%) | 109 (98%) | 2 (2%) | 54 | 75 |
| 102 | n3 | 111/112 (99%) | 109 (98%) | 2 (2%) | 54 | 75 |
| 103 | N4 | 463/463 (100%) | 455 (98%) | 8 (2%) | 56 | 76 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 103 | n4 | 463/463 (100%) | 455 (98%) | 8 (2%) | 56 | 76 |
| 104 | N5 | 653/694 (94%) | 640 (98%) | 13 (2%) | 50 | 72 |
| 104 | n5 | 653/694 (94%) | 641 (98%) | 12 (2%) | 54 | 75 |
| 105 | N6 | 244/244 (100%) | 242 (99%) | 2 (1%) | 79 | 88 |
| 105 | n6 | 244/244 (100%) | 242 (99%) | 2 (1%) | 79 | 88 |
| 106 | P1 | 207/223 (93%) | 205 (99%) | 2 (1%) | 73 | 85 |
| 106 | p1 | 207/223 (93%) | 205 (99%) | 2 (1%) | 73 | 85 |
| 107 | P2 | 158/178 (89%) | 154 (98%) | 4 (2%) | 42 | 66 |
| 107 | p2 | 158/178 (89%) | 157 (99%) | 1 (1%) | 84 | 91 |
| 108 | QA | 385/409 (94%) | 383 (100%) | 2 (0%) | 86 | 93 |
| 108 | Qa | 385/409 (94%) | 379 (98%) | 6 (2%) | 58 | 77 |
| 108 | qA | 385/409 (94%) | 383 (100%) | 2 (0%) | 86 | 93 |
| 108 | qa | 385/409 (94%) | 378 (98%) | 7 (2%) | 54 | 75 |
| 109 | QB | 411/440 (93%) | 405 (98%) | 6 (2%) | 60 | 78 |
| 109 | Qb | 411/440 (93%) | 401 (98%) | 10 (2%) | 44 | 68 |
| 109 | qB | 411/440 (93%) | 406 (99%) | 5 (1%) | 67 | 82 |
| 109 | qb | 411/440 (93%) | 402 (98%) | 9 (2%) | 47 | 69 |
| 110 | QC | 386/386 (100%) | 378 (98%) | 8 (2%) | 48 | 70 |
| 110 | Qc | 385/386 (100%) | 374 (97%) | 11 (3%) | 37 | 61 |
| 110 | qC | 386/386 (100%) | 379 (98%) | 7 (2%) | 54 | 75 |
| 110 | qc | 385/386 (100%) | 375 (97%) | 10 (3%) | 41 | 65 |
| 111 | QD | 255/274 (93%) | 252 (99%) | 3 (1%) | 67 | 82 |
| 111 | Qd | 255/274 (93%) | 253 (99%) | 2 (1%) | 79 | 88 |
| 111 | qD | 255/274 (93%) | 252 (99%) | 3 (1%) | 67 | 82 |
| 111 | qd | 255/274 (93%) | 254 (100%) | 1 (0%) | 89 | 95 |
| 112 | QE | 109/237 (46%) | 106 (97%) | 3 (3%) | 38 | 63 |
| 112 | Qe | 99/237 (42%) | 97 (98%) | 2 (2%) | 50 | 72 |
| 112 | qE | 109/237 (46%) | 106 (97%) | 3 (3%) | 38 | 63 |
| 112 | qe | 99/237 (42%) | 97 (98%) | 2 (2%) | 50 | 72 |
| 113 | QF | 80/81 (99%) | 79 (99%) | 1 (1%) | 65 | 80 |
| 113 | Qf | 72/81 (89%) | 72 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 113 | qF | 80/81 (99%) | 79 (99%) | 1 (1%) | 65 | 80 |
| 113 | qf | 72/81 (89%) | 72 (100%) | 0 | 100 | 100 |
| 114 | QG | 288/289 (100%) | 282 (98%) | 6 (2%) | 48 | 70 |
| 114 | Qg | 287/289 (99%) | 282 (98%) | 5 (2%) | 56 | 76 |
| 114 | qG | 288/289 (100%) | 283 (98%) | 5 (2%) | 56 | 76 |
| 114 | qg | 287/289 (99%) | 282 (98%) | 5 (2%) | 56 | 76 |
| 115 | QH | 117/118 (99%) | 116 (99%) | 1 (1%) | 75 | 86 |
| 115 | Qh | 117/118 (99%) | 117 (100%) | 0 | 100 | 100 |
| 115 | qH | 117/118 (99%) | 116 (99%) | 1 (1%) | 75 | 86 |
| 115 | qh | 117/118 (99%) | 117 (100%) | 0 | 100 | 100 |
| 116 | QI | 104/109 (95%) | 103 (99%) | 1 (1%) | 73 | 85 |
| 116 | Qi | 104/109 (95%) | 103 (99%) | 1 (1%) | 73 | 85 |
| 116 | qI | 104/109 (95%) | 102 (98%) | 2 (2%) | 52 | 73 |
| 116 | qi | 104/109 (95%) | 103 (99%) | 1 (1%) | 73 | 85 |
| 117 | QJ | 51/56 (91%) | 51 (100%) | 0 | 100 | 100 |
| 117 | Qj | 53/56 (95%) | 52 (98%) | 1 (2%) | 52 | 73 |
| 117 | qJ | 51/56 (91%) | 51 (100%) | 0 | 100 | 100 |
| 117 | qj | 53/56 (95%) | 52 (98%) | 1 (2%) | 52 | 73 |
| 118 | QL | 28/36 (78%) | 28 (100%) | 0 | 100 | 100 |
| 118 | Ql | 28/36 (78%) | 28 (100%) | 0 | 100 | 100 |
| 118 | qL | 28/36 (78%) | 28 (100%) | 0 | 100 | 100 |
| 118 | ql | 28/36 (78%) | 28 (100%) | 0 | 100 | 100 |
| 120 | S1 | 590/617 (96%) | 583 (99%) | 7 (1%) | 67 | 82 |
| 120 | s1 | 590/617 (96%) | 585 (99%) | 5 (1%) | 79 | 88 |
| 121 | S2 | 399/399 (100%) | 387 (97%) | 12 (3%) | 36 | 60 |
| 121 | s2 | 399/399 (100%) | 389 (98%) | 10 (2%) | 42 | 66 |
| 122 | S3 | 191/191 (100%) | 187 (98%) | 4 (2%) | 48 | 70 |
| 122 | s3 | 191/191 (100%) | 187 (98%) | 4 (2%) | 48 | 70 |
| 123 | S4 | 160/163 (98%) | 156 (98%) | 4 (2%) | 42 | 66 |
| 123 | s4 | 160/163 (98%) | 156 (98%) | 4 (2%) | 42 | 66 |
| 124 | S5 | 82/83 (99%) | 79 (96%) | 3 (4%) | 29 | 54 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 124 | s5 | 82/83 (99%) | 80 (98%) | 2 (2%) | 44 | 68 |
| 125 | S6 | 82/116 (71%) | 80 (98%) | 2 (2%) | 44 | 68 |
| 125 | s6 | 82/116 (71%) | 81 (99%) | 1 (1%) | 67 | 82 |
| 126 | S7 | 136/137 (99%) | 129 (95%) | 7 (5%) | 20 | 43 |
| 126 | s7 | 136/137 (99%) | 130 (96%) | 6 (4%) | 24 | 49 |
| 127 | S8 | 197/215 (92%) | 197 (100%) | 0 | 100 | 100 |
| 127 | s8 | 197/215 (92%) | 197 (100%) | 0 | 100 | 100 |
| 128 | T1 | 440/454 (97%) | 433 (98%) | 7 (2%) | 58 | 77 |
| 128 | t1 | 440/454 (97%) | 432 (98%) | 8 (2%) | 54 | 75 |
| 129 | T2 | 237/280 (85%) | 232 (98%) | 5 (2%) | 48 | 70 |
| 129 | t2 | 237/280 (85%) | 232 (98%) | 5 (2%) | 48 | 70 |
| 130 | T3 | 272/275 (99%) | 268 (98%) | 4 (2%) | 60 | 78 |
| 130 | t3 | 272/275 (99%) | 268 (98%) | 4 (2%) | 60 | 78 |
| 131 | T4 | 178/190 (94%) | 177 (99%) | 1 (1%) | 84 | 91 |
| 131 | t4 | 178/190 (94%) | 177 (99%) | 1 (1%) | 84 | 91 |
| 132 | T5 | 119/179 (66%) | 118 (99%) | 1 (1%) | 79 | 88 |
| 132 | t5 | 119/179 (66%) | 118 (99%) | 1 (1%) | 79 | 88 |
| 133 | T6 | 97/131 (74%) | 96 (99%) | 1 (1%) | 73 | 85 |
| 133 | t6 | 97/131 (74%) | 96 (99%) | 1 (1%) | 73 | 85 |
| 134 | T7 | 124/125 (99%) | 122 (98%) | 2 (2%) | 58 | 77 |
| 134 | t7 | 124/125 (99%) | 123 (99%) | 1 (1%) | 79 | 88 |
| 135 | T8 | 118/122 (97%) | 118 (100%) | 0 | 100 | 100 |
| 135 | t8 | 118/122 (97%) | 118 (100%) | 0 | 100 | 100 |
| 136 | T9 | 118/122 (97%) | 117 (99%) | 1 (1%) | 79 | 88 |
| 136 | t9 | 118/122 (97%) | 118 (100%) | 0 | 100 | 100 |
| 137 | TA | 94/117 (80%) | 93 (99%) | 1 (1%) | 70 | 83 |
| 137 | ta | 94/117 (80%) | 93 (99%) | 1 (1%) | 70 | 83 |
| 138 | TB | 82/97 (84%) | 82 (100%) | 0 | 100 | 100 |
| 138 | tb | 82/97 (84%) | 82 (100%) | 0 | 100 | 100 |
| 139 | TC | 83/84 (99%) | 82 (99%) | 1 (1%) | 67 | 82 |
| 139 | tc | 83/84 (99%) | 82 (99%) | 1 (1%) | 67 | 82 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|-------------|-----|
| 140 | TD | 64/65 (98%) | 64 (100%) | 0 | 100 | 100 |
| 140 | td | 64/65 (98%) | 64 (100%) | 0 | 100 | 100 |
| 141 | TE | 45/63 (71%) | 45 (100%) | 0 | 100 | 100 |
| 141 | te | 45/63 (71%) | 45 (100%) | 0 | 100 | 100 |
| 142 | TF | 195/212 (92%) | 194 (100%) | 1 (0%) | 86 | 93 |
| 142 | tf | 195/212 (92%) | 194 (100%) | 1 (0%) | 86 | 93 |
| 143 | TG | 121/122 (99%) | 115 (95%) | 6 (5%) | 20 | 44 |
| 143 | tg | 121/122 (99%) | 117 (97%) | 4 (3%) | 33 | 58 |
| 144 | TH | 108/108 (100%) | 107 (99%) | 1 (1%) | 75 | 86 |
| 144 | th | 108/108 (100%) | 107 (99%) | 1 (1%) | 75 | 86 |
| 145 | TX | 128/147 (87%) | 126 (98%) | 2 (2%) | 58 | 77 |
| 145 | tx | 128/147 (87%) | 127 (99%) | 1 (1%) | 79 | 88 |
| 146 | V1 | 362/392 (92%) | 359 (99%) | 3 (1%) | 79 | 88 |
| 146 | v1 | 362/392 (92%) | 358 (99%) | 4 (1%) | 70 | 83 |
| 147 | V2 | 205/236 (87%) | 204 (100%) | 1 (0%) | 86 | 93 |
| 147 | v2 | 205/236 (87%) | 204 (100%) | 1 (0%) | 86 | 93 |
| 148 | X1 | 132/133 (99%) | 131 (99%) | 1 (1%) | 79 | 88 |
| 148 | x1 | 132/133 (99%) | 131 (99%) | 1 (1%) | 79 | 88 |
| 149 | C | 106/178 (60%) | 104 (98%) | 2 (2%) | 52 | 73 |
| 149 | c | 106/178 (60%) | 104 (98%) | 2 (2%) | 52 | 73 |
| All | All | 58230/65244 (89%) | 57534 (99%) | 696 (1%) | 66 | 82 |

5 of 696 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 82 | AL | 37 | ARG |
| 114 | QG | 326 | PHE |
| 90 | B8 | 129 | LYS |
| 81 | AC | 64 | LEU |
| 103 | N4 | 205 | TRP |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 977 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 140 | td | 73 | GLN |
| 122 | S3 | 3 | ASN |
| 34 | F | 267 | ASN |
| 120 | S1 | 598 | GLN |
| 140 | TD | 73 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 59 | SEP | VB | 520 | 59 | 8,9,10 | 0.88 | 0 | 8,12,14 | 0.75 | 0 |
| 24 | SEP | 7C | 120 | 24 | 8,9,10 | 0.87 | 0 | 8,12,14 | 0.67 | 0 |
| 59 | TPO | VB | 387 | 59 | 8,10,11 | 1.21 | 1 (12%) | 10,14,16 | 1.05 | 0 |
| 24 | SEP | 7c | 120 | 24 | 8,9,10 | 0.87 | 0 | 8,12,14 | 0.67 | 0 |
| 59 | SEP | vb | 520 | 59 | 8,9,10 | 0.88 | 0 | 8,12,14 | 0.76 | 0 |
| 59 | TPO | vb | 387 | 59 | 8,10,11 | 1.21 | 1 (12%) | 10,14,16 | 1.05 | 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 |
|-----|------|-------|-----|------|---------|-----------|-------|
| 59 | SEP | VB | 520 | 59 | - | 3/5/8/10 | - |
| 24 | SEP | 7C | 120 | 24 | - | 3/5/8/10 | - |
| 59 | TPO | VB | 387 | 59 | - | 1/9/11/13 | - |
| 24 | SEP | 7c | 120 | 24 | - | 3/5/8/10 | - |
| 59 | SEP | vb | 520 | 59 | - | 3/5/8/10 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|-------|
| 59 | TPO | vb | 387 | 59 | - | 1/9/11/13 | - |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 59 | VB | 387 | TPO | P-OG1 | 3.02 | 1.65 | 1.59 |
| 59 | vb | 387 | TPO | P-OG1 | 3.01 | 1.65 | 1.59 |

There are no bond angle outliers.

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 24 | 7c | 120 | SEP | CB-OG-P-O1P |
| 24 | 7c | 120 | SEP | CB-OG-P-O2P |
| 24 | 7c | 120 | SEP | CB-OG-P-O3P |
| 59 | vb | 387 | TPO | O-C-CA-CB |
| 59 | vb | 520 | SEP | CB-OG-P-O1P |

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 510 ligands modelled in this entry, 14 are monoatomic - leaving 496 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 |
| 152 | PC1 | n5 | 803 | - | 52,52,53 | 0.29 | 0 | 58,60,61 | 0.29 | 0 |
| 153 | CDL | T | 201 | - | 58,58,99 | 0.38 | 0 | 64,70,111 | 0.32 | 0 |
| 152 | PC1 | c4 | 403 | - | 40,40,53 | 0.33 | 0 | 46,48,61 | 0.30 | 0 |
| 158 | 3PE | T8 | 602 | - | 38,38,50 | 0.34 | 0 | 41,43,55 | 0.36 | 0 |
| 157 | FES | fs | 201 | 35 | 0,4,4 | - | - | - | | |
| 153 | CDL | QB | 601 | - | 67,67,99 | 0.35 | 0 | 73,79,111 | 0.30 | 0 |
| 158 | 3PE | bm | 302 | - | 29,29,50 | 0.39 | 0 | 32,34,55 | 0.46 | 0 |
| 162 | SF4 | s7 | 201 | 126 | 0,12,12 | - | - | - | | |
| 153 | CDL | c | 301 | - | 63,63,99 | 0.37 | 0 | 69,75,111 | 0.43 | 0 |
| 153 | CDL | u | 201 | - | 59,59,99 | 0.38 | 0 | 65,71,111 | 0.32 | 0 |
| 153 | CDL | 2o | 101 | - | 49,49,99 | 0.41 | 0 | 55,61,111 | 0.35 | 0 |
| 153 | CDL | m1 | 404 | - | 90,90,99 | 0.32 | 0 | 96,102,111 | 0.28 | 0 |
| 153 | CDL | N | 304 | - | 83,83,99 | 0.33 | 0 | 89,95,111 | 0.32 | 0 |
| 152 | PC1 | B9 | 201 | - | 33,33,53 | 0.38 | 0 | 39,41,61 | 0.52 | 0 |
| 152 | PC1 | 7C | 303 | - | 42,42,53 | 0.32 | 0 | 48,50,61 | 0.32 | 0 |
| 153 | CDL | M2 | 403 | - | 65,65,99 | 0.36 | 0 | 71,77,111 | 0.30 | 0 |
| 152 | PC1 | t4 | 303 | - | 53,53,53 | 0.30 | 0 | 59,61,61 | 0.35 | 0 |
| 152 | PC1 | Qg | 401 | - | 31,31,53 | 0.36 | 0 | 37,39,61 | 0.33 | 0 |
| 157 | FES | QE | 302 | - | 0,4,4 | - | - | - | | |
| 152 | PC1 | f | 402 | - | 37,37,53 | 0.34 | 0 | 43,45,61 | 0.28 | 0 |
| 153 | CDL | E | 401 | - | 59,59,99 | 0.37 | 0 | 65,71,111 | 0.34 | 0 |
| 153 | CDL | 2b | 201 | - | 86,86,99 | 0.32 | 0 | 92,98,111 | 0.36 | 0 |
| 153 | CDL | q | 203 | - | 85,85,99 | 0.33 | 0 | 91,97,111 | 0.31 | 0 |
| 153 | CDL | qG | 402 | - | 85,85,99 | 0.32 | 0 | 91,97,111 | 0.28 | 0 |
| 153 | CDL | A1 | 101 | - | 65,65,99 | 0.36 | 0 | 71,77,111 | 0.33 | 0 |
| 157 | FES | V2 | 300 | 147 | 0,4,4 | - | - | - | | |
| 152 | PC1 | N | 303 | - | 35,35,53 | 0.34 | 0 | 41,43,61 | 0.33 | 0 |
| 153 | CDL | b4 | 201 | - | 36,36,99 | 0.43 | 0 | 42,48,111 | 0.40 | 0 |
| 152 | PC1 | m1 | 401 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.28 | 0 |
| 152 | PC1 | V | 201 | - | 34,34,53 | 0.35 | 0 | 40,42,61 | 0.32 | 0 |
| 152 | PC1 | I | 301 | - | 38,38,53 | 0.34 | 0 | 44,46,61 | 0.32 | 0 |
| 153 | CDL | m | 306 | - | 65,65,99 | 0.36 | 0 | 71,77,111 | 0.31 | 0 |
| 153 | CDL | p1 | 402 | - | 62,62,99 | 0.37 | 0 | 68,74,111 | 0.31 | 0 |
| 153 | CDL | t1 | 601 | - | 54,54,99 | 0.39 | 0 | 60,66,111 | 0.36 | 0 |
| 152 | PC1 | n5 | 804 | - | 38,38,53 | 0.33 | 0 | 44,46,61 | 0.32 | 0 |
| 152 | PC1 | 6c | 203 | - | 32,32,53 | 0.36 | 0 | 38,40,61 | 0.35 | 0 |
| 152 | PC1 | qc | 509 | - | 46,46,53 | 0.31 | 0 | 52,54,61 | 0.34 | 0 |
| 153 | CDL | a | 502 | - | 50,50,99 | 0.41 | 0 | 56,62,111 | 0.47 | 0 |
| 153 | CDL | B4 | 201 | - | 36,36,99 | 0.43 | 0 | 42,48,111 | 0.40 | 0 |
| 153 | CDL | qH | 201 | - | 93,93,99 | 0.31 | 0 | 99,105,111 | 0.26 | 0 |
| 153 | CDL | T | 202 | - | 74,74,99 | 0.34 | 0 | 80,86,111 | 0.34 | 0 |
| 171 | FMN | v1 | 501 | - | 33,33,33 | 0.20 | 0 | 48,50,50 | 0.42 | 0 |
| 152 | PC1 | qE | 301 | - | 23,23,53 | 0.40 | 0 | 29,31,61 | 0.36 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 153 | CDL | B | 501 | - | 61,61,99 | 0.37 | 0 | 67,73,111 | 0.32 | 0 |
| 153 | CDL | A9 | 402 | - | 75,75,99 | 0.34 | 0 | 81,87,111 | 0.35 | 0 |
| 152 | PC1 | fs | 204 | - | 39,39,53 | 0.34 | 0 | 45,47,61 | 0.27 | 0 |
| 153 | CDL | qB | 601 | - | 67,67,99 | 0.35 | 0 | 73,79,111 | 0.30 | 0 |
| 157 | FES | FS | 203 | 35 | 0,4,4 | - | - | - | | |
| 152 | PC1 | b9 | 201 | - | 33,33,53 | 0.38 | 0 | 39,41,61 | 0.52 | 0 |
| 153 | CDL | 6a | 201 | - | 73,73,99 | 0.35 | 0 | 79,85,111 | 0.41 | 0 |
| 153 | CDL | W | 202 | - | 83,83,99 | 0.33 | 0 | 89,95,111 | 0.33 | 0 |
| 153 | CDL | a | 505 | - | 81,81,99 | 0.33 | 0 | 87,93,111 | 0.29 | 0 |
| 153 | CDL | z | 101 | - | 66,66,99 | 0.36 | 0 | 72,78,111 | 0.30 | 0 |
| 153 | CDL | TE | 101 | - | 52,52,99 | 0.40 | 0 | 58,64,111 | 0.33 | 0 |
| 158 | 3PE | N5 | 802 | - | 35,35,50 | 0.36 | 0 | 38,40,55 | 0.31 | 0 |
| 153 | CDL | q | 201 | - | 62,62,99 | 0.37 | 0 | 68,74,111 | 0.38 | 0 |
| 152 | PC1 | d | 501 | - | 34,34,53 | 0.36 | 0 | 40,42,61 | 0.38 | 0 |
| 153 | CDL | td | 101 | - | 65,65,99 | 0.36 | 0 | 71,77,111 | 0.33 | 0 |
| 153 | CDL | R | 201 | - | 64,64,99 | 0.36 | 0 | 70,76,111 | 0.31 | 0 |
| 153 | CDL | 6c | 202 | - | 81,81,99 | 0.32 | 0 | 87,93,111 | 0.30 | 0 |
| 152 | PC1 | qb | 602 | - | 42,42,53 | 0.32 | 0 | 48,50,61 | 0.30 | 0 |
| 153 | CDL | 2k | 101 | - | 97,97,99 | 0.31 | 0 | 103,109,111 | 0.35 | 0 |
| 167 | NDP | a9 | 401 | - | 45,52,52 | 0.52 | 0 | 53,80,80 | 0.54 | 1 (1%) |
| 171 | FMN | V1 | 501 | - | 33,33,33 | 0.20 | 0 | 48,50,50 | 0.42 | 0 |
| 153 | CDL | qb | 601 | - | 67,67,99 | 0.36 | 0 | 73,79,111 | 0.30 | 0 |
| 152 | PC1 | QG | 401 | - | 31,31,53 | 0.37 | 0 | 37,39,61 | 0.40 | 0 |
| 152 | PC1 | c3 | 601 | - | 51,51,53 | 0.30 | 0 | 57,59,61 | 0.34 | 0 |
| 153 | CDL | 2G | 203 | - | 54,54,99 | 0.39 | 0 | 60,66,111 | 0.36 | 0 |
| 162 | SF4 | s8 | 302 | 127 | 0,12,12 | - | - | - | | |
| 152 | PC1 | m2 | 402 | - | 31,31,53 | 0.36 | 0 | 37,39,61 | 0.38 | 0 |
| 152 | PC1 | C3 | 606 | - | 48,48,53 | 0.31 | 0 | 54,56,61 | 0.35 | 0 |
| 152 | PC1 | n | 302 | - | 31,31,53 | 0.36 | 0 | 37,39,61 | 0.32 | 0 |
| 153 | CDL | a1 | 101 | - | 66,66,99 | 0.36 | 0 | 72,78,111 | 0.37 | 0 |
| 152 | PC1 | qg | 401 | - | 31,31,53 | 0.36 | 0 | 37,39,61 | 0.33 | 0 |
| 153 | CDL | U | 201 | - | 59,59,99 | 0.38 | 0 | 65,71,111 | 0.32 | 0 |
| 153 | CDL | 2g | 204 | - | 62,62,99 | 0.37 | 0 | 68,74,111 | 0.32 | 0 |
| 153 | CDL | fs | 203 | - | 46,46,99 | 0.42 | 0 | 52,58,111 | 0.35 | 0 |
| 153 | CDL | 7C | 302 | - | 50,50,99 | 0.40 | 0 | 56,62,111 | 0.35 | 0 |
| 158 | 3PE | an | 301 | - | 44,44,50 | 0.32 | 0 | 47,49,55 | 0.27 | 0 |
| 152 | PC1 | Qe | 303 | - | 42,42,53 | 0.33 | 0 | 48,50,61 | 0.44 | 0 |
| 152 | PC1 | S8 | 301 | - | 29,29,53 | 0.38 | 0 | 35,37,61 | 0.33 | 0 |
| 153 | CDL | E | 403 | - | 62,62,99 | 0.37 | 0 | 68,74,111 | 0.30 | 0 |
| 152 | PC1 | N5 | 805 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.32 | 0 |
| 153 | CDL | r | 201 | - | 64,64,99 | 0.36 | 0 | 70,76,111 | 0.31 | 0 |
| 153 | CDL | AN | 302 | - | 86,86,99 | 0.32 | 0 | 92,98,111 | 0.29 | 0 |
| 152 | PC1 | qI | 201 | - | 29,29,53 | 0.38 | 0 | 35,37,61 | 0.32 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 152 | PC1 | qC | 508 | - | 35,35,53 | 0.35 | 0 | 41,43,61 | 0.34 | 0 |
| 152 | PC1 | Qc | 506 | - | 37,37,53 | 0.34 | 0 | 43,45,61 | 0.31 | 0 |
| 153 | CDL | N5 | 806 | - | 89,89,99 | 0.31 | 0 | 95,101,111 | 0.28 | 0 |
| 154 | HEA | c1 | 708 | 29 | 57,67,67 | 2.02 | 18 (31%) | 61,103,103 | 2.76 | 26 (42%) |
| 152 | PC1 | N1 | 301 | - | 35,35,53 | 0.35 | 0 | 41,43,61 | 0.33 | 0 |
| 169 | T7X | b6 | 201 | - | 55,55,61 | 1.51 | 5 (9%) | 64,67,73 | 1.08 | 4 (6%) |
| 152 | PC1 | N | 301 | - | 40,40,53 | 0.33 | 0 | 46,48,61 | 0.29 | 0 |
| 152 | PC1 | FS | 201 | - | 39,39,53 | 0.34 | 0 | 45,47,61 | 0.27 | 0 |
| 170 | ADP | b9 | 202 | - | 24,29,29 | 0.94 | 1 (4%) | 29,45,45 | 1.46 | 4 (13%) |
| 152 | PC1 | 2f | 301 | - | 46,46,53 | 0.32 | 0 | 52,54,61 | 0.50 | 0 |
| 158 | 3PE | g2 | 301 | - | 50,50,50 | 0.30 | 0 | 53,55,55 | 0.29 | 0 |
| 164 | U10 | b8 | 301 | - | 63,63,63 | 2.15 | 21 (33%) | 76,79,79 | 1.68 | 21 (27%) |
| 153 | CDL | C1 | 708 | - | 62,62,99 | 0.37 | 0 | 68,74,111 | 0.39 | 0 |
| 152 | PC1 | T4 | 301 | - | 47,47,53 | 0.31 | 0 | 53,55,61 | 0.36 | 0 |
| 152 | PC1 | Qb | 602 | - | 42,42,53 | 0.32 | 0 | 48,50,61 | 0.30 | 0 |
| 153 | CDL | qI | 203 | - | 70,70,99 | 0.35 | 0 | 76,82,111 | 0.31 | 0 |
| 153 | CDL | B3 | 101 | - | 57,57,99 | 0.38 | 0 | 63,69,111 | 0.32 | 0 |
| 153 | CDL | j | 301 | - | 69,69,99 | 0.35 | 0 | 75,81,111 | 0.29 | 0 |
| 153 | CDL | Qc | 508 | - | 46,46,99 | 0.42 | 0 | 52,58,111 | 0.42 | 0 |
| 158 | 3PE | AN | 303 | - | 44,44,50 | 0.32 | 0 | 47,49,55 | 0.29 | 0 |
| 152 | PC1 | Qj | 101 | - | 35,35,53 | 0.35 | 0 | 41,43,61 | 0.32 | 0 |
| 153 | CDL | M | 301 | - | 65,65,99 | 0.36 | 0 | 71,77,111 | 0.31 | 0 |
| 152 | PC1 | qC | 507 | - | 49,49,53 | 0.30 | 0 | 55,57,61 | 0.30 | 0 |
| 157 | FES | qe | 302 | - | 0,4,4 | - | - | - | - | - |
| 158 | 3PE | S8 | 304 | - | 40,40,50 | 0.33 | 0 | 43,45,55 | 0.31 | 0 |
| 152 | PC1 | a | 501 | - | 40,40,53 | 0.34 | 0 | 46,48,61 | 0.35 | 0 |
| 162 | SF4 | S8 | 302 | 127 | 0,12,12 | - | - | - | - | - |
| 157 | FES | fs | 202 | 35 | 0,4,4 | - | - | - | - | - |
| 153 | CDL | QG | 402 | - | 85,85,99 | 0.32 | 0 | 91,97,111 | 0.28 | 0 |
| 153 | CDL | e | 401 | - | 59,59,99 | 0.37 | 0 | 65,71,111 | 0.34 | 0 |
| 152 | PC1 | C1 | 711 | - | 38,38,53 | 0.34 | 0 | 44,46,61 | 0.32 | 0 |
| 152 | PC1 | n5 | 805 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.32 | 0 |
| 153 | CDL | AM | 201 | - | 55,55,99 | 0.39 | 0 | 61,67,111 | 0.33 | 0 |
| 152 | PC1 | 5B | 202 | - | 46,46,53 | 0.32 | 0 | 52,54,61 | 0.28 | 0 |
| 152 | PC1 | v | 201 | - | 34,34,53 | 0.35 | 0 | 40,42,61 | 0.31 | 0 |
| 164 | U10 | qc | 507 | - | 29,29,63 | 2.68 | 11 (37%) | 35,38,79 | 1.53 | 7 (20%) |
| 151 | HEC | qD | 401 | 111 | 32,50,50 | 2.03 | 4 (12%) | 24,82,82 | 2.31 | 14 (58%) |
| 152 | PC1 | w | 205 | - | 42,42,53 | 0.32 | 0 | 48,50,61 | 0.30 | 0 |
| 153 | CDL | qD | 402 | - | 60,60,99 | 0.37 | 0 | 66,72,111 | 0.31 | 0 |
| 153 | CDL | 6A | 201 | - | 73,73,99 | 0.35 | 0 | 79,85,111 | 0.41 | 0 |
| 153 | CDL | U1 | 101 | - | 56,56,99 | 0.38 | 0 | 62,68,111 | 0.31 | 0 |
| 152 | PC1 | AN | 304 | - | 35,35,53 | 0.36 | 0 | 41,43,61 | 0.33 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 153 | CDL | t | 202 | - | 74,74,99 | 0.34 | 0 | 80,86,111 | 0.34 | 0 |
| 157 | FES | fx | 201 | 95 | 0,4,4 | - | - | - | | |
| 152 | PC1 | w | 204 | - | 33,33,53 | 0.36 | 0 | 39,41,61 | 0.34 | 0 |
| 152 | PC1 | AM | 202 | - | 38,38,53 | 0.34 | 0 | 44,46,61 | 0.31 | 0 |
| 153 | CDL | TH | 200 | - | 83,83,99 | 0.32 | 0 | 89,95,111 | 0.28 | 0 |
| 153 | CDL | M2 | 404 | - | 73,73,99 | 0.34 | 0 | 79,85,111 | 0.34 | 0 |
| 158 | 3PE | ta | 201 | - | 25,25,50 | 0.41 | 0 | 28,30,55 | 0.40 | 0 |
| 152 | PC1 | C3 | 603 | - | 30,30,53 | 0.37 | 0 | 36,38,61 | 0.34 | 0 |
| 152 | PC1 | J1 | 400 | - | 39,39,53 | 0.33 | 0 | 45,47,61 | 0.33 | 0 |
| 153 | CDL | t5 | 301 | - | 95,95,99 | 0.31 | 0 | 101,107,111 | 0.31 | 0 |
| 153 | CDL | I | 302 | - | 76,76,99 | 0.33 | 0 | 82,88,111 | 0.31 | 0 |
| 151 | HEC | Qd | 401 | 111 | 32,50,50 | 2.03 | 4 (12%) | 24,82,82 | 2.27 | 14 (58%) |
| 157 | FES | FS | 202 | 35 | 0,4,4 | - | - | - | | |
| 153 | CDL | 2M | 101 | - | 95,95,99 | 0.31 | 0 | 101,107,111 | 0.30 | 0 |
| 158 | 3PE | an | 306 | - | 28,28,50 | 0.40 | 0 | 31,33,55 | 0.42 | 0 |
| 153 | CDL | 2G | 204 | - | 62,62,99 | 0.37 | 0 | 68,74,111 | 0.32 | 0 |
| 152 | PC1 | qj | 101 | - | 35,35,53 | 0.35 | 0 | 41,43,61 | 0.32 | 0 |
| 153 | CDL | QD | 402 | - | 60,60,99 | 0.37 | 0 | 66,72,111 | 0.31 | 0 |
| 164 | U10 | SC | 102 | - | 63,63,63 | 2.17 | 21 (33%) | 76,79,79 | 1.65 | 20 (26%) |
| 152 | PC1 | tc | 102 | - | 46,46,53 | 0.31 | 0 | 52,54,61 | 0.30 | 0 |
| 153 | CDL | C1 | 701 | - | 78,78,99 | 0.33 | 0 | 84,90,111 | 0.32 | 0 |
| 153 | CDL | B8 | 302 | - | 68,68,99 | 0.35 | 0 | 74,80,111 | 0.31 | 0 |
| 166 | HEM | QC | 502 | 110 | 41,50,50 | 1.25 | 3 (7%) | 45,82,82 | 1.67 | 10 (22%) |
| 153 | CDL | an | 302 | - | 86,86,99 | 0.32 | 0 | 92,98,111 | 0.29 | 0 |
| 152 | PC1 | M2 | 402 | - | 31,31,53 | 0.36 | 0 | 37,39,61 | 0.38 | 0 |
| 153 | CDL | AL | 301 | - | 52,52,99 | 0.40 | 0 | 58,64,111 | 0.33 | 0 |
| 158 | 3PE | M3 | 402 | - | 37,37,50 | 0.35 | 0 | 40,42,55 | 0.31 | 0 |
| 158 | 3PE | T4 | 302 | - | 24,24,50 | 0.42 | 0 | 27,29,55 | 0.36 | 0 |
| 152 | PC1 | n5 | 801 | - | 51,51,53 | 0.30 | 0 | 57,59,61 | 0.29 | 0 |
| 152 | PC1 | C1 | 710 | - | 37,37,53 | 0.34 | 0 | 43,45,61 | 0.31 | 0 |
| 166 | HEM | qC | 501 | 110 | 41,50,50 | 1.22 | 4 (9%) | 45,82,82 | 1.68 | 9 (20%) |
| 152 | PC1 | C3 | 601 | - | 51,51,53 | 0.30 | 0 | 57,59,61 | 0.34 | 0 |
| 153 | CDL | q | 202 | - | 71,71,99 | 0.35 | 0 | 77,83,111 | 0.30 | 0 |
| 152 | PC1 | c3 | 606 | - | 48,48,53 | 0.31 | 0 | 54,56,61 | 0.35 | 0 |
| 152 | PC1 | M | 303 | - | 44,44,53 | 0.32 | 0 | 50,52,61 | 0.37 | 0 |
| 152 | PC1 | F | 401 | - | 37,37,53 | 0.34 | 0 | 43,45,61 | 0.28 | 0 |
| 152 | PC1 | m | 301 | - | 44,44,53 | 0.32 | 0 | 50,52,61 | 0.37 | 0 |
| 158 | 3PE | an | 305 | - | 32,32,50 | 0.37 | 0 | 35,37,55 | 0.34 | 0 |
| 158 | 3PE | n5 | 802 | - | 35,35,50 | 0.36 | 0 | 38,40,55 | 0.31 | 0 |
| 153 | CDL | P1 | 402 | - | 62,62,99 | 0.37 | 0 | 68,74,111 | 0.31 | 0 |
| 152 | PC1 | 7c | 303 | - | 42,42,53 | 0.32 | 0 | 48,50,61 | 0.32 | 0 |
| 153 | CDL | M3 | 401 | - | 62,62,99 | 0.37 | 0 | 68,74,111 | 0.32 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 152 | PC1 | al | 302 | - | 25,25,53 | 0.40 | 0 | 31,33,61 | 0.37 | 0 |
| 158 | 3PE | G2 | 301 | - | 50,50,50 | 0.30 | 0 | 53,55,55 | 0.29 | 0 |
| 152 | PC1 | M2 | 407 | - | 45,45,53 | 0.32 | 0 | 51,53,61 | 0.37 | 0 |
| 152 | PC1 | 2f | 303 | - | 31,31,53 | 0.37 | 0 | 37,39,61 | 0.31 | 0 |
| 152 | PC1 | c3 | 602 | - | 38,38,53 | 0.33 | 0 | 44,46,61 | 0.30 | 0 |
| 164 | U10 | qc | 501 | - | 25,25,63 | 2.22 | 5 (20%) | 27,29,79 | 1.83 | 8 (29%) |
| 158 | 3PE | I | 304 | - | 31,31,50 | 0.37 | 0 | 34,36,55 | 0.32 | 0 |
| 153 | CDL | vb | 701 | - | 61,61,99 | 0.37 | 0 | 67,73,111 | 0.32 | 0 |
| 153 | CDL | 7C | 301 | - | 84,84,99 | 0.32 | 0 | 90,96,111 | 0.33 | 0 |
| 153 | CDL | f | 401 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.29 | 0 |
| 153 | CDL | m2 | 404 | - | 73,73,99 | 0.35 | 0 | 79,85,111 | 0.34 | 0 |
| 157 | FES | s1 | 803 | 120 | 0,4,4 | - | - | - | - | - |
| 153 | CDL | qc | 505 | - | 55,55,99 | 0.38 | 0 | 61,67,111 | 0.36 | 0 |
| 152 | PC1 | W | 205 | - | 42,42,53 | 0.32 | 0 | 48,50,61 | 0.29 | 0 |
| 152 | PC1 | Qe | 301 | - | 32,32,53 | 0.36 | 0 | 38,40,61 | 0.34 | 0 |
| 158 | 3PE | m2 | 408 | - | 30,30,50 | 0.38 | 0 | 33,35,55 | 0.36 | 0 |
| 152 | PC1 | P1 | 401 | - | 39,39,53 | 0.33 | 0 | 45,47,61 | 0.30 | 0 |
| 152 | PC1 | Qc | 509 | - | 46,46,53 | 0.31 | 0 | 52,54,61 | 0.34 | 0 |
| 158 | 3PE | a3 | 201 | - | 44,44,50 | 0.33 | 0 | 47,49,55 | 0.55 | 1 (2%) |
| 152 | PC1 | c3 | 605 | - | 38,38,53 | 0.33 | 0 | 44,46,61 | 0.32 | 0 |
| 152 | PC1 | v | 202 | - | 48,48,53 | 0.31 | 0 | 54,56,61 | 0.32 | 0 |
| 152 | PC1 | w | 201 | - | 48,48,53 | 0.30 | 0 | 54,56,61 | 0.29 | 0 |
| 158 | 3PE | AN | 301 | - | 44,44,50 | 0.32 | 0 | 47,49,55 | 0.28 | 0 |
| 152 | PC1 | c2 | 703 | - | 35,35,53 | 0.35 | 0 | 41,43,61 | 0.31 | 0 |
| 152 | PC1 | 6a | 202 | - | 34,34,53 | 0.36 | 0 | 40,42,61 | 0.34 | 0 |
| 152 | PC1 | m1 | 403 | - | 41,41,53 | 0.33 | 0 | 47,49,61 | 0.38 | 0 |
| 153 | CDL | Y5 | 201 | - | 69,69,99 | 0.35 | 0 | 75,81,111 | 0.30 | 0 |
| 152 | PC1 | qc | 506 | - | 37,37,53 | 0.34 | 0 | 43,45,61 | 0.31 | 0 |
| 153 | CDL | b3 | 102 | - | 81,81,99 | 0.33 | 0 | 87,93,111 | 0.30 | 0 |
| 152 | PC1 | qI | 202 | - | 42,42,53 | 0.32 | 0 | 48,50,61 | 0.31 | 0 |
| 158 | 3PE | n4 | 601 | - | 35,35,50 | 0.35 | 0 | 38,40,55 | 0.36 | 0 |
| 162 | SF4 | v1 | 500 | 146 | 0,12,12 | - | - | - | - | - |
| 153 | CDL | T1 | 601 | - | 54,54,99 | 0.39 | 0 | 60,66,111 | 0.36 | 0 |
| 152 | PC1 | J | 302 | - | 36,36,53 | 0.34 | 0 | 42,44,61 | 0.31 | 0 |
| 153 | CDL | M3 | 403 | - | 54,54,99 | 0.39 | 0 | 60,66,111 | 0.38 | 0 |
| 162 | SF4 | S1 | 802 | 120 | 0,12,12 | - | - | - | - | - |
| 158 | 3PE | t8 | 601 | - | 46,46,50 | 0.33 | 0 | 49,51,55 | 0.40 | 0 |
| 153 | CDL | qc | 504 | - | 63,63,99 | 0.37 | 0 | 69,75,111 | 0.34 | 0 |
| 152 | PC1 | qi | 201 | - | 29,29,53 | 0.39 | 0 | 35,37,61 | 0.41 | 0 |
| 151 | HEC | qd | 401 | 111 | 32,50,50 | 2.03 | 4 (12%) | 24,82,82 | 2.28 | 14 (58%) |
| 152 | PC1 | qE | 303 | - | 38,38,53 | 0.34 | 0 | 44,46,61 | 0.32 | 0 |
| 153 | CDL | c1 | 701 | - | 78,78,99 | 0.33 | 0 | 84,90,111 | 0.32 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 151 | HEC | QD | 401 | 111 | 32,50,50 | 2.02 | 4 (12%) | 24,82,82 | 2.30 | 14 (58%) |
| 153 | CDL | BM | 301 | - | 85,85,99 | 0.32 | 0 | 91,97,111 | 0.30 | 0 |
| 152 | PC1 | 7a | 202 | - | 44,44,53 | 0.31 | 0 | 50,52,61 | 0.31 | 0 |
| 152 | PC1 | p1 | 401 | - | 39,39,53 | 0.33 | 0 | 45,47,61 | 0.30 | 0 |
| 158 | 3PE | c4 | 402 | - | 50,50,50 | 0.30 | 0 | 53,55,55 | 0.31 | 0 |
| 152 | PC1 | M2 | 405 | - | 53,53,53 | 0.30 | 0 | 59,61,61 | 0.26 | 0 |
| 153 | CDL | b | 501 | - | 61,61,99 | 0.37 | 0 | 67,73,111 | 0.32 | 0 |
| 152 | PC1 | j | 302 | - | 36,36,53 | 0.34 | 0 | 42,44,61 | 0.31 | 0 |
| 153 | CDL | B3 | 102 | - | 81,81,99 | 0.33 | 0 | 87,93,111 | 0.29 | 0 |
| 153 | CDL | C1 | 712 | - | 94,94,99 | 0.31 | 0 | 100,106,111 | 0.32 | 0 |
| 153 | CDL | Qc | 505 | - | 55,55,99 | 0.38 | 0 | 61,67,111 | 0.36 | 0 |
| 153 | CDL | T | 204 | - | 89,89,99 | 0.33 | 0 | 95,101,111 | 0.32 | 0 |
| 153 | CDL | VB | 706 | - | 66,66,99 | 0.36 | 0 | 72,78,111 | 0.30 | 0 |
| 152 | PC1 | n3 | 201 | - | 30,30,53 | 0.37 | 0 | 36,38,61 | 0.36 | 0 |
| 152 | PC1 | TC | 101 | - | 41,41,53 | 0.32 | 0 | 47,49,61 | 0.28 | 0 |
| 153 | CDL | VB | 703 | - | 85,85,99 | 0.33 | 0 | 91,97,111 | 0.31 | 0 |
| 158 | 3PE | s8 | 304 | - | 40,40,50 | 0.33 | 0 | 43,45,55 | 0.31 | 0 |
| 166 | HEM | y5 | 203 | - | 41,50,50 | 1.21 | 4 (9%) | 45,82,82 | 1.70 | 7 (15%) |
| 152 | PC1 | 6A | 202 | - | 34,34,53 | 0.36 | 0 | 40,42,61 | 0.34 | 0 |
| 153 | CDL | 7c | 302 | - | 50,50,99 | 0.40 | 0 | 56,62,111 | 0.35 | 0 |
| 153 | CDL | m2 | 403 | - | 65,65,99 | 0.36 | 0 | 71,77,111 | 0.30 | 0 |
| 153 | CDL | L | 301 | - | 73,73,99 | 0.34 | 0 | 79,85,111 | 0.29 | 0 |
| 152 | PC1 | m2 | 407 | - | 45,45,53 | 0.32 | 0 | 51,53,61 | 0.37 | 0 |
| 170 | ADP | B9 | 202 | - | 24,29,29 | 0.94 | 1 (4%) | 29,45,45 | 1.46 | 4 (13%) |
| 153 | CDL | c4 | 401 | - | 97,97,99 | 0.30 | 0 | 103,109,111 | 0.31 | 0 |
| 152 | PC1 | 2f | 302 | - | 41,41,53 | 0.33 | 0 | 47,49,61 | 0.40 | 0 |
| 152 | PC1 | QE | 303 | - | 38,38,53 | 0.34 | 0 | 44,46,61 | 0.32 | 0 |
| 153 | CDL | qg | 402 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.30 | 0 |
| 158 | 3PE | vb | 705 | - | 27,27,50 | 0.39 | 0 | 30,32,55 | 0.34 | 0 |
| 153 | CDL | a | 504 | - | 93,93,99 | 0.31 | 0 | 99,105,111 | 0.27 | 0 |
| 152 | PC1 | QI | 202 | - | 42,42,53 | 0.32 | 0 | 48,50,61 | 0.31 | 0 |
| 153 | CDL | Qb | 601 | - | 67,67,99 | 0.36 | 0 | 73,79,111 | 0.30 | 0 |
| 153 | CDL | c3 | 604 | - | 67,67,99 | 0.36 | 0 | 73,79,111 | 0.31 | 0 |
| 152 | PC1 | m | 307 | - | 35,35,53 | 0.35 | 0 | 41,43,61 | 0.33 | 0 |
| 152 | PC1 | m2 | 405 | - | 53,53,53 | 0.30 | 0 | 59,61,61 | 0.26 | 0 |
| 153 | CDL | y5 | 201 | - | 69,69,99 | 0.35 | 0 | 75,81,111 | 0.30 | 0 |
| 152 | PC1 | 2j | 201 | - | 41,41,53 | 0.33 | 0 | 47,49,61 | 0.36 | 0 |
| 153 | CDL | u1 | 101 | - | 56,56,99 | 0.38 | 0 | 62,68,111 | 0.31 | 0 |
| 153 | CDL | m2 | 401 | - | 53,53,99 | 0.39 | 0 | 59,65,111 | 0.40 | 0 |
| 153 | CDL | a9 | 403 | - | 86,86,99 | 0.32 | 0 | 92,98,111 | 0.27 | 0 |
| 152 | PC1 | W | 204 | - | 33,33,53 | 0.36 | 0 | 39,41,61 | 0.34 | 0 |
| 162 | SF4 | S8 | 303 | 127 | 0,12,12 | - | - | - | - | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 153 | CDL | qi | 202 | - | 70,70,99 | 0.35 | 0 | 76,82,111 | 0.35 | 0 |
| 153 | CDL | M | 305 | - | 82,82,99 | 0.33 | 0 | 88,94,111 | 0.31 | 0 |
| 153 | CDL | QC | 504 | - | 55,55,99 | 0.38 | 0 | 61,67,111 | 0.40 | 0 |
| 152 | PC1 | M | 307 | - | 34,34,53 | 0.35 | 0 | 40,42,61 | 0.34 | 0 |
| 160 | PX2 | Y5 | 204 | - | 20,20,35 | 1.28 | 4 (20%) | 24,25,40 | 1.25 | 2 (8%) |
| 153 | CDL | P1 | 403 | - | 57,57,99 | 0.39 | 0 | 63,69,111 | 0.40 | 0 |
| 166 | HEM | Qc | 502 | 110 | 41,50,50 | 1.22 | 4 (9%) | 45,82,82 | 1.67 | 8 (17%) |
| 152 | PC1 | D | 501 | - | 34,34,53 | 0.36 | 0 | 40,42,61 | 0.38 | 0 |
| 153 | CDL | 7c | 301 | - | 84,84,99 | 0.32 | 0 | 90,96,111 | 0.33 | 0 |
| 161 | FAD | sa | 701 | - | 53,58,58 | 0.48 | 0 | 68,89,89 | 0.52 | 2 (2%) |
| 158 | 3PE | BM | 302 | - | 29,29,50 | 0.39 | 0 | 32,34,55 | 0.46 | 0 |
| 152 | PC1 | qJ | 101 | - | 37,37,53 | 0.34 | 0 | 43,45,61 | 0.36 | 0 |
| 152 | PC1 | QC | 508 | - | 35,35,53 | 0.35 | 0 | 41,43,61 | 0.34 | 0 |
| 153 | CDL | 2g | 203 | - | 54,54,99 | 0.39 | 0 | 60,66,111 | 0.36 | 0 |
| 152 | PC1 | te | 102 | - | 31,31,53 | 0.37 | 0 | 37,39,61 | 0.40 | 0 |
| 153 | CDL | M1 | 404 | - | 90,90,99 | 0.32 | 0 | 96,102,111 | 0.28 | 0 |
| 164 | U10 | B8 | 301 | - | 63,63,63 | 2.15 | 21 (33%) | 76,79,79 | 1.68 | 21 (27%) |
| 153 | CDL | SD | 101 | - | 75,75,99 | 0.34 | 0 | 81,87,111 | 0.31 | 0 |
| 158 | 3PE | t4 | 302 | - | 24,24,50 | 0.42 | 0 | 27,29,55 | 0.36 | 0 |
| 153 | CDL | A1 | 102 | - | 66,66,99 | 0.36 | 0 | 72,78,111 | 0.37 | 0 |
| 161 | FAD | SA | 701 | - | 53,58,58 | 0.48 | 0 | 68,89,89 | 0.52 | 2 (2%) |
| 152 | PC1 | TC | 102 | - | 46,46,53 | 0.31 | 0 | 52,54,61 | 0.30 | 0 |
| 152 | PC1 | s8 | 301 | - | 29,29,53 | 0.38 | 0 | 35,37,61 | 0.33 | 0 |
| 153 | CDL | VB | 705 | - | 81,81,99 | 0.33 | 0 | 87,93,111 | 0.29 | 0 |
| 153 | CDL | e | 402 | - | 71,71,99 | 0.35 | 0 | 77,83,111 | 0.35 | 0 |
| 153 | CDL | bm | 301 | - | 85,85,99 | 0.32 | 0 | 91,97,111 | 0.30 | 0 |
| 154 | HEA | c1 | 702 | 29 | 57,67,67 | 2.04 | 17 (29%) | 61,103,103 | 2.75 | 29 (47%) |
| 153 | CDL | 6C | 203 | - | 81,81,99 | 0.32 | 0 | 87,93,111 | 0.30 | 0 |
| 153 | CDL | 7A | 201 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.28 | 0 |
| 157 | FES | SB | 401 | 53 | 0,4,4 | - | - | - | - | - |
| 158 | 3PE | M2 | 408 | - | 30,30,50 | 0.38 | 0 | 33,35,55 | 0.36 | 0 |
| 153 | CDL | M2 | 401 | - | 53,53,99 | 0.39 | 0 | 59,65,111 | 0.40 | 0 |
| 157 | FES | qE | 302 | - | 0,4,4 | - | - | - | - | - |
| 152 | PC1 | V | 202 | - | 48,48,53 | 0.31 | 0 | 54,56,61 | 0.32 | 0 |
| 153 | CDL | e | 403 | - | 62,62,99 | 0.37 | 0 | 68,74,111 | 0.30 | 0 |
| 153 | CDL | 2g | 201 | - | 88,88,99 | 0.32 | 0 | 94,100,111 | 0.28 | 0 |
| 153 | CDL | VB | 701 | - | 61,61,99 | 0.37 | 0 | 67,73,111 | 0.32 | 0 |
| 166 | HEM | Qc | 503 | 110 | 41,50,50 | 1.25 | 3 (7%) | 45,82,82 | 1.70 | 10 (22%) |
| 153 | CDL | T5 | 301 | - | 95,95,99 | 0.31 | 0 | 101,107,111 | 0.31 | 0 |
| 152 | PC1 | W | 201 | - | 48,48,53 | 0.30 | 0 | 54,56,61 | 0.29 | 0 |
| 158 | 3PE | AN | 305 | - | 32,32,50 | 0.37 | 0 | 35,37,55 | 0.34 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 158 | 3PE | a3 | 202 | - | 43,43,50 | 0.32 | 0 | 46,48,55 | 0.29 | 0 |
| 169 | T7X | B6 | 201 | - | 55,55,61 | 1.51 | 5 (9%) | 64,67,73 | 1.08 | 4 (6%) |
| 162 | SF4 | sb | 402 | 53 | 0,12,12 | - | - | - | - | - |
| 157 | FES | v2 | 300 | 147 | 0,4,4 | - | - | - | - | - |
| 152 | PC1 | n1 | 301 | - | 35,35,53 | 0.35 | 0 | 41,43,61 | 0.33 | 0 |
| 151 | HEC | 2e | 401 | 2 | 32,50,50 | 2.04 | 4 (12%) | 24,82,82 | 2.40 | 13 (54%) |
| 153 | CDL | QC | 503 | - | 63,63,99 | 0.37 | 0 | 69,75,111 | 0.31 | 0 |
| 152 | PC1 | m | 305 | - | 34,34,53 | 0.35 | 0 | 40,42,61 | 0.33 | 0 |
| 152 | PC1 | t1 | 602 | - | 32,32,53 | 0.36 | 0 | 38,40,61 | 0.34 | 0 |
| 152 | PC1 | 7A | 202 | - | 44,44,53 | 0.31 | 0 | 50,52,61 | 0.31 | 0 |
| 153 | CDL | al | 301 | - | 52,52,99 | 0.40 | 0 | 58,64,111 | 0.33 | 0 |
| 153 | CDL | m3 | 403 | - | 54,54,99 | 0.39 | 0 | 60,66,111 | 0.38 | 0 |
| 153 | CDL | b8 | 302 | - | 68,68,99 | 0.35 | 0 | 74,80,111 | 0.31 | 0 |
| 152 | PC1 | c1 | 704 | - | 48,48,53 | 0.31 | 0 | 54,56,61 | 0.27 | 0 |
| 159 | P5S | M2 | 406 | - | 34,35,53 | 1.34 | 4 (11%) | 38,42,60 | 1.04 | 2 (5%) |
| 152 | PC1 | A | 503 | - | 40,40,53 | 0.34 | 0 | 46,48,61 | 0.35 | 0 |
| 153 | CDL | Q | 201 | - | 62,62,99 | 0.37 | 0 | 68,74,111 | 0.38 | 0 |
| 153 | CDL | F | 402 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.29 | 0 |
| 152 | PC1 | 2F | 301 | - | 46,46,53 | 0.32 | 0 | 52,54,61 | 0.50 | 0 |
| 152 | PC1 | C3 | 605 | - | 38,38,53 | 0.33 | 0 | 44,46,61 | 0.32 | 0 |
| 151 | HEC | 2E | 401 | 2 | 32,50,50 | 2.10 | 6 (18%) | 24,82,82 | 2.34 | 14 (58%) |
| 160 | PX2 | r | 202 | - | 32,32,35 | 1.02 | 4 (12%) | 36,37,40 | 0.98 | 2 (5%) |
| 153 | CDL | M | 306 | - | 63,63,99 | 0.36 | 0 | 69,75,111 | 0.32 | 0 |
| 160 | PX2 | y5 | 204 | - | 20,20,35 | 1.28 | 4 (20%) | 24,25,40 | 1.26 | 2 (8%) |
| 152 | PC1 | 5b | 202 | - | 46,46,53 | 0.32 | 0 | 52,54,61 | 0.28 | 0 |
| 153 | CDL | C | 301 | - | 63,63,99 | 0.37 | 0 | 69,75,111 | 0.43 | 0 |
| 153 | CDL | n6 | 302 | - | 89,89,99 | 0.32 | 0 | 95,101,111 | 0.36 | 0 |
| 152 | PC1 | Qi | 201 | - | 29,29,53 | 0.39 | 0 | 35,37,61 | 0.41 | 0 |
| 152 | PC1 | c1 | 707 | - | 37,37,53 | 0.34 | 0 | 43,45,61 | 0.31 | 0 |
| 153 | CDL | Qg | 402 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.30 | 0 |
| 166 | HEM | qc | 502 | 110 | 41,50,50 | 1.23 | 4 (9%) | 45,82,82 | 1.67 | 8 (17%) |
| 152 | PC1 | qi | 203 | - | 41,41,53 | 0.33 | 0 | 47,49,61 | 0.35 | 0 |
| 158 | 3PE | SC | 101 | - | 39,39,50 | 0.34 | 0 | 42,44,55 | 0.30 | 0 |
| 153 | CDL | m | 303 | - | 82,82,99 | 0.33 | 0 | 88,94,111 | 0.30 | 0 |
| 152 | PC1 | C4 | 403 | - | 40,40,53 | 0.33 | 0 | 46,48,61 | 0.30 | 0 |
| 153 | CDL | n5 | 806 | - | 89,89,99 | 0.31 | 0 | 95,101,111 | 0.28 | 0 |
| 164 | U10 | sc | 102 | - | 63,63,63 | 2.18 | 21 (33%) | 76,79,79 | 1.64 | 20 (26%) |
| 152 | PC1 | 2F | 303 | - | 31,31,53 | 0.37 | 0 | 37,39,61 | 0.31 | 0 |
| 152 | PC1 | M1 | 403 | - | 41,41,53 | 0.33 | 0 | 47,49,61 | 0.38 | 0 |
| 152 | PC1 | n | 303 | - | 35,35,53 | 0.35 | 0 | 41,43,61 | 0.32 | 0 |
| 153 | CDL | 2G | 201 | - | 88,88,99 | 0.32 | 0 | 94,100,111 | 0.28 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 158 | 3PE | m3 | 402 | - | 37,37,50 | 0.35 | 0 | 40,42,55 | 0.31 | 0 |
| 153 | CDL | J | 301 | - | 69,69,99 | 0.35 | 0 | 75,81,111 | 0.29 | 0 |
| 152 | PC1 | T4 | 303 | - | 53,53,53 | 0.30 | 0 | 59,61,61 | 0.35 | 0 |
| 158 | 3PE | sc | 101 | - | 39,39,50 | 0.34 | 0 | 42,44,55 | 0.31 | 0 |
| 164 | U10 | qC | 506 | - | 29,29,63 | 2.68 | 10 (34%) | 35,38,79 | 1.55 | 7 (20%) |
| 162 | SF4 | S1 | 801 | 120 | 0,12,12 | - | - | - | | |
| 158 | 3PE | A3 | 201 | - | 44,44,50 | 0.33 | 0 | 47,49,55 | 0.55 | 1 (2%) |
| 158 | 3PE | AN | 306 | - | 28,28,50 | 0.40 | 0 | 31,33,55 | 0.42 | 0 |
| 153 | CDL | c1 | 703 | - | 64,64,99 | 0.36 | 0 | 70,76,111 | 0.31 | 0 |
| 153 | CDL | A | 504 | - | 93,93,99 | 0.31 | 0 | 99,105,111 | 0.27 | 0 |
| 152 | PC1 | 6C | 201 | - | 32,32,53 | 0.36 | 0 | 38,40,61 | 0.35 | 0 |
| 152 | PC1 | am | 202 | - | 38,38,53 | 0.33 | 0 | 44,46,61 | 0.32 | 0 |
| 163 | F3S | SB | 403 | 53 | 0,9,9 | - | - | - | | |
| 157 | FES | FX | 201 | 95 | 0,4,4 | - | - | - | | |
| 158 | 3PE | w | 203 | - | 33,33,50 | 0.36 | 0 | 36,38,55 | 0.31 | 0 |
| 158 | 3PE | i | 303 | - | 31,31,50 | 0.37 | 0 | 34,36,55 | 0.32 | 0 |
| 153 | CDL | sd | 101 | - | 75,75,99 | 0.34 | 0 | 81,87,111 | 0.31 | 0 |
| 152 | PC1 | 2F | 302 | - | 41,41,53 | 0.33 | 0 | 47,49,61 | 0.40 | 0 |
| 153 | CDL | m3 | 401 | - | 62,62,99 | 0.37 | 0 | 68,74,111 | 0.32 | 0 |
| 153 | CDL | am | 201 | - | 55,55,99 | 0.39 | 0 | 61,67,111 | 0.33 | 0 |
| 158 | 3PE | Y5 | 202 | - | 27,27,50 | 0.40 | 0 | 30,32,55 | 0.34 | 0 |
| 152 | PC1 | C2 | 701 | - | 35,35,53 | 0.35 | 0 | 41,43,61 | 0.31 | 0 |
| 158 | 3PE | b4 | 202 | - | 47,47,50 | 0.32 | 0 | 50,52,55 | 0.28 | 0 |
| 152 | PC1 | 2G | 202 | - | 49,49,53 | 0.31 | 0 | 55,57,61 | 0.40 | 0 |
| 152 | PC1 | TE | 102 | - | 31,31,53 | 0.37 | 0 | 37,39,61 | 0.40 | 0 |
| 153 | CDL | t | 204 | - | 89,89,99 | 0.33 | 0 | 95,101,111 | 0.32 | 0 |
| 153 | CDL | 7A | 203 | - | 61,61,99 | 0.37 | 0 | 67,73,111 | 0.34 | 0 |
| 158 | 3PE | TA | 201 | - | 25,25,50 | 0.41 | 0 | 28,30,55 | 0.40 | 0 |
| 152 | PC1 | c1 | 706 | - | 44,44,53 | 0.32 | 0 | 50,52,61 | 0.42 | 0 |
| 152 | PC1 | tc | 101 | - | 41,41,53 | 0.32 | 0 | 47,49,61 | 0.28 | 0 |
| 153 | CDL | i | 301 | - | 76,76,99 | 0.33 | 0 | 82,88,111 | 0.31 | 0 |
| 153 | CDL | QH | 201 | - | 93,93,99 | 0.31 | 0 | 99,105,111 | 0.26 | 0 |
| 152 | PC1 | C1 | 709 | - | 44,44,53 | 0.32 | 0 | 50,52,61 | 0.42 | 0 |
| 152 | PC1 | qB | 602 | - | 43,43,53 | 0.32 | 0 | 49,51,61 | 0.29 | 0 |
| 160 | PX2 | Qh | 201 | - | 35,35,35 | 0.98 | 4 (11%) | 39,40,40 | 1.02 | 2 (5%) |
| 153 | CDL | 2O | 101 | - | 49,49,99 | 0.41 | 0 | 55,61,111 | 0.35 | 0 |
| 154 | HEA | C1 | 703 | 29 | 57,67,67 | 2.08 | 17 (29%) | 61,103,103 | 2.72 | 22 (36%) |
| 163 | F3S | sb | 403 | 53 | 0,9,9 | - | - | - | | |
| 153 | CDL | M | 304 | - | 63,63,99 | 0.37 | 0 | 69,75,111 | 0.31 | 0 |
| 152 | PC1 | a | 503 | - | 40,40,53 | 0.34 | 0 | 46,48,61 | 0.35 | 0 |
| 152 | PC1 | qG | 401 | - | 31,31,53 | 0.37 | 0 | 37,39,61 | 0.40 | 0 |
| 153 | CDL | 6C | 202 | - | 74,74,99 | 0.34 | 0 | 80,86,111 | 0.32 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 153 | CDL | m1 | 402 | - | 65,65,99 | 0.36 | 0 | 71,77,111 | 0.31 | 0 |
| 153 | CDL | b3 | 101 | - | 57,57,99 | 0.38 | 0 | 63,69,111 | 0.32 | 0 |
| 162 | SF4 | V1 | 500 | 146 | 0,12,12 | - | - | - | | |
| 153 | CDL | m | 302 | - | 63,63,99 | 0.37 | 0 | 69,75,111 | 0.31 | 0 |
| 152 | PC1 | C1 | 706 | - | 48,48,53 | 0.31 | 0 | 54,56,61 | 0.27 | 0 |
| 153 | CDL | T7 | 201 | - | 72,72,99 | 0.34 | 0 | 78,84,111 | 0.29 | 0 |
| 167 | NDP | A9 | 401 | - | 45,52,52 | 0.52 | 0 | 53,80,80 | 0.54 | 1 (1%) |
| 164 | U10 | Qc | 507 | - | 29,29,63 | 2.68 | 11 (37%) | 35,38,79 | 1.53 | 7 (20%) |
| 153 | CDL | t7 | 201 | - | 72,72,99 | 0.35 | 0 | 78,84,111 | 0.29 | 0 |
| 158 | 3PE | B4 | 202 | - | 47,47,50 | 0.32 | 0 | 50,52,55 | 0.28 | 0 |
| 152 | PC1 | N5 | 801 | - | 51,51,53 | 0.30 | 0 | 57,59,61 | 0.29 | 0 |
| 168 | ZMP | ab | 201 | 80 | 33,36,36 | 0.67 | 1 (3%) | 42,45,45 | 0.75 | 0 |
| 153 | CDL | Q | 202 | - | 71,71,99 | 0.35 | 0 | 77,83,111 | 0.30 | 0 |
| 153 | CDL | A | 502 | - | 50,50,99 | 0.41 | 0 | 56,62,111 | 0.47 | 0 |
| 164 | U10 | QC | 506 | - | 29,29,63 | 2.68 | 10 (34%) | 35,38,79 | 1.55 | 7 (20%) |
| 152 | PC1 | n6 | 301 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.29 | 0 |
| 153 | CDL | Y7 | 501 | - | 64,64,99 | 0.36 | 0 | 70,76,111 | 0.37 | 0 |
| 164 | U10 | Qc | 501 | - | 25,25,63 | 2.22 | 5 (20%) | 27,29,79 | 1.84 | 8 (29%) |
| 153 | CDL | qC | 503 | - | 63,63,99 | 0.37 | 0 | 69,75,111 | 0.31 | 0 |
| 166 | HEM | QC | 501 | 110 | 41,50,50 | 1.22 | 4 (9%) | 45,82,82 | 1.68 | 8 (17%) |
| 153 | CDL | Qi | 202 | - | 70,70,99 | 0.35 | 0 | 76,82,111 | 0.35 | 0 |
| 152 | PC1 | c1 | 711 | - | 38,38,53 | 0.34 | 0 | 44,46,61 | 0.32 | 0 |
| 166 | HEM | qc | 503 | 110 | 41,50,50 | 1.25 | 3 (7%) | 45,82,82 | 1.70 | 10 (22%) |
| 152 | PC1 | QE | 301 | - | 23,23,53 | 0.40 | 0 | 29,31,61 | 0.36 | 0 |
| 153 | CDL | M1 | 402 | - | 65,65,99 | 0.36 | 0 | 71,77,111 | 0.31 | 0 |
| 153 | CDL | C1 | 707 | - | 64,64,99 | 0.36 | 0 | 70,76,111 | 0.31 | 0 |
| 152 | PC1 | c3 | 603 | - | 30,30,53 | 0.37 | 0 | 36,38,61 | 0.34 | 0 |
| 152 | PC1 | Qi | 203 | - | 41,41,53 | 0.33 | 0 | 47,49,61 | 0.35 | 0 |
| 152 | PC1 | qE | 304 | - | 27,27,53 | 0.39 | 0 | 33,35,61 | 0.43 | 0 |
| 153 | CDL | 7a | 201 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.28 | 0 |
| 157 | FES | Qe | 302 | - | 0,4,4 | - | - | - | | |
| 153 | CDL | 2K | 101 | - | 97,97,99 | 0.31 | 0 | 103,109,111 | 0.35 | 0 |
| 153 | CDL | I | 303 | - | 74,74,99 | 0.34 | 0 | 80,86,111 | 0.29 | 0 |
| 158 | 3PE | T8 | 601 | - | 46,46,50 | 0.33 | 0 | 49,51,55 | 0.40 | 0 |
| 152 | PC1 | N5 | 803 | - | 52,52,53 | 0.29 | 0 | 58,60,61 | 0.29 | 0 |
| 157 | FES | sb | 401 | 53 | 0,4,4 | - | - | - | | |
| 153 | CDL | N6 | 302 | - | 89,89,99 | 0.32 | 0 | 95,101,111 | 0.36 | 0 |
| 158 | 3PE | A3 | 202 | - | 43,43,50 | 0.32 | 0 | 46,48,55 | 0.29 | 0 |
| 158 | 3PE | VB | 707 | - | 27,27,50 | 0.39 | 0 | 30,32,55 | 0.34 | 0 |
| 153 | CDL | w | 202 | - | 83,83,99 | 0.33 | 0 | 89,95,111 | 0.33 | 0 |
| 153 | CDL | t | 201 | - | 58,58,99 | 0.38 | 0 | 64,70,111 | 0.32 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 153 | CDL | 2B | 201 | - | 86,86,99 | 0.32 | 0 | 92,98,111 | 0.36 | 0 |
| 153 | CDL | y7 | 501 | - | 64,64,99 | 0.36 | 0 | 70,76,111 | 0.37 | 0 |
| 153 | CDL | m | 304 | - | 63,63,99 | 0.36 | 0 | 69,75,111 | 0.32 | 0 |
| 153 | CDL | n | 304 | - | 83,83,99 | 0.33 | 0 | 89,95,111 | 0.32 | 0 |
| 152 | PC1 | QI | 201 | - | 29,29,53 | 0.38 | 0 | 35,37,61 | 0.32 | 0 |
| 152 | PC1 | qe | 303 | - | 42,42,53 | 0.33 | 0 | 48,50,61 | 0.44 | 0 |
| 152 | PC1 | t4 | 301 | - | 47,47,53 | 0.31 | 0 | 53,55,61 | 0.36 | 0 |
| 153 | CDL | a9 | 402 | - | 75,75,99 | 0.34 | 0 | 81,87,111 | 0.35 | 0 |
| 152 | PC1 | 2g | 202 | - | 49,49,53 | 0.31 | 0 | 55,57,61 | 0.40 | 0 |
| 158 | 3PE | an | 303 | - | 44,44,50 | 0.32 | 0 | 47,49,55 | 0.29 | 0 |
| 153 | CDL | FS | 204 | - | 46,46,99 | 0.42 | 0 | 52,58,111 | 0.35 | 0 |
| 153 | CDL | th | 200 | - | 83,83,99 | 0.32 | 0 | 89,95,111 | 0.28 | 0 |
| 152 | PC1 | AL | 302 | - | 25,25,53 | 0.40 | 0 | 31,33,61 | 0.37 | 0 |
| 159 | P5S | m2 | 406 | - | 34,35,53 | 1.34 | 4 (11%) | 38,42,60 | 1.04 | 2 (5%) |
| 152 | PC1 | C3 | 602 | - | 38,38,53 | 0.34 | 0 | 44,46,61 | 0.30 | 0 |
| 152 | PC1 | QJ | 102 | - | 37,37,53 | 0.34 | 0 | 43,45,61 | 0.36 | 0 |
| 153 | CDL | C4 | 401 | - | 97,97,99 | 0.30 | 0 | 103,109,111 | 0.30 | 0 |
| 152 | PC1 | M | 302 | - | 35,35,53 | 0.35 | 0 | 41,43,61 | 0.33 | 0 |
| 158 | 3PE | y5 | 202 | - | 27,27,50 | 0.40 | 0 | 30,32,55 | 0.34 | 0 |
| 153 | CDL | Z | 101 | - | 66,66,99 | 0.36 | 0 | 72,78,111 | 0.30 | 0 |
| 158 | 3PE | W | 203 | - | 33,33,50 | 0.36 | 0 | 36,38,55 | 0.31 | 0 |
| 152 | PC1 | A | 501 | - | 40,40,53 | 0.34 | 0 | 46,48,61 | 0.35 | 0 |
| 158 | 3PE | t8 | 602 | - | 38,38,50 | 0.34 | 0 | 41,43,55 | 0.36 | 0 |
| 158 | 3PE | N4 | 601 | - | 35,35,50 | 0.35 | 0 | 38,40,55 | 0.36 | 0 |
| 153 | CDL | 7a | 203 | - | 61,61,99 | 0.37 | 0 | 67,73,111 | 0.34 | 0 |
| 153 | CDL | qC | 504 | - | 55,55,99 | 0.38 | 0 | 61,67,111 | 0.40 | 0 |
| 162 | SF4 | SB | 402 | 53 | 0,12,12 | - | - | - | - | - |
| 152 | PC1 | QC | 507 | - | 49,49,53 | 0.30 | 0 | 55,57,61 | 0.29 | 0 |
| 162 | SF4 | s1 | 801 | 120 | 0,12,12 | - | - | - | - | - |
| 152 | PC1 | QJ | 101 | - | 27,27,53 | 0.39 | 0 | 33,35,61 | 0.43 | 0 |
| 160 | PX2 | R | 202 | - | 32,32,35 | 1.01 | 4 (12%) | 36,37,40 | 0.91 | 2 (5%) |
| 152 | PC1 | M1 | 401 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.28 | 0 |
| 166 | HEM | qC | 502 | 110 | 41,50,50 | 1.25 | 3 (7%) | 45,82,82 | 1.67 | 10 (22%) |
| 152 | PC1 | j1 | 400 | - | 39,39,53 | 0.33 | 0 | 45,47,61 | 0.33 | 0 |
| 154 | HEA | C1 | 702 | 29 | 57,67,67 | 2.03 | 16 (28%) | 61,103,103 | 2.64 | 27 (44%) |
| 152 | PC1 | n | 301 | - | 40,40,53 | 0.33 | 0 | 46,48,61 | 0.29 | 0 |
| 168 | ZMP | AB | 201 | 80 | 33,36,36 | 0.67 | 1 (3%) | 42,45,45 | 0.75 | 0 |
| 153 | CDL | 2m | 101 | - | 95,95,99 | 0.31 | 0 | 101,107,111 | 0.30 | 0 |
| 153 | CDL | 6c | 201 | - | 74,74,99 | 0.34 | 0 | 80,86,111 | 0.32 | 0 |
| 162 | SF4 | s1 | 802 | 120 | 0,12,12 | - | - | - | - | - |
| 153 | CDL | QI | 203 | - | 70,70,99 | 0.35 | 0 | 76,82,111 | 0.30 | 0 |
| 153 | CDL | qc | 508 | - | 46,46,99 | 0.42 | 0 | 52,58,111 | 0.42 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 153 | CDL | Qc | 504 | - | 63,63,99 | 0.37 | 0 | 69,75,111 | 0.34 | 0 |
| 153 | CDL | C3 | 604 | - | 67,67,99 | 0.36 | 0 | 73,79,111 | 0.31 | 0 |
| 160 | PX2 | qh | 201 | - | 35,35,35 | 0.98 | 4 (11%) | 39,40,40 | 0.99 | 2 (5%) |
| 152 | PC1 | qC | 505 | - | 37,37,53 | 0.34 | 0 | 43,45,61 | 0.29 | 0 |
| 153 | CDL | te | 101 | - | 52,52,99 | 0.40 | 0 | 58,64,111 | 0.33 | 0 |
| 153 | CDL | c1 | 712 | - | 94,94,99 | 0.31 | 0 | 100,106,111 | 0.32 | 0 |
| 152 | PC1 | N5 | 804 | - | 38,38,53 | 0.33 | 0 | 44,46,61 | 0.32 | 0 |
| 162 | SF4 | S7 | 201 | 126 | 0,12,12 | - | - | - | - | - |
| 153 | CDL | 5B | 201 | - | 80,80,99 | 0.34 | 0 | 86,92,111 | 0.33 | 0 |
| 153 | CDL | E | 402 | - | 71,71,99 | 0.35 | 0 | 77,83,111 | 0.34 | 0 |
| 152 | PC1 | QC | 505 | - | 37,37,53 | 0.34 | 0 | 43,45,61 | 0.29 | 0 |
| 153 | CDL | p1 | 403 | - | 57,57,99 | 0.39 | 0 | 63,69,111 | 0.40 | 0 |
| 153 | CDL | m1 | 405 | - | 56,56,99 | 0.38 | 0 | 62,68,111 | 0.37 | 0 |
| 152 | PC1 | an | 304 | - | 35,35,53 | 0.36 | 0 | 41,43,61 | 0.33 | 0 |
| 153 | CDL | vb | 704 | - | 66,66,99 | 0.36 | 0 | 72,78,111 | 0.30 | 0 |
| 153 | CDL | l | 301 | - | 73,73,99 | 0.34 | 0 | 79,85,111 | 0.29 | 0 |
| 152 | PC1 | 2J | 201 | - | 41,41,53 | 0.33 | 0 | 47,49,61 | 0.36 | 0 |
| 152 | PC1 | qe | 301 | - | 32,32,53 | 0.36 | 0 | 38,40,61 | 0.34 | 0 |
| 152 | PC1 | N | 302 | - | 31,31,53 | 0.36 | 0 | 37,39,61 | 0.32 | 0 |
| 153 | CDL | A9 | 403 | - | 86,86,99 | 0.32 | 0 | 92,98,111 | 0.27 | 0 |
| 166 | HEM | Y5 | 203 | - | 41,50,50 | 1.21 | 4 (9%) | 45,82,82 | 1.70 | 7 (15%) |
| 152 | PC1 | N3 | 201 | - | 30,30,53 | 0.37 | 0 | 36,38,61 | 0.36 | 0 |
| 152 | PC1 | N6 | 301 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.29 | 0 |
| 152 | PC1 | QB | 602 | - | 43,43,53 | 0.32 | 0 | 49,51,61 | 0.29 | 0 |
| 153 | CDL | t | 203 | - | 70,70,99 | 0.35 | 0 | 76,82,111 | 0.32 | 0 |
| 157 | FES | S1 | 803 | 120 | 0,4,4 | - | - | - | - | - |
| 152 | PC1 | i | 304 | - | 38,38,53 | 0.34 | 0 | 44,46,61 | 0.32 | 0 |
| 153 | CDL | M1 | 405 | - | 56,56,99 | 0.38 | 0 | 62,68,111 | 0.37 | 0 |
| 153 | CDL | i | 302 | - | 74,74,99 | 0.34 | 0 | 80,86,111 | 0.29 | 0 |
| 153 | CDL | T | 203 | - | 70,70,99 | 0.35 | 0 | 76,82,111 | 0.32 | 0 |
| 158 | 3PE | C4 | 402 | - | 50,50,50 | 0.30 | 0 | 53,55,55 | 0.31 | 0 |
| 153 | CDL | 5b | 201 | - | 80,80,99 | 0.34 | 0 | 86,92,111 | 0.33 | 0 |
| 162 | SF4 | s8 | 303 | 127 | 0,12,12 | - | - | - | - | - |
| 153 | CDL | c1 | 709 | - | 62,62,99 | 0.37 | 0 | 68,74,111 | 0.39 | 0 |
| 152 | PC1 | T1 | 602 | - | 32,32,53 | 0.36 | 0 | 38,40,61 | 0.34 | 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 |
|-----|------|-------|-----|------|---------|----------------|---------|
| 152 | PC1 | n5 | 803 | - | - | 9/56/56/57 | - |
| 153 | CDL | T | 201 | - | - | 12/69/69/110 | - |
| 152 | PC1 | c4 | 403 | - | - | 5/44/44/57 | - |
| 158 | 3PE | T8 | 602 | - | - | 11/42/42/54 | - |
| 157 | FES | fs | 201 | 35 | - | - | 0/1/1/1 |
| 153 | CDL | QB | 601 | - | - | 12/78/78/110 | - |
| 158 | 3PE | bm | 302 | - | - | 8/33/33/54 | - |
| 162 | SF4 | s7 | 201 | 126 | - | - | 0/6/5/5 |
| 153 | CDL | c | 301 | - | - | 13/74/74/110 | - |
| 153 | CDL | u | 201 | - | - | 12/70/70/110 | - |
| 153 | CDL | 2o | 101 | - | - | 19/60/60/110 | - |
| 153 | CDL | m1 | 404 | - | - | 17/101/101/110 | - |
| 153 | CDL | N | 304 | - | - | 33/94/94/110 | - |
| 152 | PC1 | B9 | 201 | - | - | 13/37/37/57 | - |
| 152 | PC1 | 7C | 303 | - | - | 7/46/46/57 | - |
| 153 | CDL | M2 | 403 | - | - | 19/76/76/110 | - |
| 152 | PC1 | t4 | 303 | - | - | 12/57/57/57 | - |
| 152 | PC1 | Qg | 401 | - | - | 7/35/35/57 | - |
| 157 | FES | QE | 302 | - | - | - | 0/1/1/1 |
| 152 | PC1 | f | 402 | - | - | 9/41/41/57 | - |
| 153 | CDL | E | 401 | - | - | 15/70/70/110 | - |
| 153 | CDL | 2b | 201 | - | - | 17/97/97/110 | - |
| 153 | CDL | q | 203 | - | - | 16/96/96/110 | - |
| 153 | CDL | qG | 402 | - | - | 18/96/96/110 | - |
| 153 | CDL | A1 | 101 | - | - | 17/76/76/110 | - |
| 157 | FES | V2 | 300 | 147 | - | - | 0/1/1/1 |
| 152 | PC1 | N | 303 | - | - | 6/39/39/57 | - |
| 153 | CDL | b4 | 201 | - | - | 9/44/44/110 | - |
| 152 | PC1 | m1 | 401 | - | - | 14/57/57/57 | - |
| 152 | PC1 | V | 201 | - | - | 4/38/38/57 | - |
| 152 | PC1 | I | 301 | - | - | 10/42/42/57 | - |
| 153 | CDL | m | 306 | - | - | 15/76/76/110 | - |
| 153 | CDL | p1 | 402 | - | - | 19/73/73/110 | - |
| 153 | CDL | t1 | 601 | - | - | 12/65/65/110 | - |
| 152 | PC1 | n5 | 804 | - | - | 12/42/42/57 | - |
| 152 | PC1 | 6c | 203 | - | - | 8/36/36/57 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------------|---------|
| 152 | PC1 | qc | 509 | - | - | 11/50/50/57 | - |
| 153 | CDL | a | 502 | - | - | 17/61/61/110 | - |
| 153 | CDL | B4 | 201 | - | - | 9/44/44/110 | - |
| 153 | CDL | qH | 201 | - | - | 13/104/104/110 | - |
| 153 | CDL | T | 202 | - | - | 14/85/85/110 | - |
| 171 | FMN | v1 | 501 | - | - | 2/18/18/18 | 0/3/3/3 |
| 152 | PC1 | qE | 301 | - | - | 8/26/26/57 | - |
| 153 | CDL | B | 501 | - | - | 16/72/72/110 | - |
| 153 | CDL | A9 | 402 | - | - | 17/86/86/110 | - |
| 152 | PC1 | fs | 204 | - | - | 6/43/43/57 | - |
| 153 | CDL | qB | 601 | - | - | 12/78/78/110 | - |
| 157 | FES | FS | 203 | 35 | - | - | 0/1/1/1 |
| 152 | PC1 | b9 | 201 | - | - | 13/37/37/57 | - |
| 153 | CDL | 6a | 201 | - | - | 21/84/84/110 | - |
| 153 | CDL | W | 202 | - | - | 17/94/94/110 | - |
| 153 | CDL | a | 505 | - | - | 20/92/92/110 | - |
| 153 | CDL | z | 101 | - | - | 13/77/77/110 | - |
| 153 | CDL | TE | 101 | - | - | 18/63/63/110 | - |
| 158 | 3PE | N5 | 802 | - | - | 7/39/39/54 | - |
| 153 | CDL | q | 201 | - | - | 13/73/73/110 | - |
| 152 | PC1 | d | 501 | - | - | 15/38/38/57 | - |
| 153 | CDL | td | 101 | - | - | 18/76/76/110 | - |
| 153 | CDL | R | 201 | - | - | 25/75/75/110 | - |
| 153 | CDL | 6c | 202 | - | - | 16/92/92/110 | - |
| 152 | PC1 | qb | 602 | - | - | 8/46/46/57 | - |
| 153 | CDL | 2k | 101 | - | - | 32/108/108/110 | - |
| 167 | NDP | a9 | 401 | - | - | 8/30/77/77 | 0/5/5/5 |
| 171 | FMN | V1 | 501 | - | - | 2/18/18/18 | 0/3/3/3 |
| 153 | CDL | qb | 601 | - | - | 9/78/78/110 | - |
| 152 | PC1 | QG | 401 | - | - | 6/35/35/57 | - |
| 152 | PC1 | c3 | 601 | - | - | 10/55/55/57 | - |
| 153 | CDL | 2G | 203 | - | - | 11/65/65/110 | - |
| 162 | SF4 | s8 | 302 | 127 | - | - | 0/6/5/5 |
| 152 | PC1 | m2 | 402 | - | - | 12/35/35/57 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------------|---------|
| 152 | PC1 | C3 | 606 | - | - | 7/52/52/57 | - |
| 152 | PC1 | n | 302 | - | - | 10/35/35/57 | - |
| 153 | CDL | a1 | 101 | - | - | 14/77/77/110 | - |
| 152 | PC1 | qg | 401 | - | - | 6/35/35/57 | - |
| 153 | CDL | U | 201 | - | - | 12/70/70/110 | - |
| 153 | CDL | 2g | 204 | - | - | 16/73/73/110 | - |
| 153 | CDL | fs | 203 | - | - | 11/57/57/110 | - |
| 153 | CDL | 7C | 302 | - | - | 11/61/61/110 | - |
| 158 | 3PE | an | 301 | - | - | 6/48/48/54 | - |
| 152 | PC1 | Qe | 303 | - | - | 12/46/46/57 | - |
| 152 | PC1 | S8 | 301 | - | - | 9/33/33/57 | - |
| 153 | CDL | E | 403 | - | - | 13/73/73/110 | - |
| 152 | PC1 | N5 | 805 | - | - | 16/57/57/57 | - |
| 153 | CDL | r | 201 | - | - | 25/75/75/110 | - |
| 153 | CDL | AN | 302 | - | - | 18/97/97/110 | - |
| 152 | PC1 | qI | 201 | - | - | 6/33/33/57 | - |
| 152 | PC1 | qC | 508 | - | - | 10/39/39/57 | - |
| 152 | PC1 | Qc | 506 | - | - | 15/41/41/57 | - |
| 153 | CDL | N5 | 806 | - | - | 21/100/100/110 | - |
| 154 | HEA | c1 | 708 | 29 | - | 15/32/76/76 | - |
| 152 | PC1 | N1 | 301 | - | - | 8/39/39/57 | - |
| 169 | T7X | b6 | 201 | - | - | 25/50/74/80 | 0/1/1/1 |
| 152 | PC1 | N | 301 | - | - | 5/44/44/57 | - |
| 152 | PC1 | FS | 201 | - | - | 6/43/43/57 | - |
| 170 | ADP | b9 | 202 | - | - | 4/12/32/32 | 0/3/3/3 |
| 152 | PC1 | 2f | 301 | - | - | 21/50/50/57 | - |
| 158 | 3PE | g2 | 301 | - | - | 15/54/54/54 | - |
| 164 | U10 | b8 | 301 | - | - | 13/63/87/87 | 0/1/1/1 |
| 153 | CDL | C1 | 708 | - | - | 25/73/73/110 | - |
| 152 | PC1 | T4 | 301 | - | - | 18/51/51/57 | - |
| 152 | PC1 | Qb | 602 | - | - | 8/46/46/57 | - |
| 153 | CDL | qI | 203 | - | - | 17/81/81/110 | - |
| 153 | CDL | B3 | 101 | - | - | 14/68/68/110 | - |
| 153 | CDL | j | 301 | - | - | 16/80/80/110 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------------|---------|
| 153 | CDL | Qc | 508 | - | - | 12/57/57/110 | - |
| 158 | 3PE | AN | 303 | - | - | 8/48/48/54 | - |
| 152 | PC1 | Qj | 101 | - | - | 11/39/39/57 | - |
| 153 | CDL | M | 301 | - | - | 15/76/76/110 | - |
| 152 | PC1 | qC | 507 | - | - | 12/53/53/57 | - |
| 157 | FES | qe | 302 | - | - | - | 0/1/1/1 |
| 158 | 3PE | S8 | 304 | - | - | 8/44/44/54 | - |
| 152 | PC1 | a | 501 | - | - | 10/44/44/57 | - |
| 162 | SF4 | S8 | 302 | 127 | - | - | 0/6/5/5 |
| 157 | FES | fs | 202 | 35 | - | - | 0/1/1/1 |
| 153 | CDL | QG | 402 | - | - | 17/96/96/110 | - |
| 153 | CDL | e | 401 | - | - | 15/70/70/110 | - |
| 152 | PC1 | C1 | 711 | - | - | 12/42/42/57 | - |
| 152 | PC1 | n5 | 805 | - | - | 16/57/57/57 | - |
| 153 | CDL | AM | 201 | - | - | 12/66/66/110 | - |
| 152 | PC1 | 5B | 202 | - | - | 12/50/50/57 | - |
| 152 | PC1 | v | 201 | - | - | 4/38/38/57 | - |
| 164 | U10 | qc | 507 | - | - | 9/23/47/87 | 0/1/1/1 |
| 151 | HEC | qD | 401 | 111 | - | 4/10/54/54 | - |
| 152 | PC1 | w | 205 | - | - | 6/46/46/57 | - |
| 153 | CDL | qD | 402 | - | - | 17/71/71/110 | - |
| 153 | CDL | 6A | 201 | - | - | 21/84/84/110 | - |
| 153 | CDL | U1 | 101 | - | - | 14/67/67/110 | - |
| 152 | PC1 | AN | 304 | - | - | 9/39/39/57 | - |
| 153 | CDL | t | 202 | - | - | 14/85/85/110 | - |
| 157 | FES | fx | 201 | 95 | - | - | 0/1/1/1 |
| 152 | PC1 | w | 204 | - | - | 7/37/37/57 | - |
| 152 | PC1 | AM | 202 | - | - | 8/42/42/57 | - |
| 153 | CDL | TH | 200 | - | - | 17/94/94/110 | - |
| 153 | CDL | M2 | 404 | - | - | 11/84/84/110 | - |
| 158 | 3PE | ta | 201 | - | - | 10/29/29/54 | - |
| 152 | PC1 | C3 | 603 | - | - | 8/34/34/57 | - |
| 152 | PC1 | J1 | 400 | - | - | 10/43/43/57 | - |
| 153 | CDL | t5 | 301 | - | - | 27/106/106/110 | - |
| 153 | CDL | I | 302 | - | - | 17/87/87/110 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------------|---------|
| 151 | HEC | Qd | 401 | 111 | - | 4/10/54/54 | - |
| 157 | FES | FS | 202 | 35 | - | - | 0/1/1/1 |
| 153 | CDL | 2M | 101 | - | - | 17/106/106/110 | - |
| 158 | 3PE | an | 306 | - | - | 6/32/32/54 | - |
| 153 | CDL | 2G | 204 | - | - | 15/73/73/110 | - |
| 152 | PC1 | qj | 101 | - | - | 11/39/39/57 | - |
| 153 | CDL | QD | 402 | - | - | 17/71/71/110 | - |
| 164 | U10 | SC | 102 | - | - | 12/63/87/87 | 0/1/1/1 |
| 152 | PC1 | tc | 102 | - | - | 15/50/50/57 | - |
| 153 | CDL | C1 | 701 | - | - | 22/89/89/110 | - |
| 153 | CDL | B8 | 302 | - | - | 11/79/79/110 | - |
| 166 | HEM | QC | 502 | 110 | - | 6/12/54/54 | - |
| 153 | CDL | an | 302 | - | - | 18/97/97/110 | - |
| 152 | PC1 | M2 | 402 | - | - | 12/35/35/57 | - |
| 153 | CDL | AL | 301 | - | - | 16/63/63/110 | - |
| 158 | 3PE | M3 | 402 | - | - | 8/41/41/54 | - |
| 158 | 3PE | T4 | 302 | - | - | 4/28/28/54 | - |
| 152 | PC1 | n5 | 801 | - | - | 11/55/55/57 | - |
| 152 | PC1 | C1 | 710 | - | - | 7/41/41/57 | - |
| 166 | HEM | qC | 501 | 110 | - | 5/12/54/54 | - |
| 152 | PC1 | C3 | 601 | - | - | 10/55/55/57 | - |
| 153 | CDL | q | 202 | - | - | 20/82/82/110 | - |
| 152 | PC1 | c3 | 606 | - | - | 7/52/52/57 | - |
| 152 | PC1 | M | 303 | - | - | 15/48/48/57 | - |
| 152 | PC1 | F | 401 | - | - | 9/41/41/57 | - |
| 152 | PC1 | m | 301 | - | - | 15/48/48/57 | - |
| 158 | 3PE | an | 305 | - | - | 5/36/36/54 | - |
| 158 | 3PE | n5 | 802 | - | - | 9/39/39/54 | - |
| 153 | CDL | P1 | 402 | - | - | 19/73/73/110 | - |
| 152 | PC1 | 7c | 303 | - | - | 7/46/46/57 | - |
| 153 | CDL | M3 | 401 | - | - | 8/73/73/110 | - |
| 152 | PC1 | al | 302 | - | - | 2/29/29/57 | - |
| 158 | 3PE | G2 | 301 | - | - | 15/54/54/54 | - |
| 152 | PC1 | M2 | 407 | - | - | 10/49/49/57 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------------|---------|
| 152 | PC1 | 2f | 303 | - | - | 10/35/35/57 | - |
| 152 | PC1 | c3 | 602 | - | - | 13/42/42/57 | - |
| 164 | U10 | qc | 501 | - | - | 9/28/28/87 | - |
| 158 | 3PE | I | 304 | - | - | 9/35/35/54 | - |
| 153 | CDL | vb | 701 | - | - | 15/72/72/110 | - |
| 153 | CDL | 7C | 301 | - | - | 23/95/95/110 | - |
| 153 | CDL | f | 401 | - | - | 17/110/110/110 | - |
| 153 | CDL | m2 | 404 | - | - | 11/84/84/110 | - |
| 157 | FES | s1 | 803 | 120 | - | - | 0/1/1/1 |
| 153 | CDL | qc | 505 | - | - | 17/66/66/110 | - |
| 152 | PC1 | W | 205 | - | - | 6/46/46/57 | - |
| 152 | PC1 | Qe | 301 | - | - | 6/36/36/57 | - |
| 158 | 3PE | m2 | 408 | - | - | 9/34/34/54 | - |
| 152 | PC1 | P1 | 401 | - | - | 10/43/43/57 | - |
| 152 | PC1 | Qc | 509 | - | - | 11/50/50/57 | - |
| 158 | 3PE | a3 | 201 | - | - | 13/48/48/54 | - |
| 152 | PC1 | c3 | 605 | - | - | 3/42/42/57 | - |
| 152 | PC1 | v | 202 | - | - | 13/52/52/57 | - |
| 152 | PC1 | w | 201 | - | - | 16/52/52/57 | - |
| 158 | 3PE | AN | 301 | - | - | 7/48/48/54 | - |
| 152 | PC1 | c2 | 703 | - | - | 11/39/39/57 | - |
| 152 | PC1 | 6a | 202 | - | - | 12/38/38/57 | - |
| 152 | PC1 | m1 | 403 | - | - | 7/45/45/57 | - |
| 153 | CDL | Y5 | 201 | - | - | 15/80/80/110 | - |
| 152 | PC1 | qc | 506 | - | - | 15/41/41/57 | - |
| 153 | CDL | b3 | 102 | - | - | 21/92/92/110 | - |
| 152 | PC1 | qI | 202 | - | - | 5/46/46/57 | - |
| 158 | 3PE | n4 | 601 | - | - | 10/39/39/54 | - |
| 162 | SF4 | v1 | 500 | 146 | - | - | 0/6/5/5 |
| 153 | CDL | T1 | 601 | - | - | 12/65/65/110 | - |
| 152 | PC1 | J | 302 | - | - | 7/40/40/57 | - |
| 153 | CDL | M3 | 403 | - | - | 14/65/65/110 | - |
| 162 | SF4 | S1 | 802 | 120 | - | - | 0/6/5/5 |
| 158 | 3PE | t8 | 601 | - | - | 12/50/50/54 | - |
| 153 | CDL | qc | 504 | - | - | 21/74/74/110 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------------|---------|
| 152 | PC1 | qi | 201 | - | - | 8/33/33/57 | - |
| 151 | HEC | qd | 401 | 111 | - | 4/10/54/54 | - |
| 152 | PC1 | qE | 303 | - | - | 2/42/42/57 | - |
| 153 | CDL | c1 | 701 | - | - | 22/89/89/110 | - |
| 151 | HEC | QD | 401 | 111 | - | 4/10/54/54 | - |
| 153 | CDL | BM | 301 | - | - | 24/96/96/110 | - |
| 152 | PC1 | 7a | 202 | - | - | 13/48/48/57 | - |
| 152 | PC1 | p1 | 401 | - | - | 10/43/43/57 | - |
| 158 | 3PE | c4 | 402 | - | - | 8/54/54/54 | - |
| 152 | PC1 | M2 | 405 | - | - | 9/57/57/57 | - |
| 153 | CDL | b | 501 | - | - | 16/72/72/110 | - |
| 152 | PC1 | j | 302 | - | - | 7/40/40/57 | - |
| 153 | CDL | B3 | 102 | - | - | 19/92/92/110 | - |
| 153 | CDL | C1 | 712 | - | - | 16/105/105/110 | - |
| 153 | CDL | Qc | 505 | - | - | 17/66/66/110 | - |
| 153 | CDL | T | 204 | - | - | 30/100/100/110 | - |
| 153 | CDL | VB | 706 | - | - | 16/77/77/110 | - |
| 152 | PC1 | n3 | 201 | - | - | 4/34/34/57 | - |
| 152 | PC1 | TC | 101 | - | - | 7/45/45/57 | - |
| 153 | CDL | VB | 703 | - | - | 17/96/96/110 | - |
| 158 | 3PE | s8 | 304 | - | - | 8/44/44/54 | - |
| 166 | HEM | y5 | 203 | - | - | 6/12/54/54 | - |
| 152 | PC1 | 6A | 202 | - | - | 12/38/38/57 | - |
| 153 | CDL | 7c | 302 | - | - | 11/61/61/110 | - |
| 153 | CDL | m2 | 403 | - | - | 19/76/76/110 | - |
| 153 | CDL | L | 301 | - | - | 24/84/84/110 | - |
| 152 | PC1 | m2 | 407 | - | - | 10/49/49/57 | - |
| 170 | ADP | B9 | 202 | - | - | 4/12/32/32 | 0/3/3/3 |
| 153 | CDL | c4 | 401 | - | - | 23/108/108/110 | - |
| 152 | PC1 | 2f | 302 | - | - | 8/45/45/57 | - |
| 152 | PC1 | QE | 303 | - | - | 2/42/42/57 | - |
| 153 | CDL | qg | 402 | - | - | 23/110/110/110 | - |
| 158 | 3PE | vb | 705 | - | - | 10/31/31/54 | - |
| 153 | CDL | a | 504 | - | - | 15/104/104/110 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------------|---------|
| 152 | PC1 | QI | 202 | - | - | 7/46/46/57 | - |
| 153 | CDL | Qb | 601 | - | - | 9/78/78/110 | - |
| 153 | CDL | c3 | 604 | - | - | 7/78/78/110 | - |
| 152 | PC1 | m | 307 | - | - | 12/39/39/57 | - |
| 152 | PC1 | m2 | 405 | - | - | 9/57/57/57 | - |
| 153 | CDL | y5 | 201 | - | - | 15/80/80/110 | - |
| 152 | PC1 | 2j | 201 | - | - | 13/45/45/57 | - |
| 153 | CDL | u1 | 101 | - | - | 14/67/67/110 | - |
| 153 | CDL | m2 | 401 | - | - | 15/64/64/110 | - |
| 153 | CDL | a9 | 403 | - | - | 20/97/97/110 | - |
| 152 | PC1 | W | 204 | - | - | 7/37/37/57 | - |
| 162 | SF4 | S8 | 303 | 127 | - | - | 0/6/5/5 |
| 153 | CDL | qi | 202 | - | - | 14/81/81/110 | - |
| 153 | CDL | M | 305 | - | - | 11/93/93/110 | - |
| 153 | CDL | QC | 504 | - | - | 11/66/66/110 | - |
| 152 | PC1 | M | 307 | - | - | 10/38/38/57 | - |
| 160 | PX2 | Y5 | 204 | - | - | 13/22/22/37 | - |
| 153 | CDL | P1 | 403 | - | - | 15/68/68/110 | - |
| 166 | HEM | Qc | 502 | 110 | - | 2/12/54/54 | - |
| 152 | PC1 | D | 501 | - | - | 15/38/38/57 | - |
| 153 | CDL | 7c | 301 | - | - | 22/95/95/110 | - |
| 161 | FAD | sa | 701 | - | - | 10/30/50/50 | 0/6/6/6 |
| 158 | 3PE | BM | 302 | - | - | 8/33/33/54 | - |
| 152 | PC1 | qJ | 101 | - | - | 13/41/41/57 | - |
| 152 | PC1 | QC | 508 | - | - | 10/39/39/57 | - |
| 153 | CDL | 2g | 203 | - | - | 11/65/65/110 | - |
| 152 | PC1 | te | 102 | - | - | 10/35/35/57 | - |
| 153 | CDL | M1 | 404 | - | - | 17/101/101/110 | - |
| 164 | U10 | B8 | 301 | - | - | 12/63/87/87 | 0/1/1/1 |
| 153 | CDL | SD | 101 | - | - | 18/86/86/110 | - |
| 158 | 3PE | t4 | 302 | - | - | 4/28/28/54 | - |
| 153 | CDL | A1 | 102 | - | - | 15/77/77/110 | - |
| 161 | FAD | SA | 701 | - | - | 10/30/50/50 | 0/6/6/6 |
| 152 | PC1 | TC | 102 | - | - | 15/50/50/57 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------------|---------|
| 152 | PC1 | s8 | 301 | - | - | 9/33/33/57 | - |
| 153 | CDL | VB | 705 | - | - | 20/92/92/110 | - |
| 153 | CDL | e | 402 | - | - | 20/82/82/110 | - |
| 153 | CDL | bm | 301 | - | - | 23/96/96/110 | - |
| 154 | HEA | c1 | 702 | 29 | - | 10/32/76/76 | - |
| 153 | CDL | 6C | 203 | - | - | 16/92/92/110 | - |
| 153 | CDL | 7A | 201 | - | - | 16/110/110/110 | - |
| 157 | FES | SB | 401 | 53 | - | - | 0/1/1/1 |
| 158 | 3PE | M2 | 408 | - | - | 9/34/34/54 | - |
| 153 | CDL | M2 | 401 | - | - | 15/64/64/110 | - |
| 157 | FES | qE | 302 | - | - | - | 0/1/1/1 |
| 152 | PC1 | V | 202 | - | - | 13/52/52/57 | - |
| 153 | CDL | e | 403 | - | - | 13/73/73/110 | - |
| 153 | CDL | 2g | 201 | - | - | 19/99/99/110 | - |
| 153 | CDL | VB | 701 | - | - | 15/72/72/110 | - |
| 166 | HEM | Qc | 503 | 110 | - | 7/12/54/54 | - |
| 153 | CDL | T5 | 301 | - | - | 27/106/106/110 | - |
| 152 | PC1 | W | 201 | - | - | 16/52/52/57 | - |
| 158 | 3PE | AN | 305 | - | - | 6/36/36/54 | - |
| 158 | 3PE | a3 | 202 | - | - | 12/47/47/54 | - |
| 169 | T7X | B6 | 201 | - | - | 25/50/74/80 | 0/1/1/1 |
| 162 | SF4 | sb | 402 | 53 | - | - | 0/6/5/5 |
| 157 | FES | v2 | 300 | 147 | - | - | 0/1/1/1 |
| 152 | PC1 | n1 | 301 | - | - | 8/39/39/57 | - |
| 151 | HEC | 2e | 401 | 2 | - | 7/10/54/54 | - |
| 153 | CDL | QC | 503 | - | - | 9/74/74/110 | - |
| 152 | PC1 | m | 305 | - | - | 10/38/38/57 | - |
| 152 | PC1 | t1 | 602 | - | - | 13/36/36/57 | - |
| 152 | PC1 | 7A | 202 | - | - | 13/48/48/57 | - |
| 153 | CDL | al | 301 | - | - | 16/63/63/110 | - |
| 153 | CDL | m3 | 403 | - | - | 14/65/65/110 | - |
| 153 | CDL | b8 | 302 | - | - | 11/79/79/110 | - |
| 152 | PC1 | c1 | 704 | - | - | 14/52/52/57 | - |
| 159 | P5S | M2 | 406 | - | - | 29/41/41/59 | - |
| 152 | PC1 | A | 503 | - | - | 7/44/44/57 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------------|---------|
| 153 | CDL | Q | 201 | - | - | 13/73/73/110 | - |
| 153 | CDL | F | 402 | - | - | 19/110/110/110 | - |
| 152 | PC1 | 2F | 301 | - | - | 21/50/50/57 | - |
| 152 | PC1 | C3 | 605 | - | - | 3/42/42/57 | - |
| 151 | HEC | 2E | 401 | 2 | - | 7/10/54/54 | - |
| 160 | PX2 | r | 202 | - | - | 23/34/34/37 | - |
| 153 | CDL | M | 306 | - | - | 12/74/74/110 | - |
| 160 | PX2 | y5 | 204 | - | - | 12/22/22/37 | - |
| 152 | PC1 | 5b | 202 | - | - | 12/50/50/57 | - |
| 153 | CDL | C | 301 | - | - | 14/74/74/110 | - |
| 153 | CDL | n6 | 302 | - | - | 19/100/100/110 | - |
| 152 | PC1 | Qi | 201 | - | - | 8/33/33/57 | - |
| 152 | PC1 | c1 | 707 | - | - | 7/41/41/57 | - |
| 153 | CDL | Qg | 402 | - | - | 23/110/110/110 | - |
| 166 | HEM | qc | 502 | 110 | - | 2/12/54/54 | - |
| 152 | PC1 | qi | 203 | - | - | 14/45/45/57 | - |
| 158 | 3PE | SC | 101 | - | - | 10/43/43/54 | - |
| 153 | CDL | m | 303 | - | - | 11/93/93/110 | - |
| 152 | PC1 | C4 | 403 | - | - | 5/44/44/57 | - |
| 153 | CDL | n5 | 806 | - | - | 21/100/100/110 | - |
| 164 | U10 | sc | 102 | - | - | 12/63/87/87 | 0/1/1/1 |
| 152 | PC1 | 2F | 303 | - | - | 10/35/35/57 | - |
| 152 | PC1 | M1 | 403 | - | - | 7/45/45/57 | - |
| 152 | PC1 | n | 303 | - | - | 7/39/39/57 | - |
| 153 | CDL | 2G | 201 | - | - | 19/99/99/110 | - |
| 158 | 3PE | m3 | 402 | - | - | 8/41/41/54 | - |
| 153 | CDL | J | 301 | - | - | 16/80/80/110 | - |
| 152 | PC1 | T4 | 303 | - | - | 12/57/57/57 | - |
| 158 | 3PE | sc | 101 | - | - | 10/43/43/54 | - |
| 164 | U10 | qC | 506 | - | - | 6/23/47/87 | 0/1/1/1 |
| 162 | SF4 | S1 | 801 | 120 | - | - | 0/6/5/5 |
| 158 | 3PE | A3 | 201 | - | - | 12/48/48/54 | - |
| 158 | 3PE | AN | 306 | - | - | 6/32/32/54 | - |
| 153 | CDL | c1 | 703 | - | - | 8/75/75/110 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------------|---------|
| 153 | CDL | A | 504 | - | - | 15/104/104/110 | - |
| 152 | PC1 | 6C | 201 | - | - | 8/36/36/57 | - |
| 152 | PC1 | am | 202 | - | - | 8/42/42/57 | - |
| 163 | F3S | SB | 403 | 53 | - | - | 0/3/3/3 |
| 157 | FES | FX | 201 | 95 | - | - | 0/1/1/1 |
| 158 | 3PE | w | 203 | - | - | 15/37/37/54 | - |
| 158 | 3PE | i | 303 | - | - | 9/35/35/54 | - |
| 153 | CDL | sd | 101 | - | - | 18/86/86/110 | - |
| 152 | PC1 | 2F | 302 | - | - | 8/45/45/57 | - |
| 153 | CDL | m3 | 401 | - | - | 8/73/73/110 | - |
| 153 | CDL | am | 201 | - | - | 11/66/66/110 | - |
| 158 | 3PE | Y5 | 202 | - | - | 8/31/31/54 | - |
| 152 | PC1 | C2 | 701 | - | - | 11/39/39/57 | - |
| 158 | 3PE | b4 | 202 | - | - | 11/51/51/54 | - |
| 152 | PC1 | 2G | 202 | - | - | 12/53/53/57 | - |
| 152 | PC1 | TE | 102 | - | - | 10/35/35/57 | - |
| 153 | CDL | t | 204 | - | - | 30/100/100/110 | - |
| 153 | CDL | 7A | 203 | - | - | 12/72/72/110 | - |
| 158 | 3PE | TA | 201 | - | - | 10/29/29/54 | - |
| 152 | PC1 | c1 | 706 | - | - | 8/48/48/57 | - |
| 152 | PC1 | tc | 101 | - | - | 7/45/45/57 | - |
| 153 | CDL | i | 301 | - | - | 17/87/87/110 | - |
| 153 | CDL | QH | 201 | - | - | 13/104/104/110 | - |
| 152 | PC1 | C1 | 709 | - | - | 8/48/48/57 | - |
| 152 | PC1 | qB | 602 | - | - | 6/47/47/57 | - |
| 160 | PX2 | Qh | 201 | - | - | 21/37/37/37 | - |
| 153 | CDL | 2O | 101 | - | - | 19/60/60/110 | - |
| 154 | HEA | C1 | 703 | 29 | - | 13/32/76/76 | - |
| 163 | F3S | sb | 403 | 53 | - | - | 0/3/3/3 |
| 153 | CDL | M | 304 | - | - | 11/74/74/110 | - |
| 152 | PC1 | a | 503 | - | - | 7/44/44/57 | - |
| 152 | PC1 | qG | 401 | - | - | 6/35/35/57 | - |
| 153 | CDL | 6C | 202 | - | - | 29/85/85/110 | - |
| 153 | CDL | m1 | 402 | - | - | 15/76/76/110 | - |
| 153 | CDL | b3 | 101 | - | - | 14/68/68/110 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------------|---------|
| 162 | SF4 | V1 | 500 | 146 | - | - | 0/6/5/5 |
| 153 | CDL | m | 302 | - | - | 11/74/74/110 | - |
| 152 | PC1 | C1 | 706 | - | - | 14/52/52/57 | - |
| 153 | CDL | T7 | 201 | - | - | 17/83/83/110 | - |
| 167 | NDP | A9 | 401 | - | - | 8/30/77/77 | 0/5/5/5 |
| 164 | U10 | Qc | 507 | - | - | 9/23/47/87 | 0/1/1/1 |
| 153 | CDL | t7 | 201 | - | - | 16/83/83/110 | - |
| 158 | 3PE | B4 | 202 | - | - | 11/51/51/54 | - |
| 152 | PC1 | N5 | 801 | - | - | 11/55/55/57 | - |
| 168 | ZMP | ab | 201 | 80 | - | 21/43/43/43 | - |
| 153 | CDL | Q | 202 | - | - | 20/82/82/110 | - |
| 153 | CDL | A | 502 | - | - | 16/61/61/110 | - |
| 164 | U10 | QC | 506 | - | - | 5/23/47/87 | 0/1/1/1 |
| 152 | PC1 | n6 | 301 | - | - | 13/57/57/57 | - |
| 153 | CDL | Y7 | 501 | - | - | 14/75/75/110 | - |
| 164 | U10 | Qc | 501 | - | - | 9/28/28/87 | - |
| 153 | CDL | qC | 503 | - | - | 9/74/74/110 | - |
| 166 | HEM | QC | 501 | 110 | - | 5/12/54/54 | - |
| 153 | CDL | Qi | 202 | - | - | 14/81/81/110 | - |
| 152 | PC1 | c1 | 711 | - | - | 12/42/42/57 | - |
| 166 | HEM | qc | 503 | 110 | - | 7/12/54/54 | - |
| 152 | PC1 | QE | 301 | - | - | 8/26/26/57 | - |
| 153 | CDL | M1 | 402 | - | - | 15/76/76/110 | - |
| 153 | CDL | C1 | 707 | - | - | 8/75/75/110 | - |
| 152 | PC1 | c3 | 603 | - | - | 8/34/34/57 | - |
| 152 | PC1 | Qi | 203 | - | - | 14/45/45/57 | - |
| 152 | PC1 | qE | 304 | - | - | 10/31/31/57 | - |
| 153 | CDL | 7a | 201 | - | - | 16/110/110/110 | - |
| 157 | FES | Qe | 302 | - | - | - | 0/1/1/1 |
| 153 | CDL | 2K | 101 | - | - | 32/108/108/110 | - |
| 153 | CDL | I | 303 | - | - | 14/85/85/110 | - |
| 158 | 3PE | T8 | 601 | - | - | 12/50/50/54 | - |
| 152 | PC1 | N5 | 803 | - | - | 9/56/56/57 | - |
| 158 | 3PE | A3 | 202 | - | - | 11/47/47/54 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------------|---------|
| 153 | CDL | N6 | 302 | - | - | 18/100/100/110 | - |
| 157 | FES | sb | 401 | 53 | - | - | 0/1/1/1 |
| 158 | 3PE | VB | 707 | - | - | 10/31/31/54 | - |
| 153 | CDL | w | 202 | - | - | 16/94/94/110 | - |
| 153 | CDL | t | 201 | - | - | 13/69/69/110 | - |
| 153 | CDL | 2B | 201 | - | - | 17/97/97/110 | - |
| 153 | CDL | y7 | 501 | - | - | 13/75/75/110 | - |
| 153 | CDL | m | 304 | - | - | 12/74/74/110 | - |
| 153 | CDL | n | 304 | - | - | 33/94/94/110 | - |
| 152 | PC1 | QI | 201 | - | - | 6/33/33/57 | - |
| 152 | PC1 | qe | 303 | - | - | 13/46/46/57 | - |
| 152 | PC1 | t4 | 301 | - | - | 18/51/51/57 | - |
| 153 | CDL | a9 | 402 | - | - | 17/86/86/110 | - |
| 152 | PC1 | 2g | 202 | - | - | 12/53/53/57 | - |
| 158 | 3PE | an | 303 | - | - | 8/48/48/54 | - |
| 153 | CDL | FS | 204 | - | - | 10/57/57/110 | - |
| 153 | CDL | th | 200 | - | - | 17/94/94/110 | - |
| 152 | PC1 | AL | 302 | - | - | 2/29/29/57 | - |
| 159 | P5S | m2 | 406 | - | - | 29/41/41/59 | - |
| 152 | PC1 | C3 | 602 | - | - | 13/42/42/57 | - |
| 152 | PC1 | QJ | 102 | - | - | 13/41/41/57 | - |
| 153 | CDL | C4 | 401 | - | - | 23/108/108/110 | - |
| 152 | PC1 | M | 302 | - | - | 12/39/39/57 | - |
| 158 | 3PE | y5 | 202 | - | - | 8/31/31/54 | - |
| 153 | CDL | Z | 101 | - | - | 13/77/77/110 | - |
| 158 | 3PE | W | 203 | - | - | 15/37/37/54 | - |
| 152 | PC1 | A | 501 | - | - | 10/44/44/57 | - |
| 158 | 3PE | t8 | 602 | - | - | 11/42/42/54 | - |
| 158 | 3PE | N4 | 601 | - | - | 9/39/39/54 | - |
| 153 | CDL | 7a | 203 | - | - | 12/72/72/110 | - |
| 153 | CDL | qC | 504 | - | - | 11/66/66/110 | - |
| 162 | SF4 | SB | 402 | 53 | - | - | 0/6/5/5 |
| 152 | PC1 | QC | 507 | - | - | 12/53/53/57 | - |
| 162 | SF4 | s1 | 801 | 120 | - | - | 0/6/5/5 |
| 152 | PC1 | QJ | 101 | - | - | 10/31/31/57 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------------|---------|
| 160 | PX2 | R | 202 | - | - | 19/34/34/37 | - |
| 152 | PC1 | M1 | 401 | - | - | 14/57/57/57 | - |
| 166 | HEM | qC | 502 | 110 | - | 6/12/54/54 | - |
| 152 | PC1 | j1 | 400 | - | - | 10/43/43/57 | - |
| 154 | HEA | C1 | 702 | 29 | - | 11/32/76/76 | - |
| 152 | PC1 | n | 301 | - | - | 5/44/44/57 | - |
| 168 | ZMP | AB | 201 | 80 | - | 21/43/43/43 | - |
| 153 | CDL | 2m | 101 | - | - | 17/106/106/110 | - |
| 153 | CDL | 6c | 201 | - | - | 29/85/85/110 | - |
| 162 | SF4 | s1 | 802 | 120 | - | - | 0/6/5/5 |
| 153 | CDL | QI | 203 | - | - | 17/81/81/110 | - |
| 153 | CDL | qc | 508 | - | - | 12/57/57/110 | - |
| 153 | CDL | Qc | 504 | - | - | 21/74/74/110 | - |
| 153 | CDL | C3 | 604 | - | - | 6/78/78/110 | - |
| 160 | PX2 | qh | 201 | - | - | 17/37/37/37 | - |
| 152 | PC1 | qC | 505 | - | - | 12/41/41/57 | - |
| 153 | CDL | te | 101 | - | - | 20/63/63/110 | - |
| 153 | CDL | c1 | 712 | - | - | 17/105/105/110 | - |
| 152 | PC1 | N5 | 804 | - | - | 12/42/42/57 | - |
| 162 | SF4 | S7 | 201 | 126 | - | - | 0/6/5/5 |
| 153 | CDL | 5B | 201 | - | - | 18/91/91/110 | - |
| 153 | CDL | E | 402 | - | - | 20/82/82/110 | - |
| 152 | PC1 | QC | 505 | - | - | 12/41/41/57 | - |
| 153 | CDL | p1 | 403 | - | - | 15/68/68/110 | - |
| 153 | CDL | m1 | 405 | - | - | 15/67/67/110 | - |
| 152 | PC1 | an | 304 | - | - | 9/39/39/57 | - |
| 153 | CDL | vb | 704 | - | - | 17/77/77/110 | - |
| 153 | CDL | l | 301 | - | - | 23/84/84/110 | - |
| 152 | PC1 | 2J | 201 | - | - | 13/45/45/57 | - |
| 152 | PC1 | qe | 301 | - | - | 6/36/36/57 | - |
| 152 | PC1 | N | 302 | - | - | 10/35/35/57 | - |
| 153 | CDL | A9 | 403 | - | - | 20/97/97/110 | - |
| 166 | HEM | Y5 | 203 | - | - | 6/12/54/54 | - |
| 152 | PC1 | N3 | 201 | - | - | 4/34/34/57 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|--------------|---------|
| 152 | PC1 | N6 | 301 | - | - | 13/57/57/57 | - |
| 152 | PC1 | QB | 602 | - | - | 6/47/47/57 | - |
| 153 | CDL | t | 203 | - | - | 23/81/81/110 | - |
| 157 | FES | S1 | 803 | 120 | - | - | 0/1/1/1 |
| 152 | PC1 | i | 304 | - | - | 10/42/42/57 | - |
| 153 | CDL | M1 | 405 | - | - | 15/67/67/110 | - |
| 153 | CDL | i | 302 | - | - | 14/85/85/110 | - |
| 153 | CDL | T | 203 | - | - | 23/81/81/110 | - |
| 158 | 3PE | C4 | 402 | - | - | 8/54/54/54 | - |
| 153 | CDL | 5b | 201 | - | - | 18/91/91/110 | - |
| 162 | SF4 | s8 | 303 | 127 | - | - | 0/6/5/5 |
| 153 | CDL | c1 | 709 | - | - | 25/73/73/110 | - |
| 152 | PC1 | T1 | 602 | - | - | 13/36/36/57 | - |

The worst 5 of 312 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 164 | sc | 102 | U10 | C6-C1 | 10.31 | 1.54 | 1.35 |
| 164 | SC | 102 | U10 | C6-C1 | 10.29 | 1.54 | 1.35 |
| 164 | qc | 507 | U10 | C6-C1 | 10.17 | 1.53 | 1.35 |
| 164 | Qc | 507 | U10 | C6-C1 | 10.17 | 1.53 | 1.35 |
| 164 | qC | 506 | U10 | C6-C1 | 10.11 | 1.53 | 1.35 |

The worst 5 of 440 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 154 | c1 | 702 | HEA | CAD-CBD-CGD | -8.19 | 95.98 | 113.60 |
| 154 | c1 | 708 | HEA | CAD-CBD-CGD | -7.89 | 96.63 | 113.60 |
| 154 | C1 | 702 | HEA | CAD-CBD-CGD | -7.46 | 97.54 | 113.60 |
| 154 | C1 | 703 | HEA | CAD-CBD-CGD | -7.18 | 98.14 | 113.60 |
| 154 | C1 | 703 | HEA | C13-C12-C11 | -6.58 | 104.46 | 114.35 |

There are no chirality outliers.

5 of 5906 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 151 | 2e | 401 | HEC | C2D-C3D-CAD-CBD |
| 151 | 2e | 401 | HEC | C4D-C3D-CAD-CBD |
| 151 | 2E | 401 | HEC | C2D-C3D-CAD-CBD |

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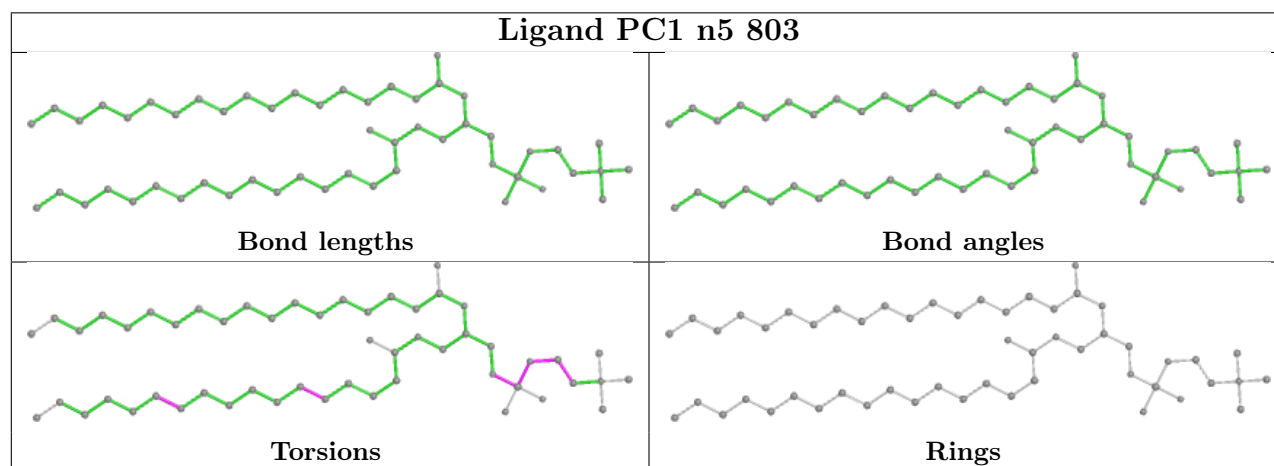
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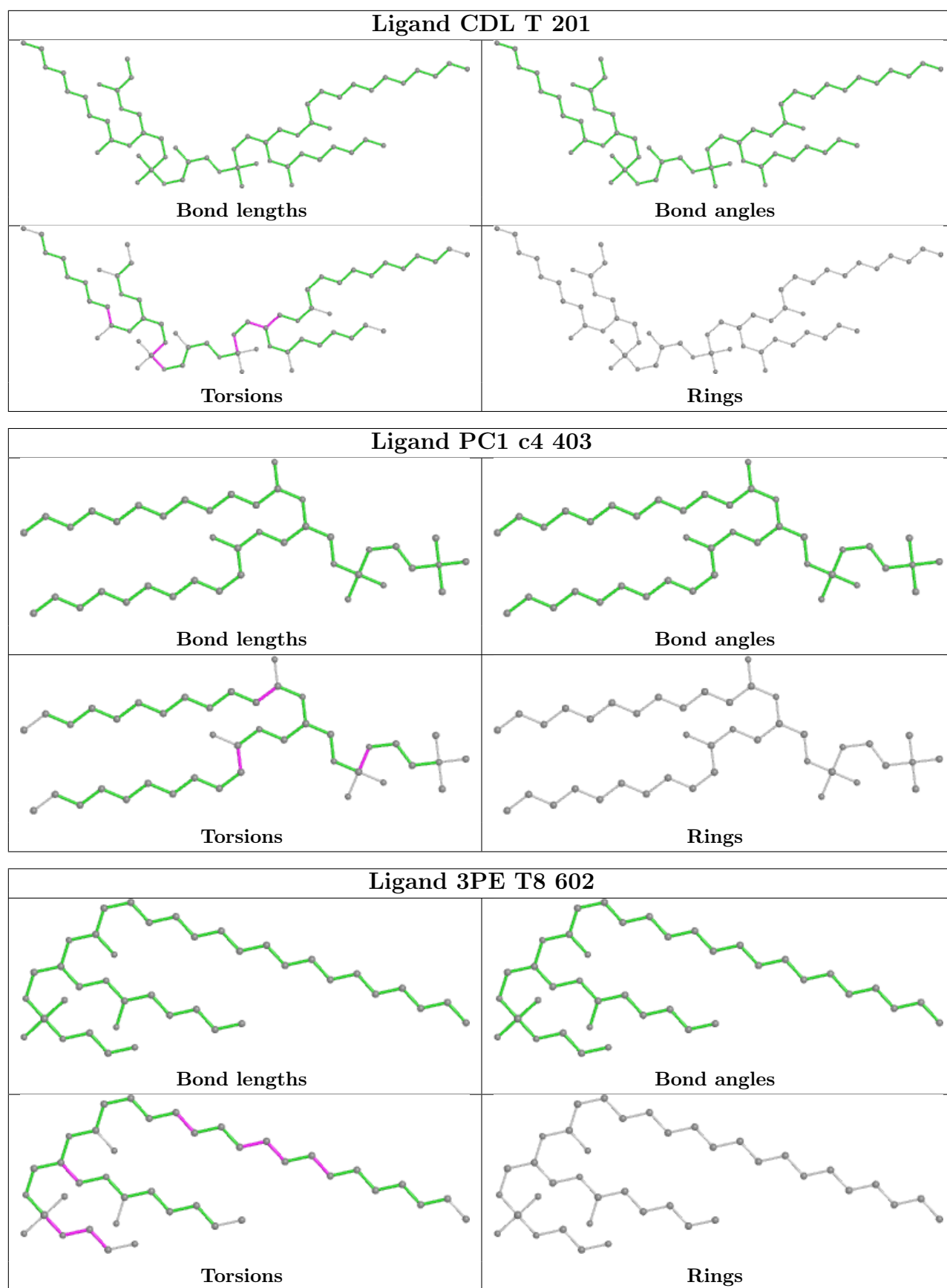
| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 151 | 2E | 401 | HEC | C4D-C3D-CAD-CBD |
| 152 | 2f | 301 | PC1 | C11-O13-P-O14 |

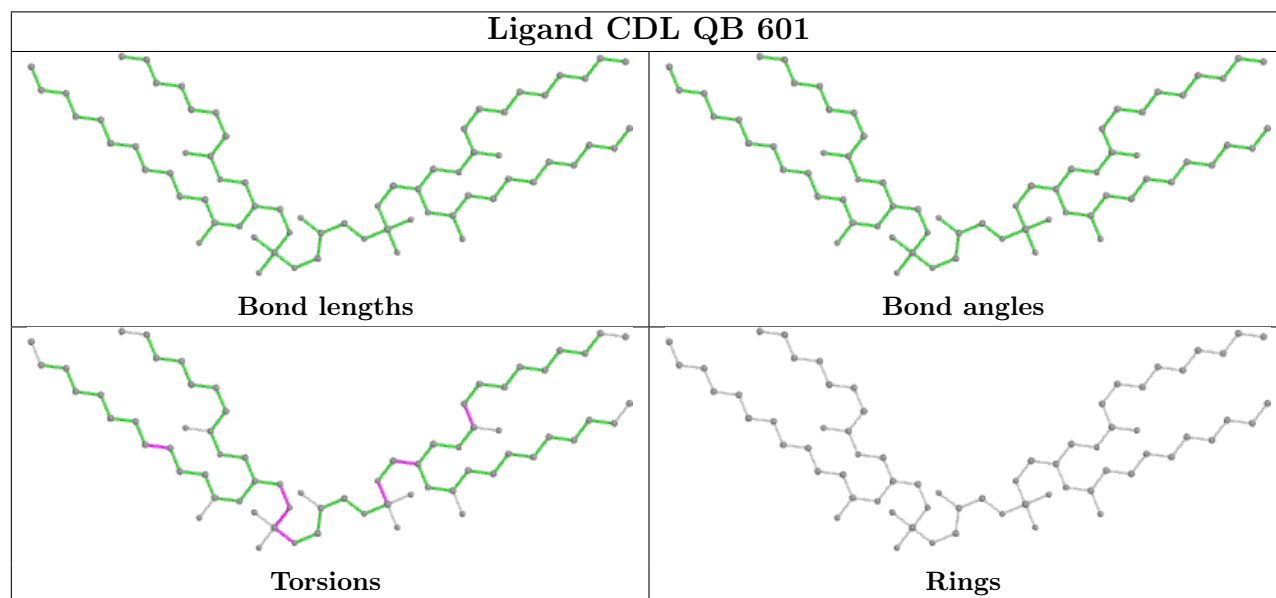
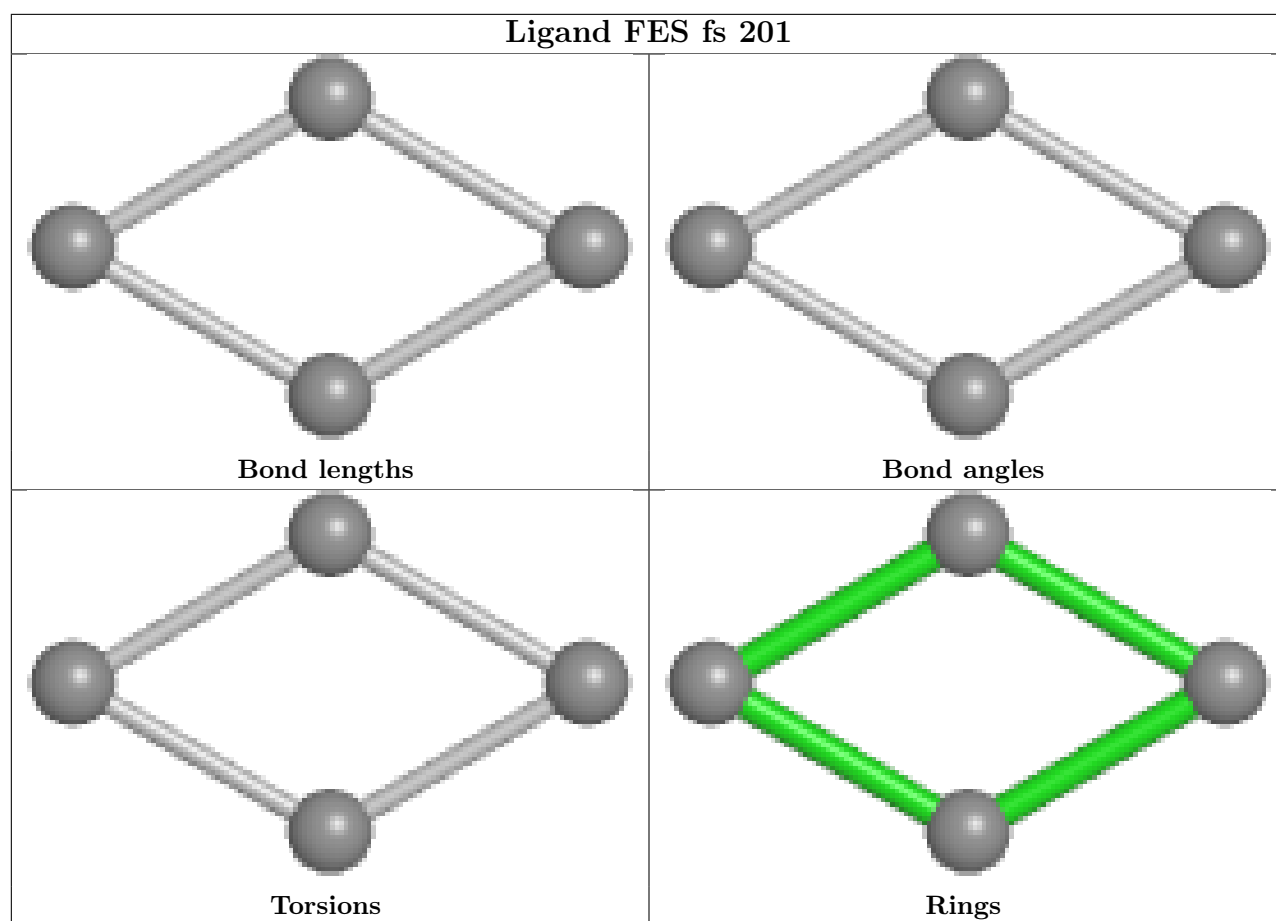
There are no ring outliers.

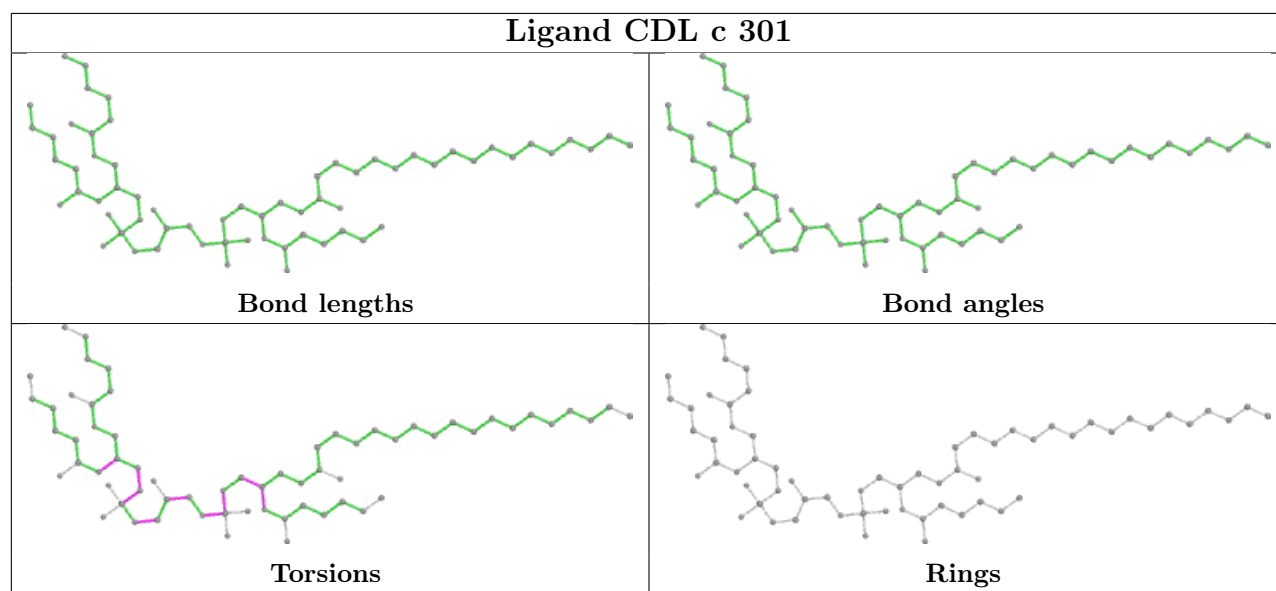
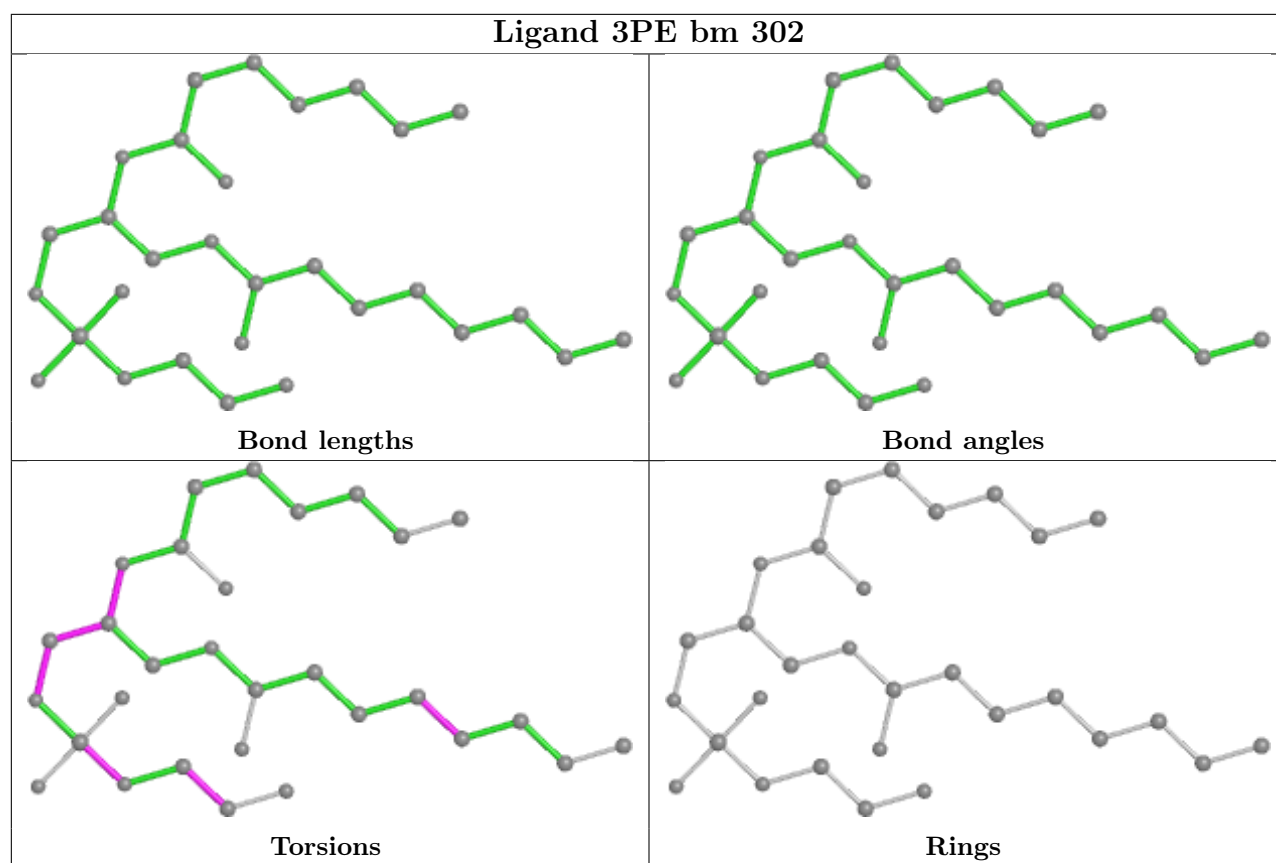
No monomer is involved in short contacts.

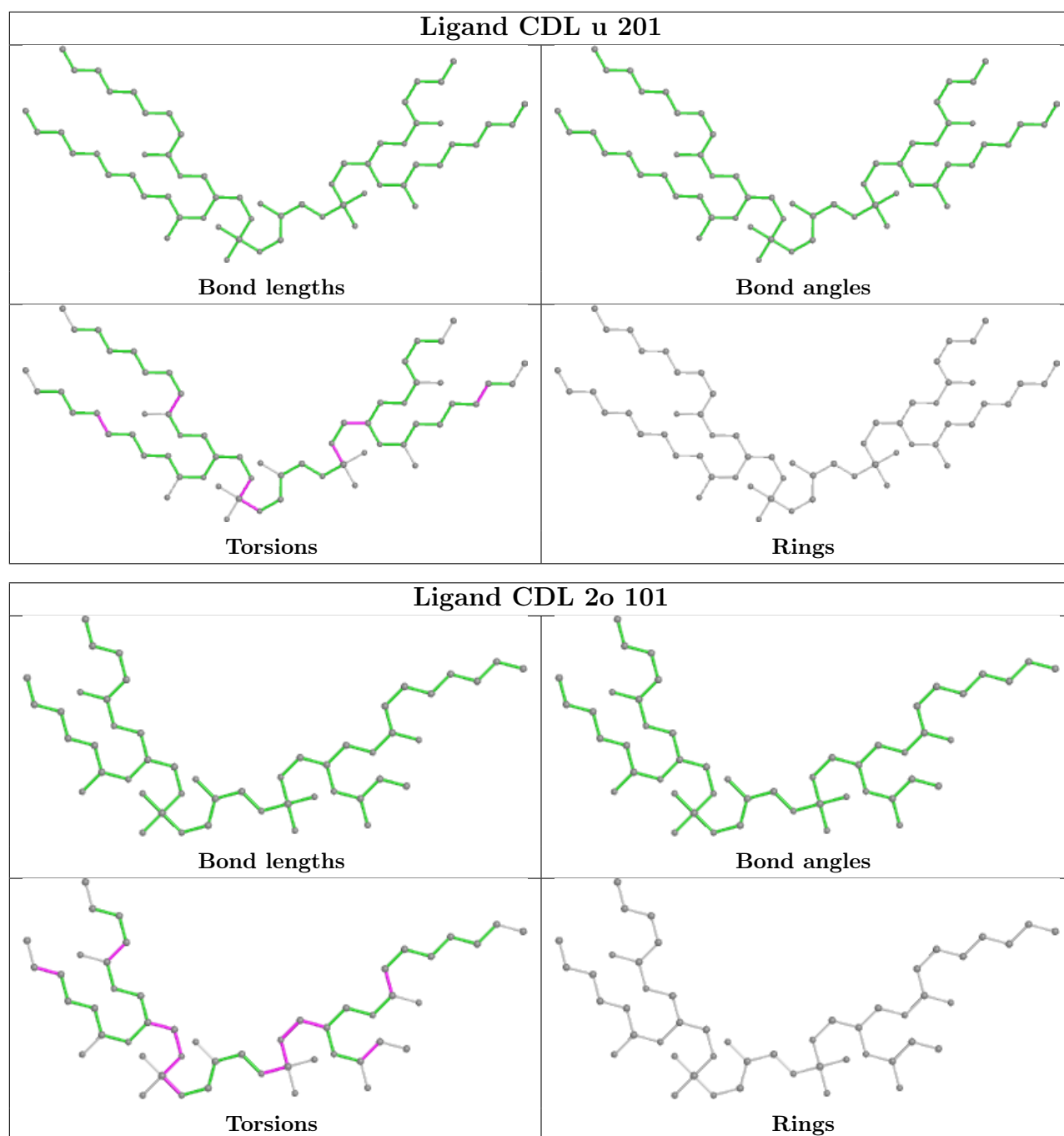
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

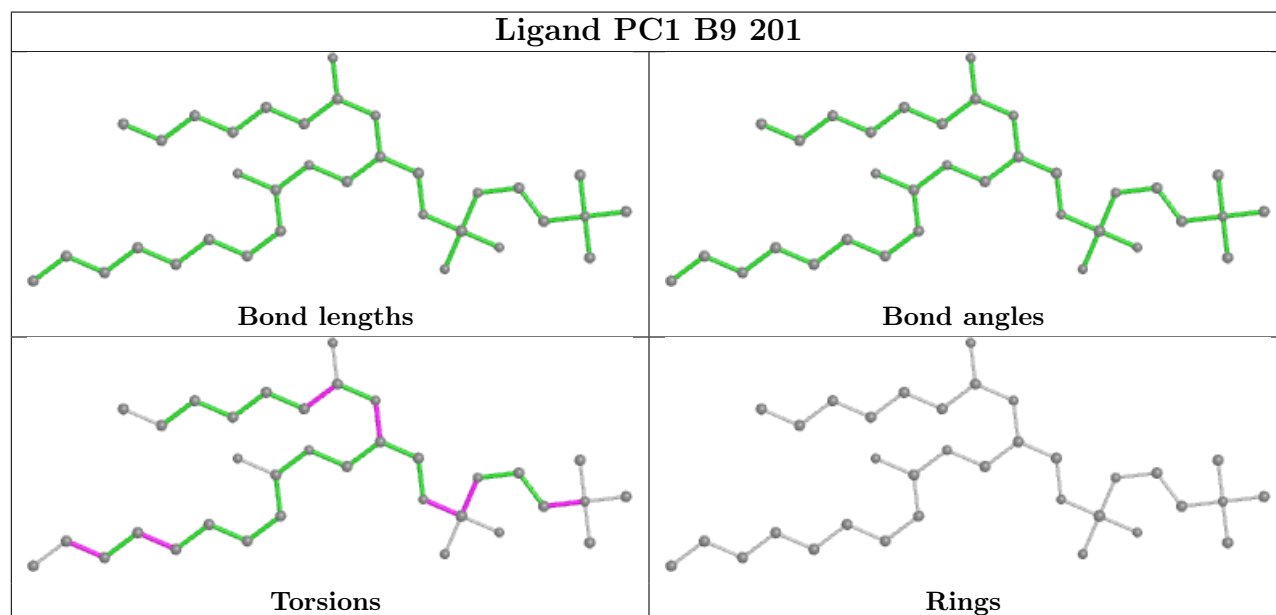
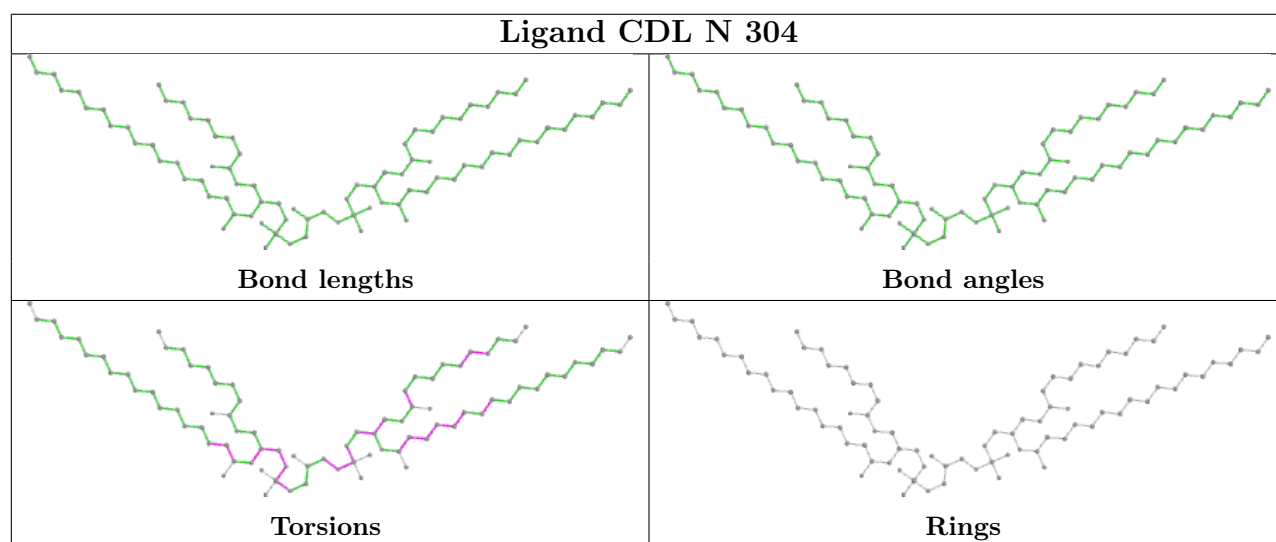
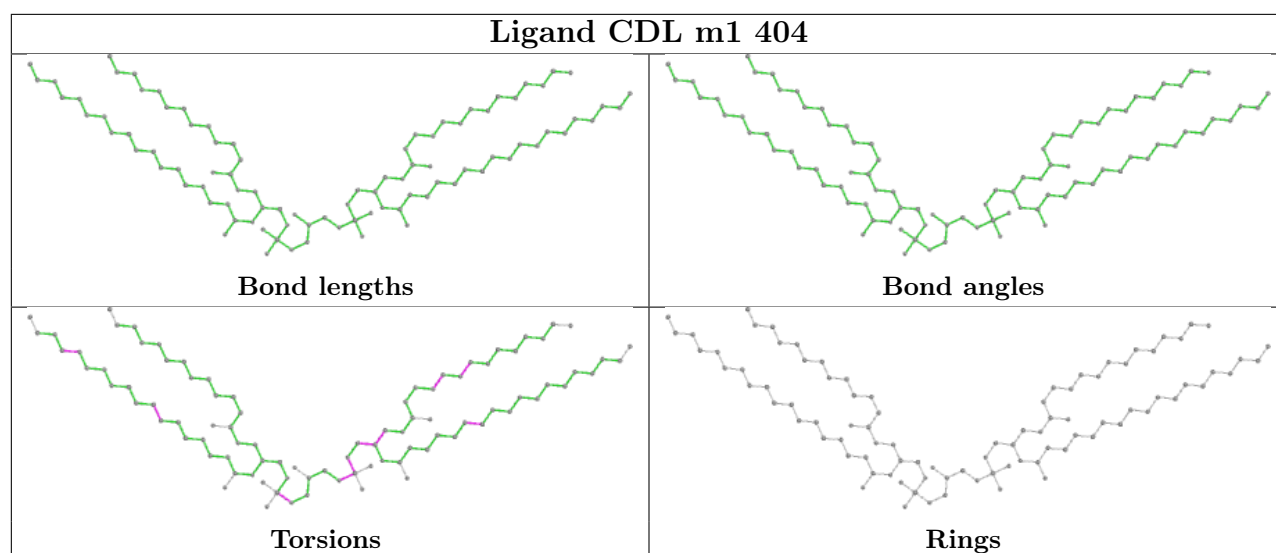


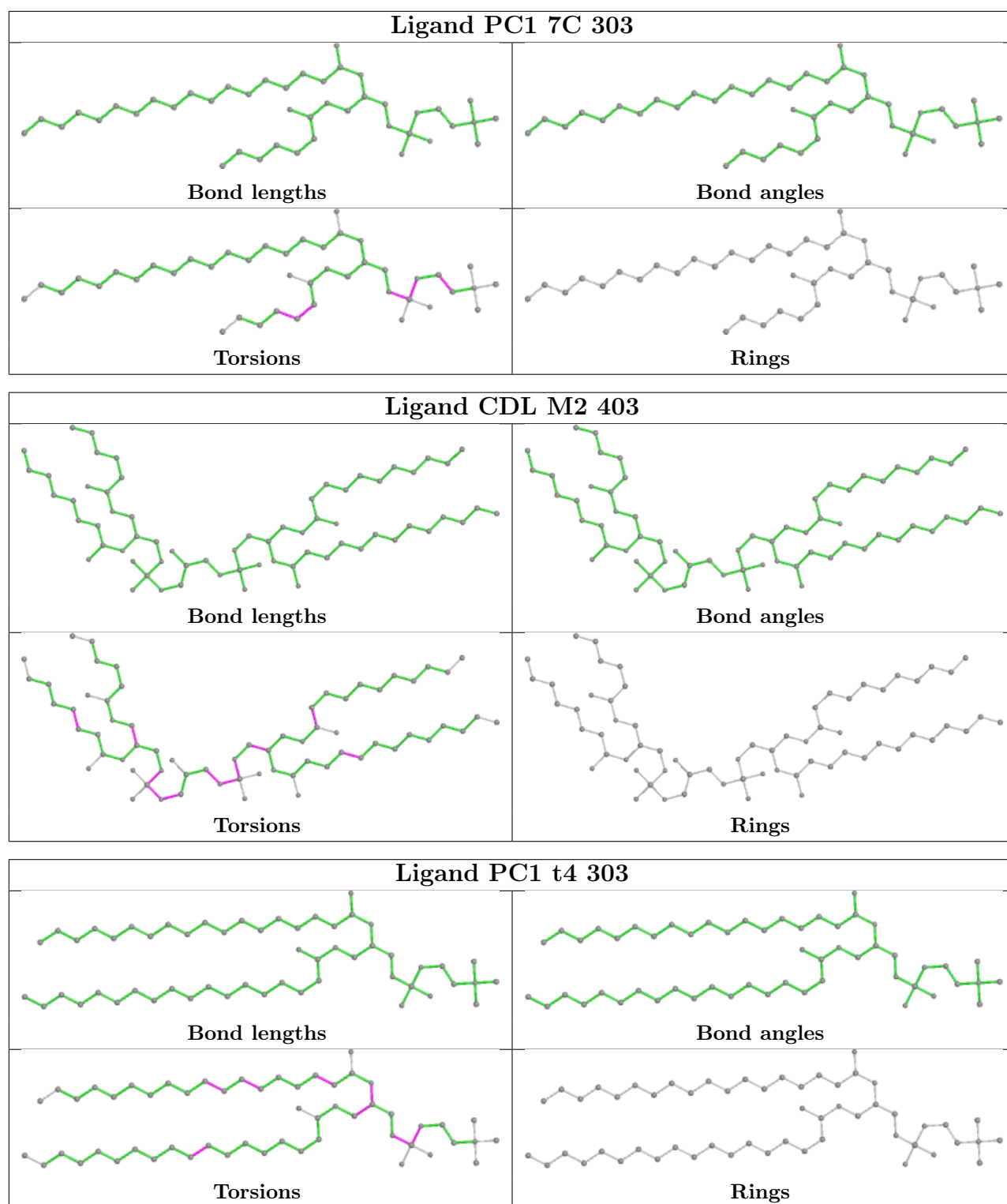


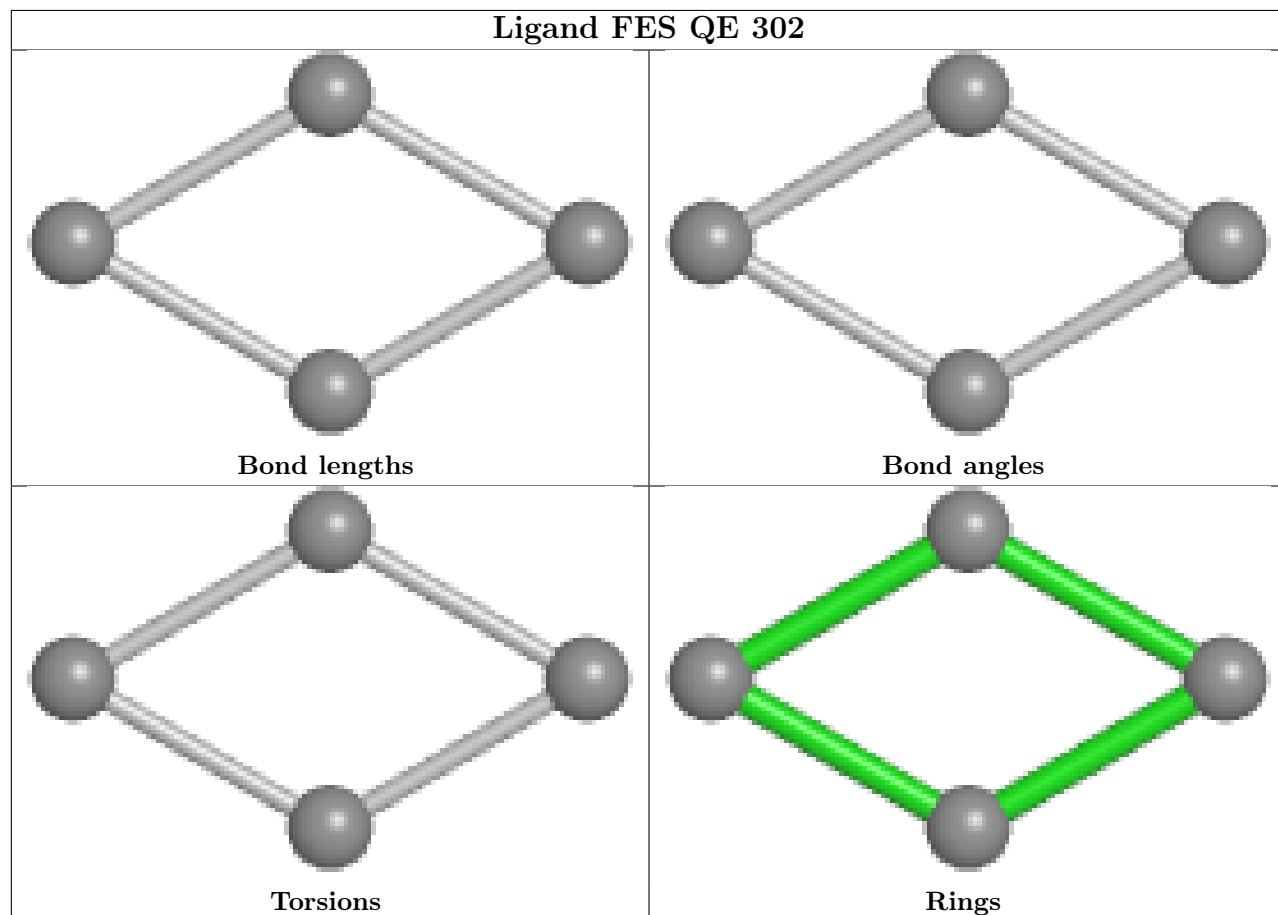
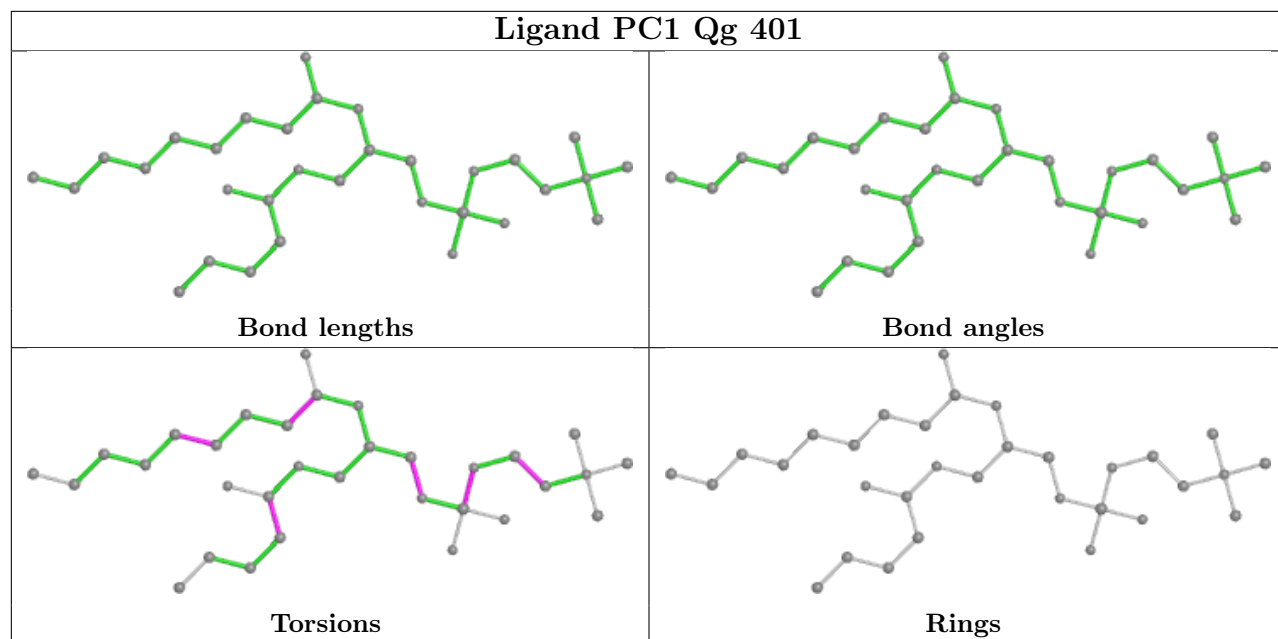


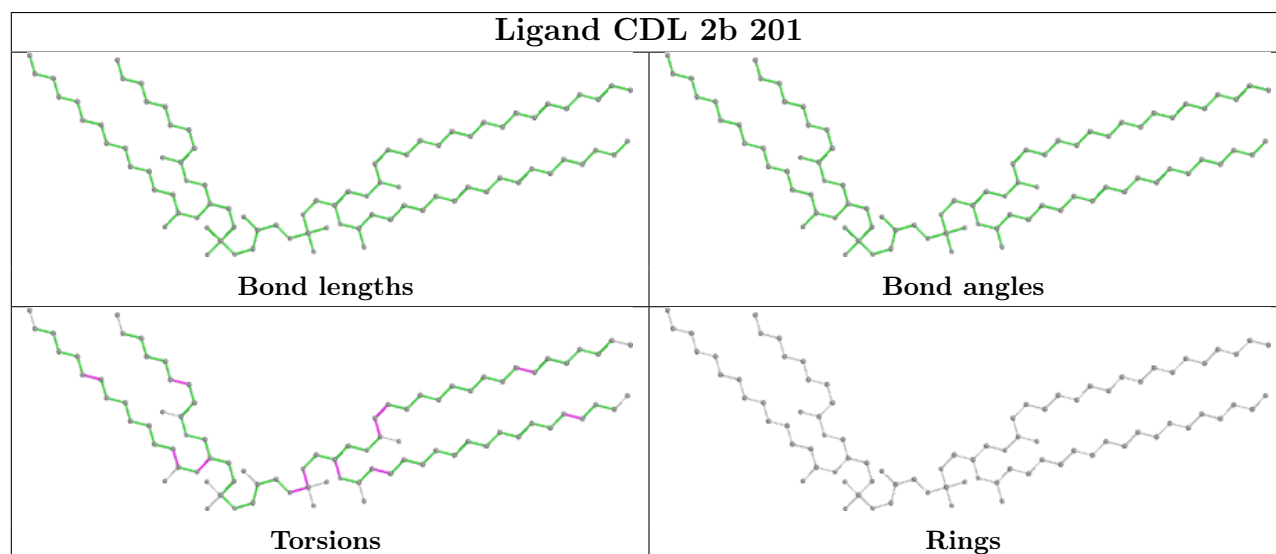
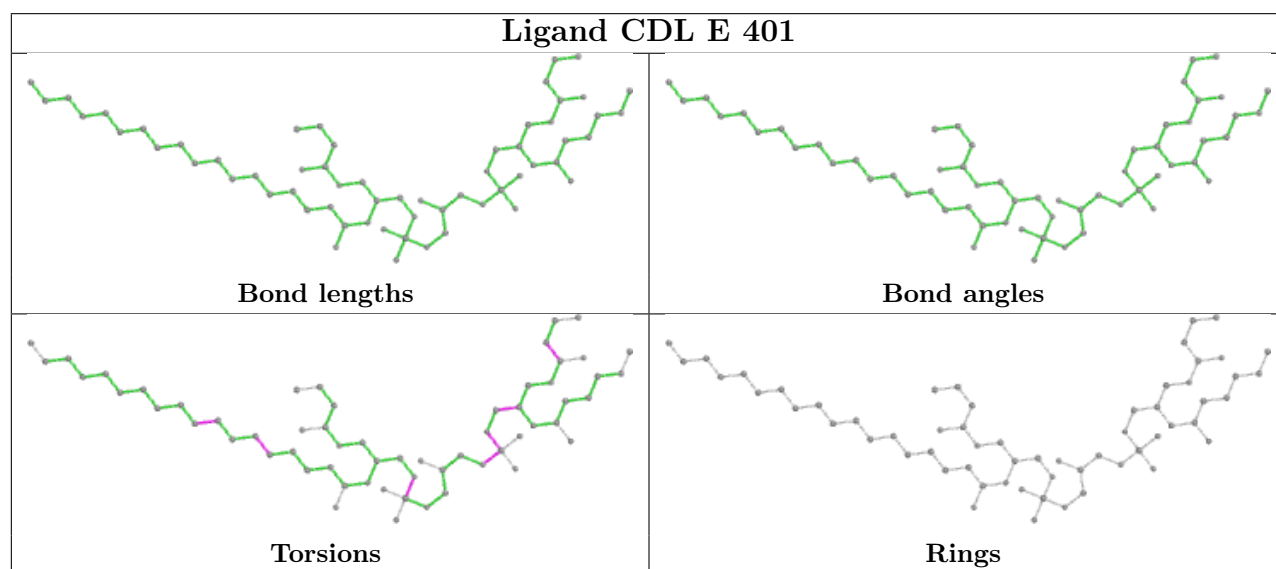
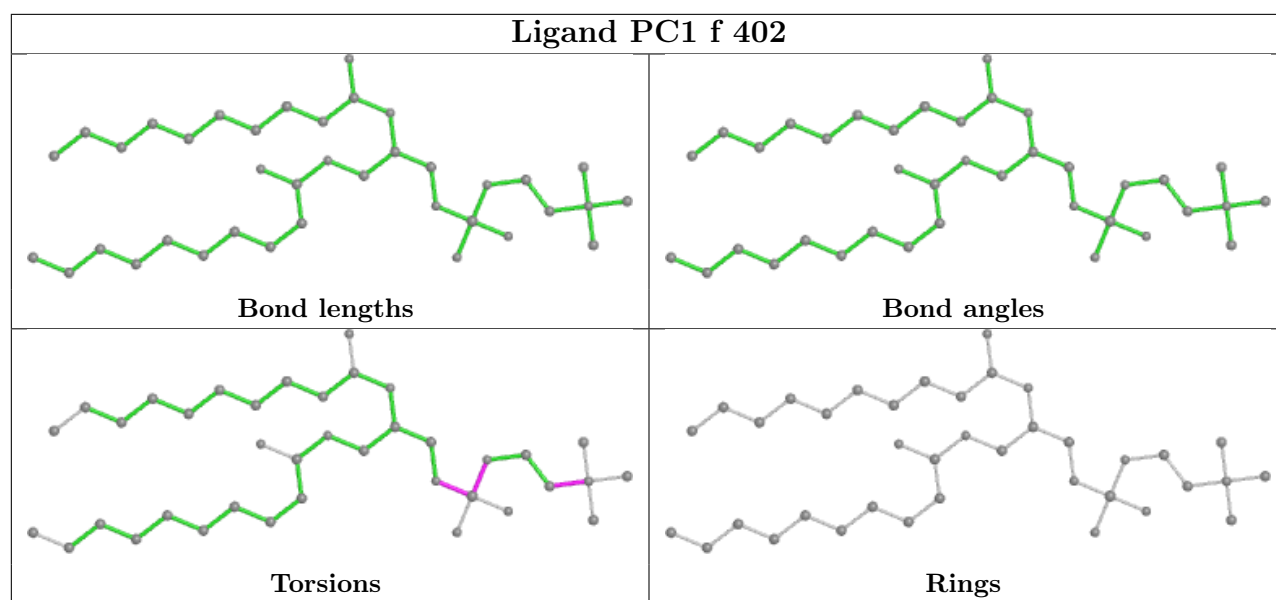


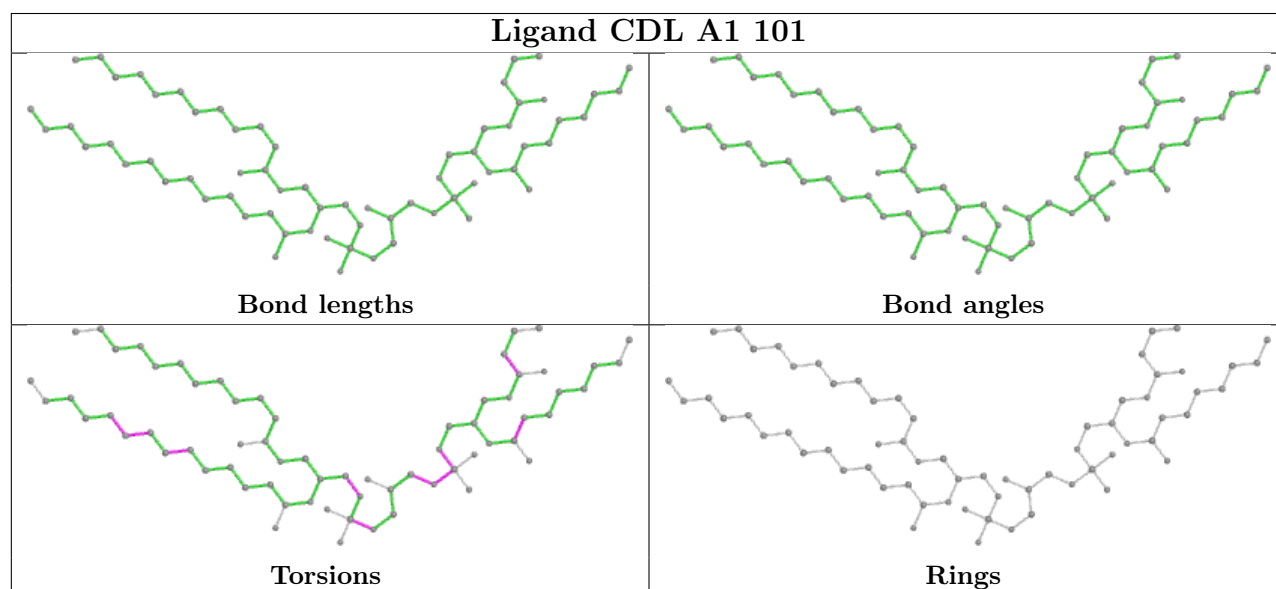
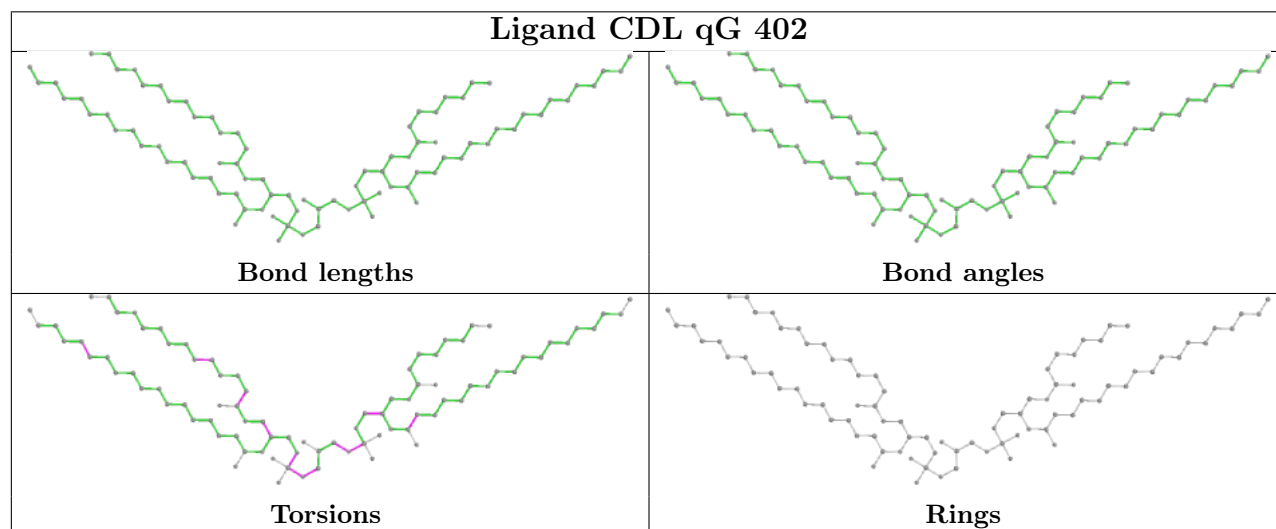
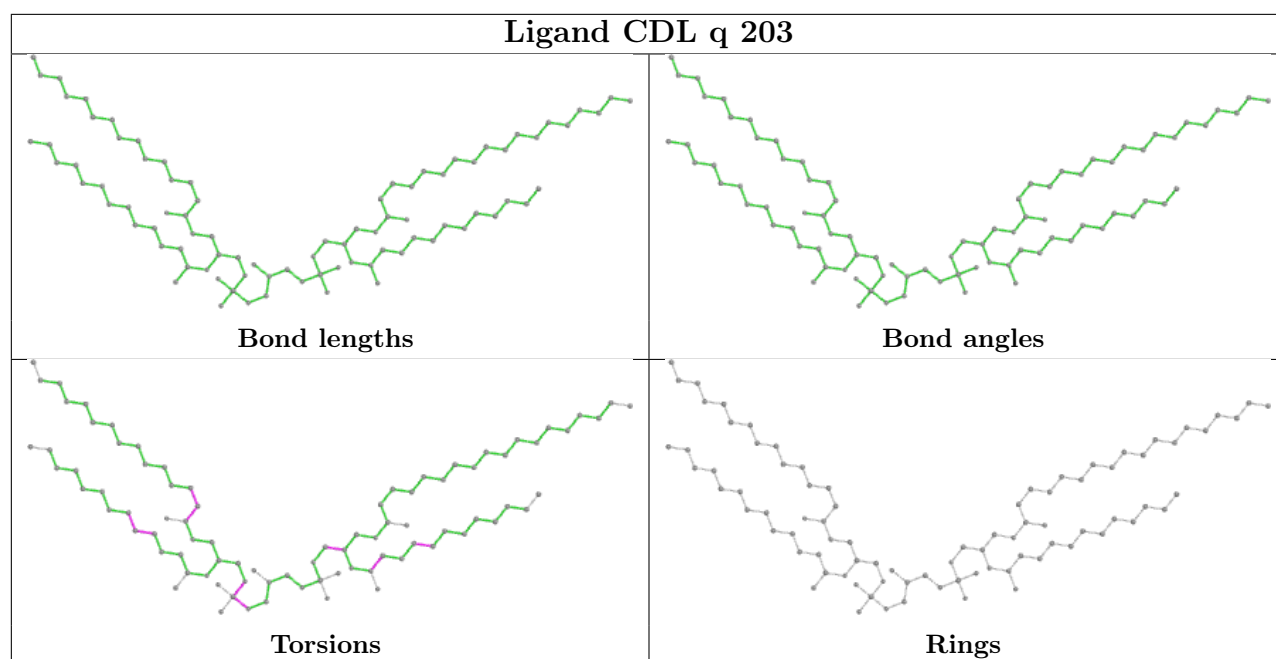


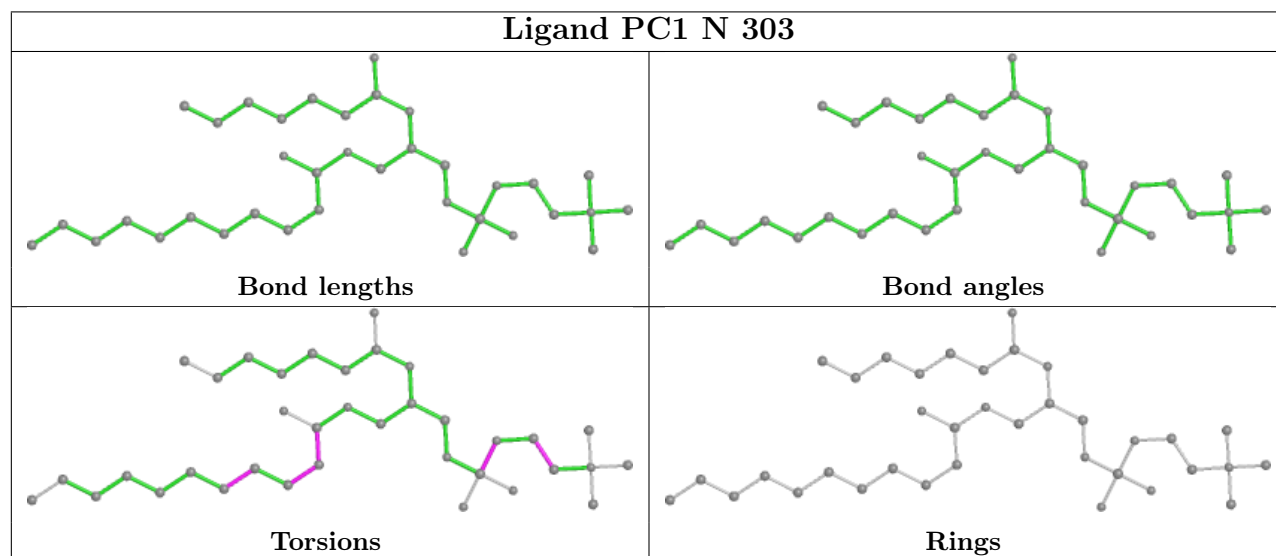
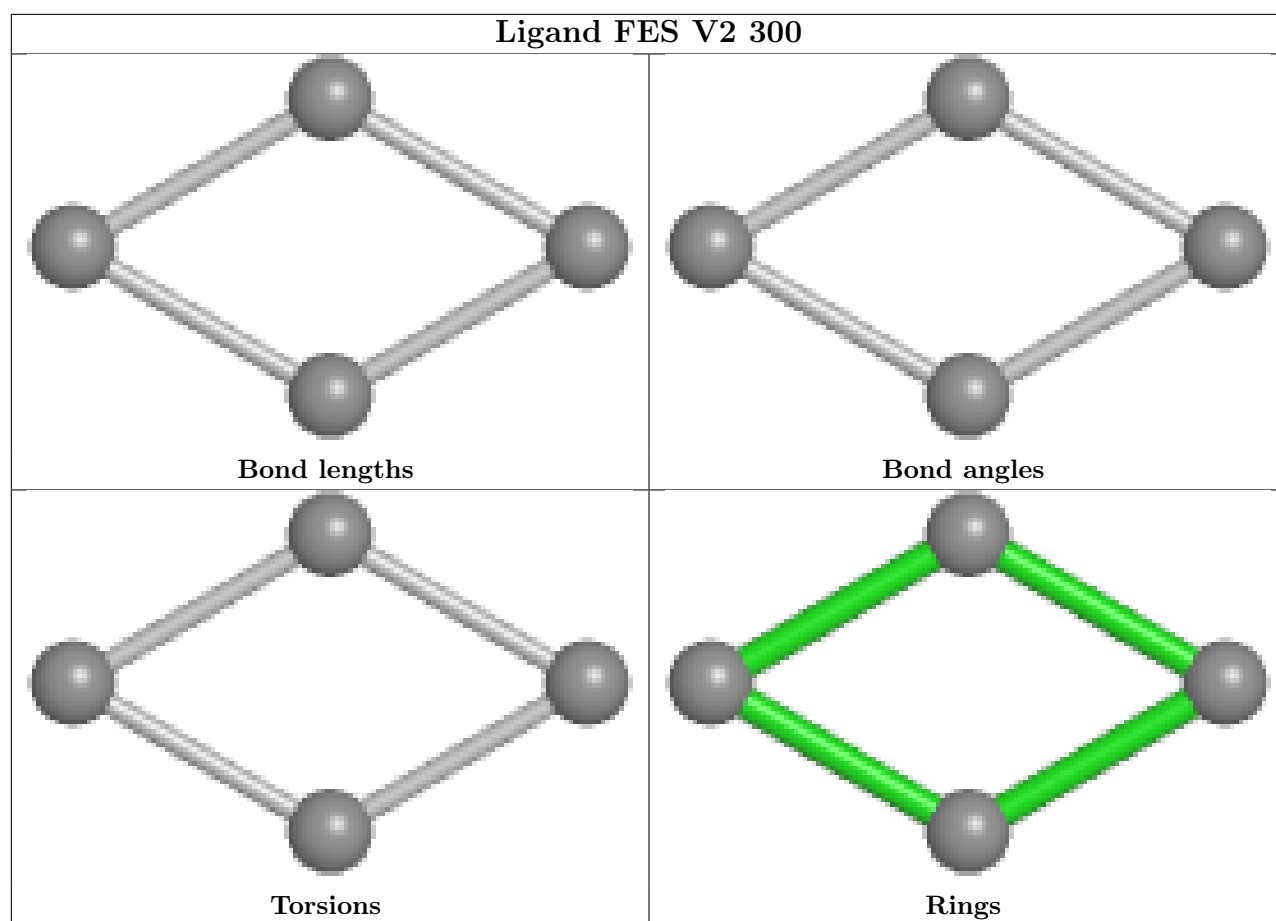


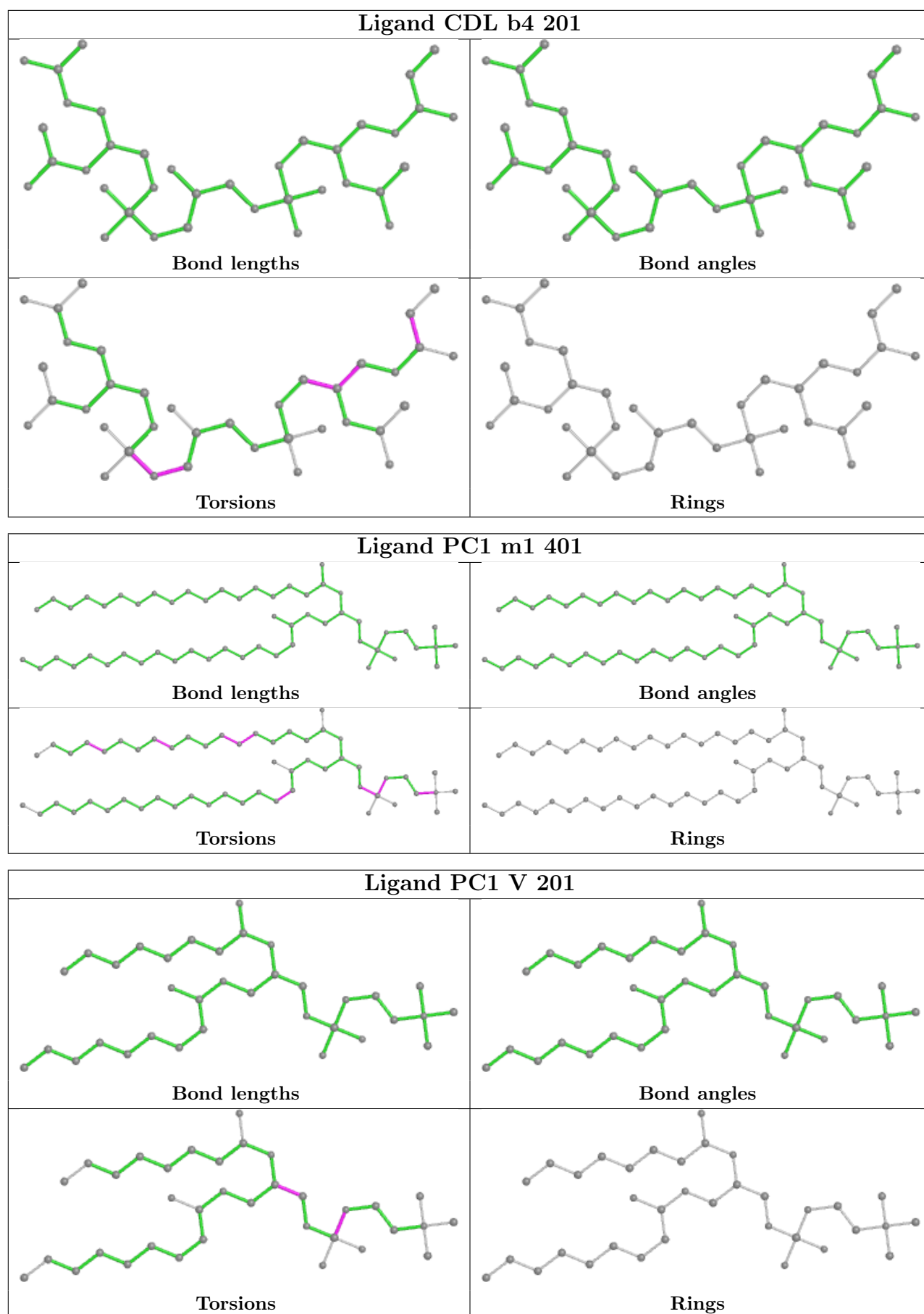


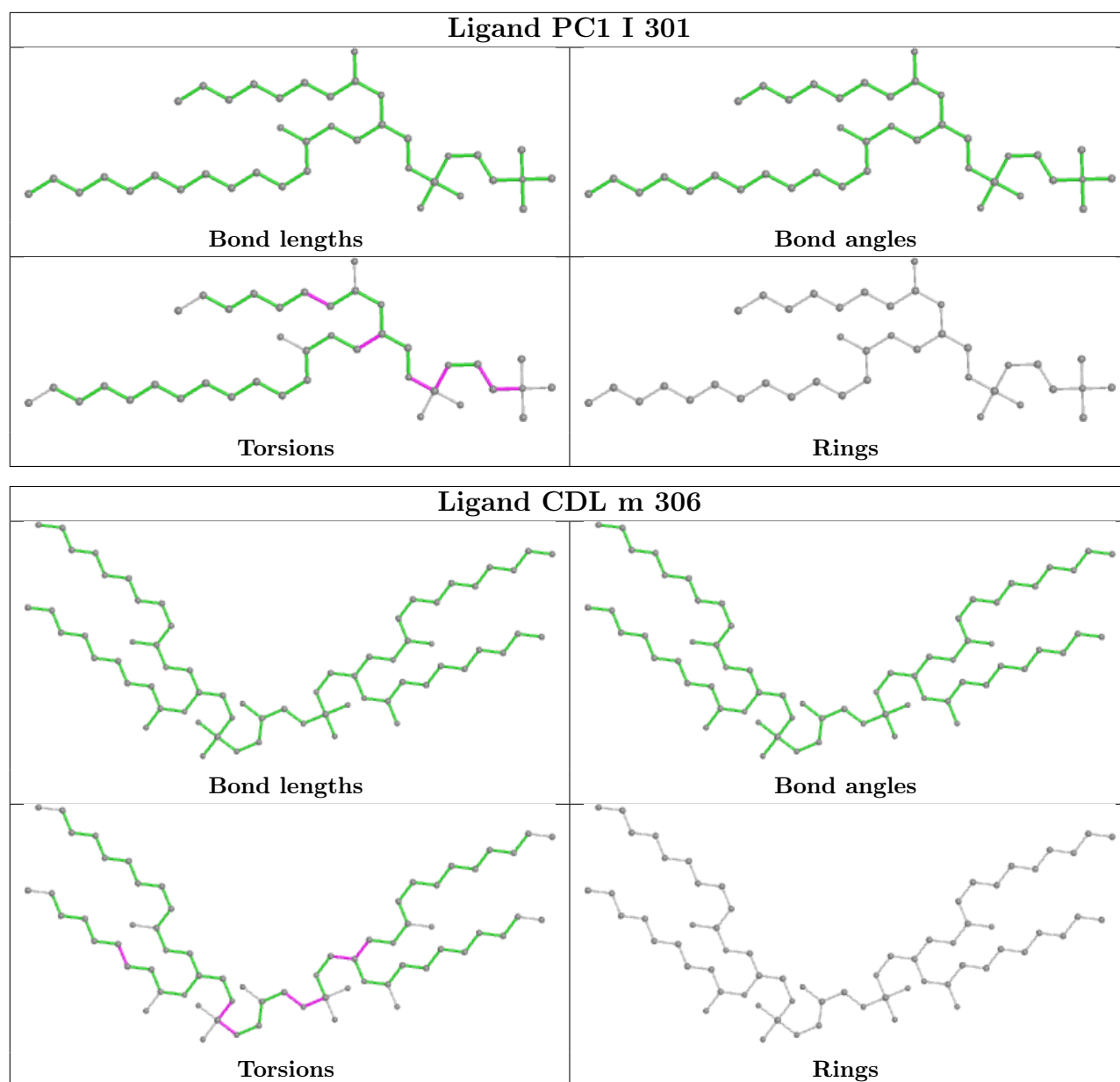


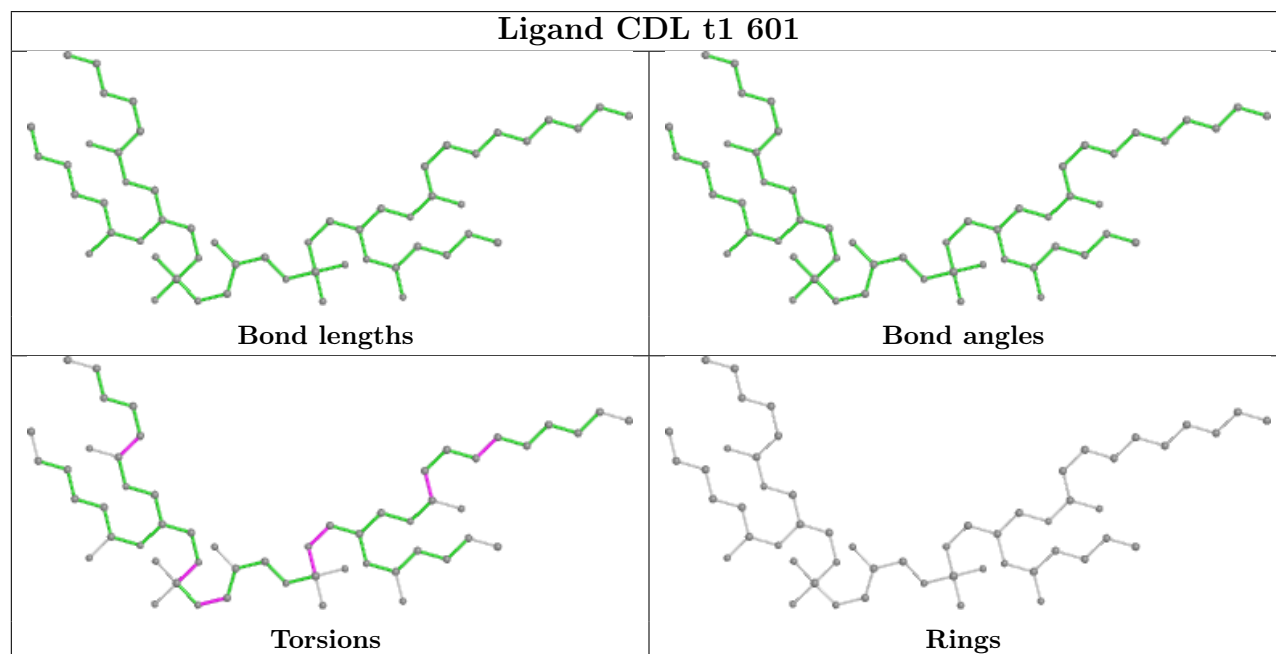
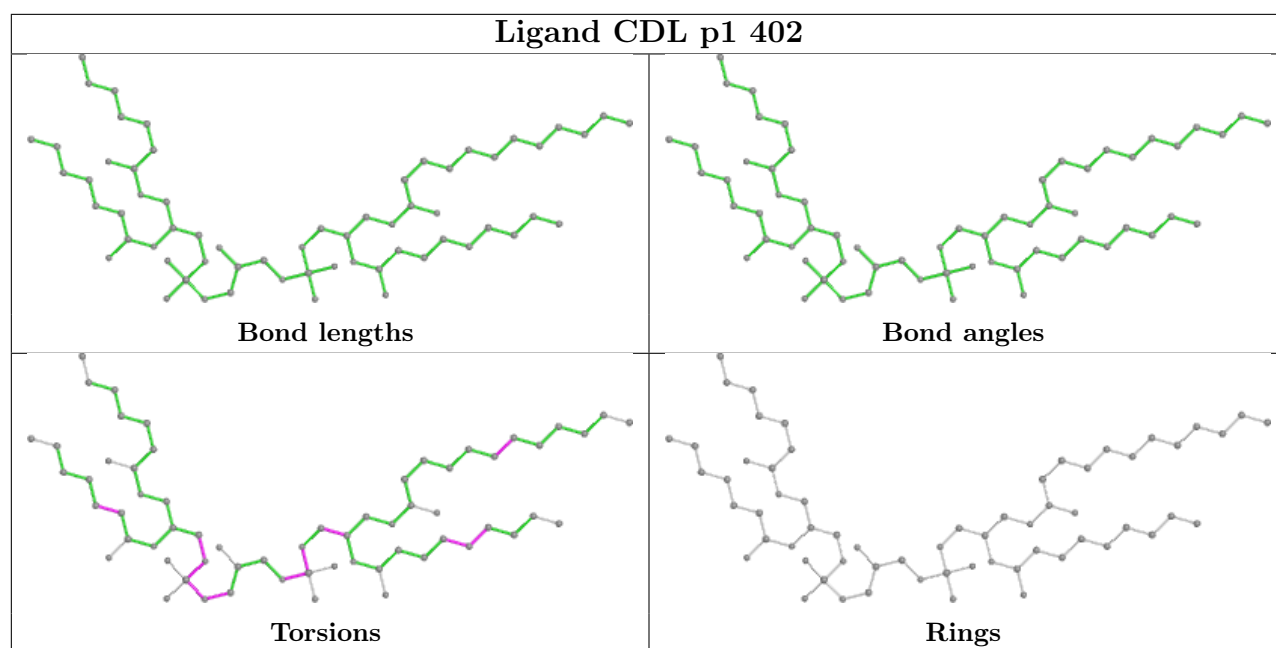


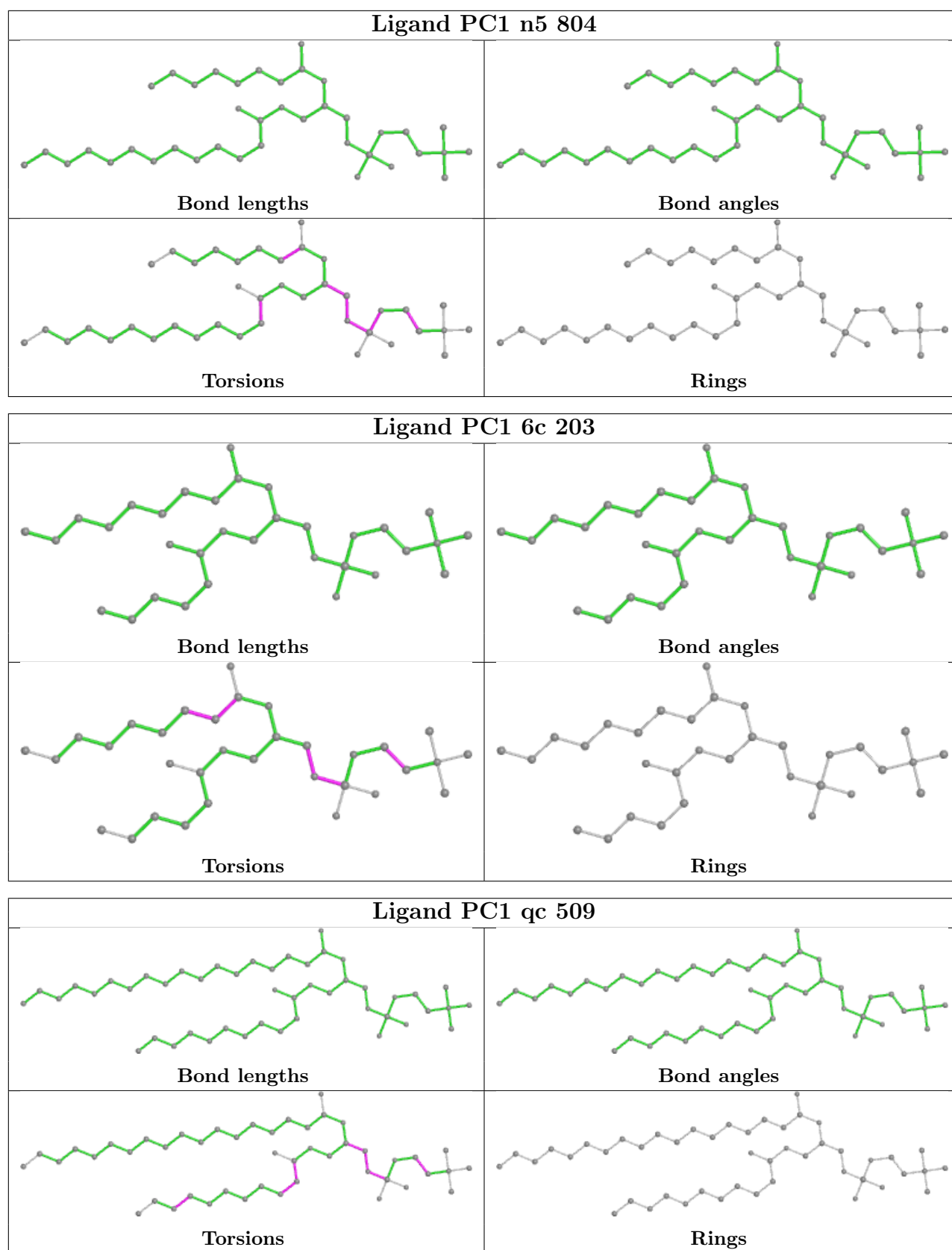


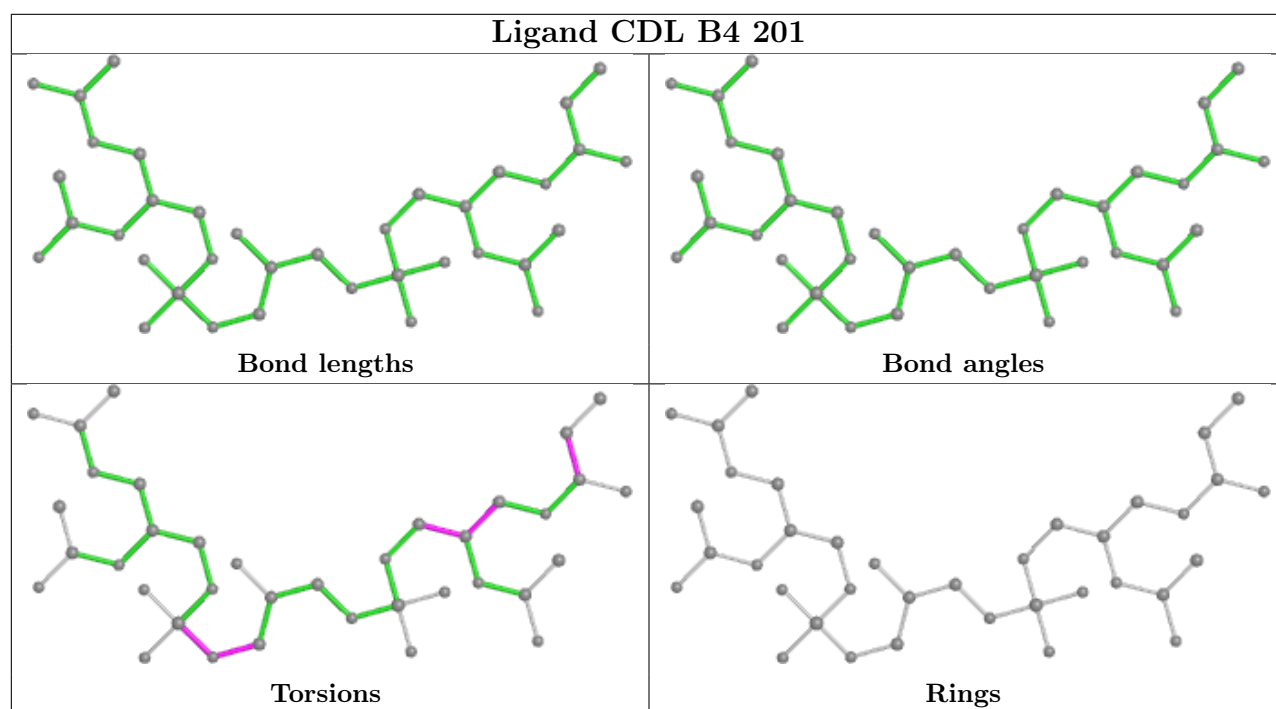
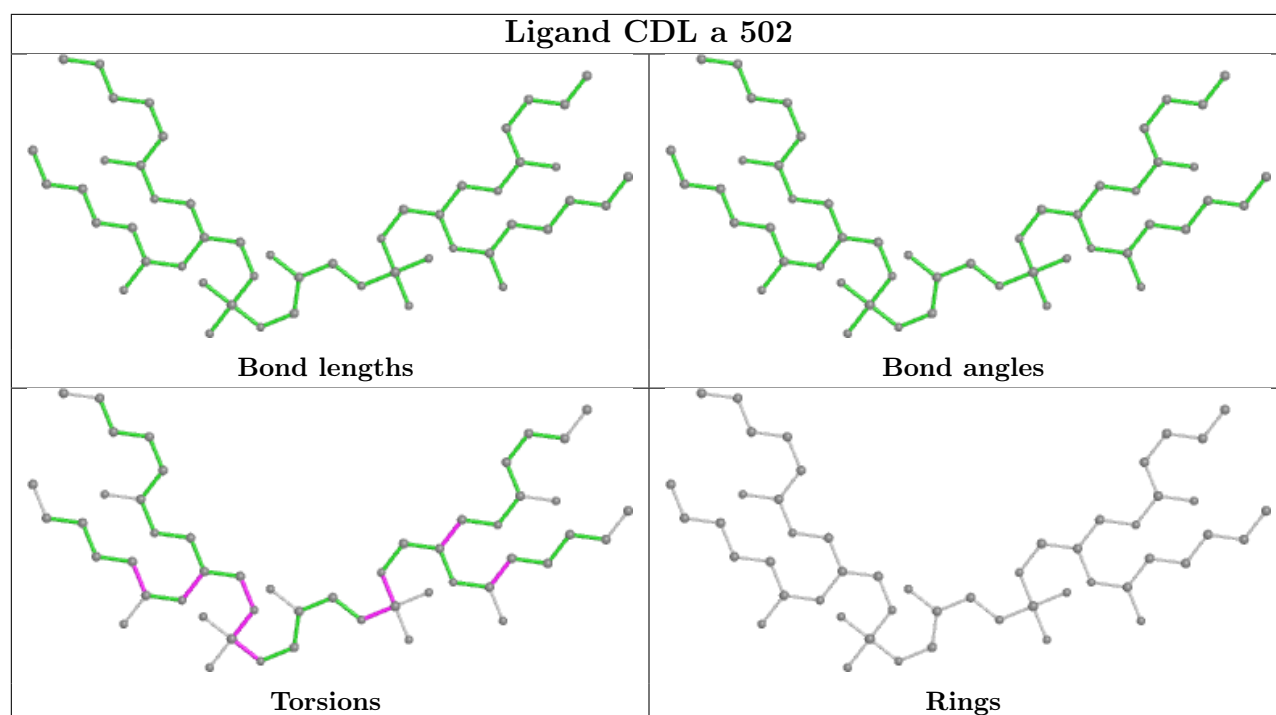


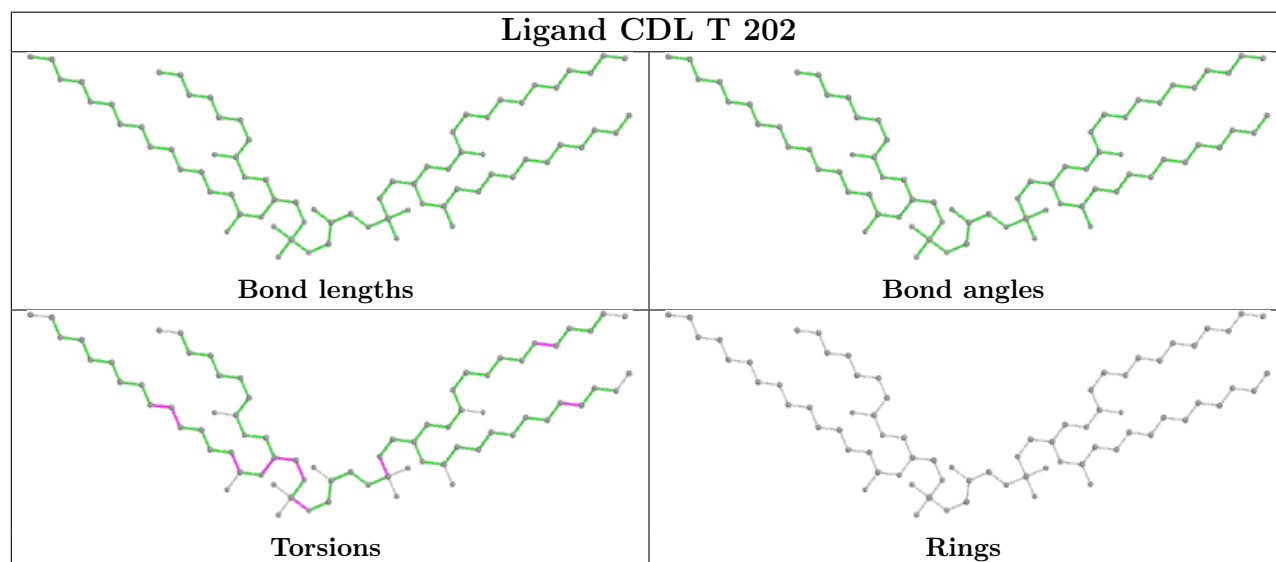
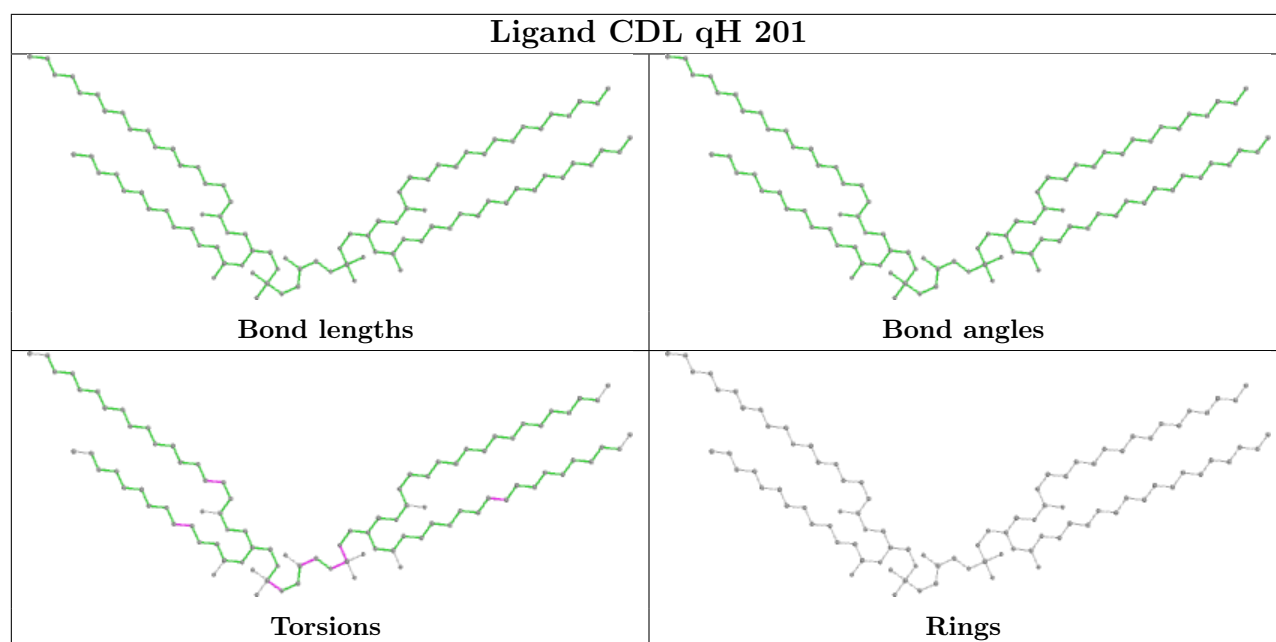


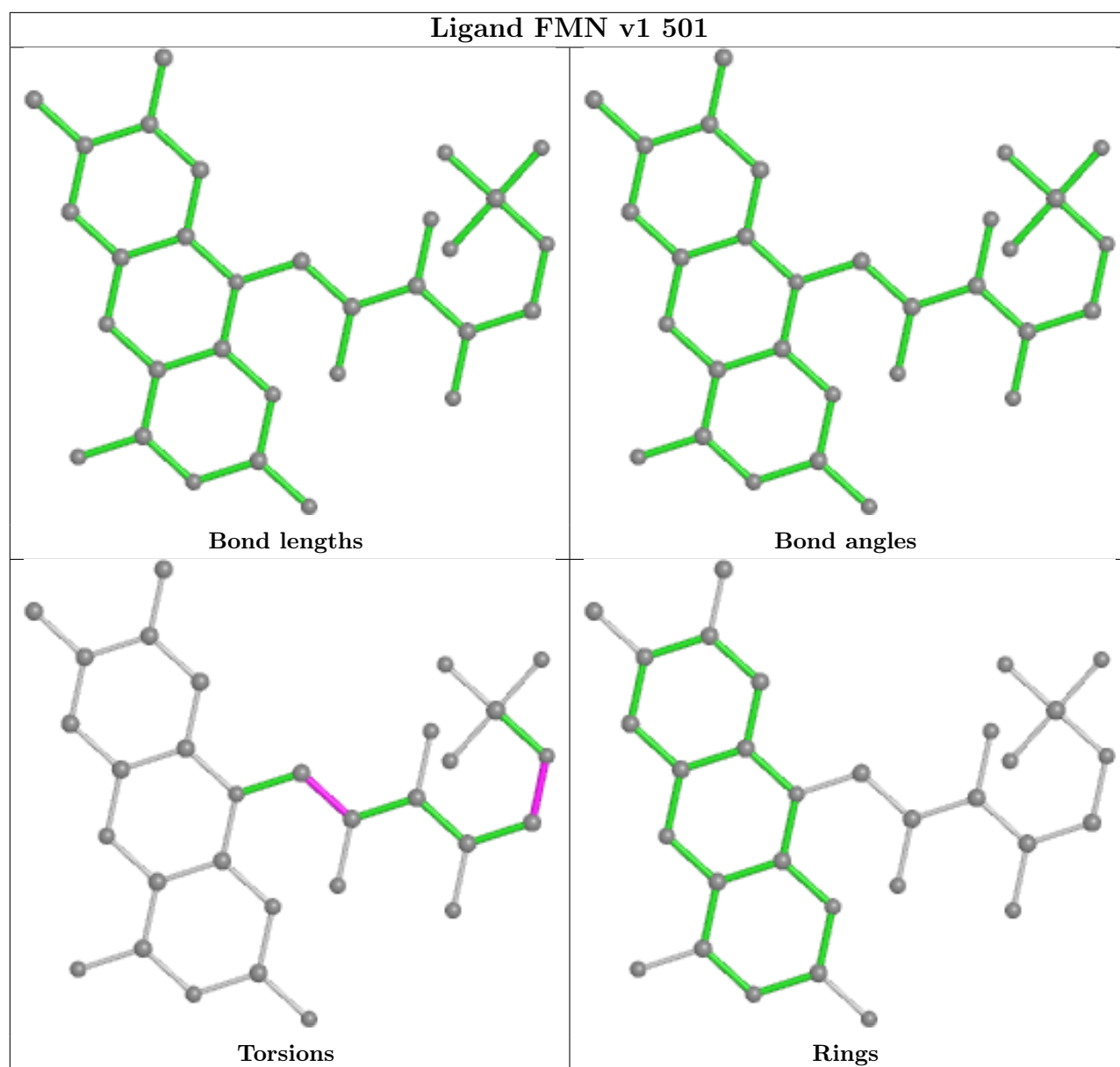


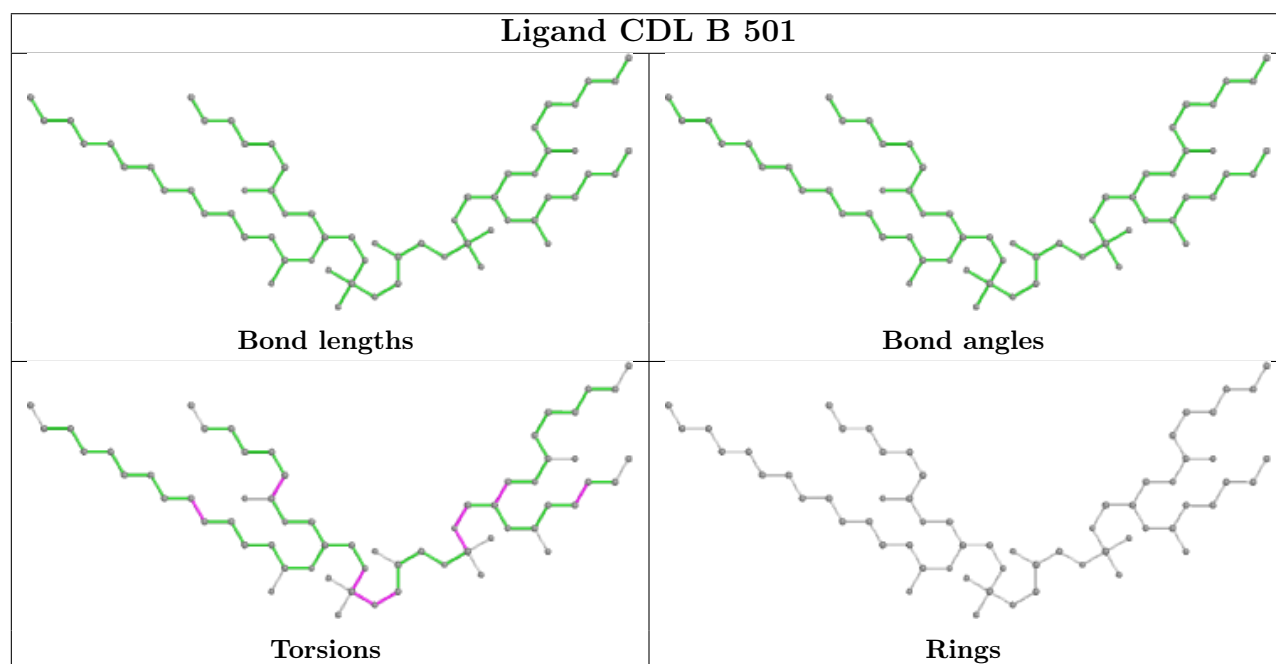
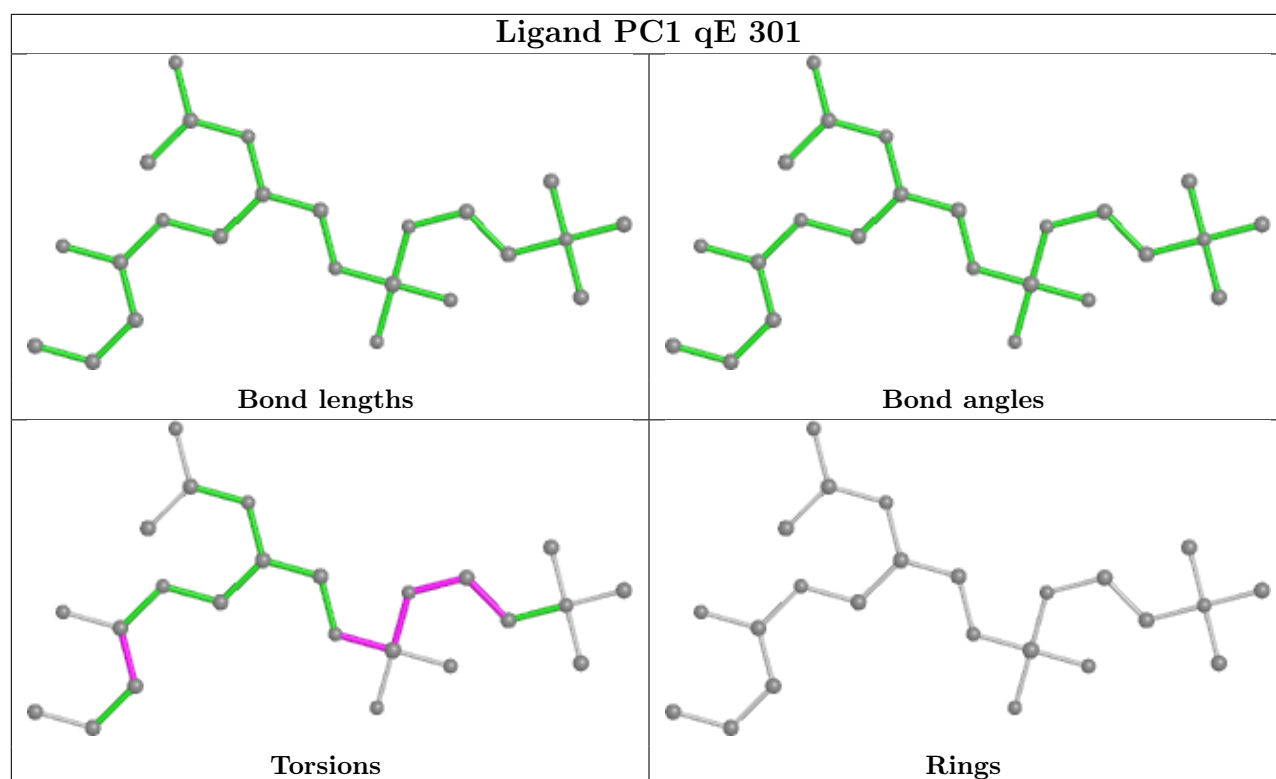


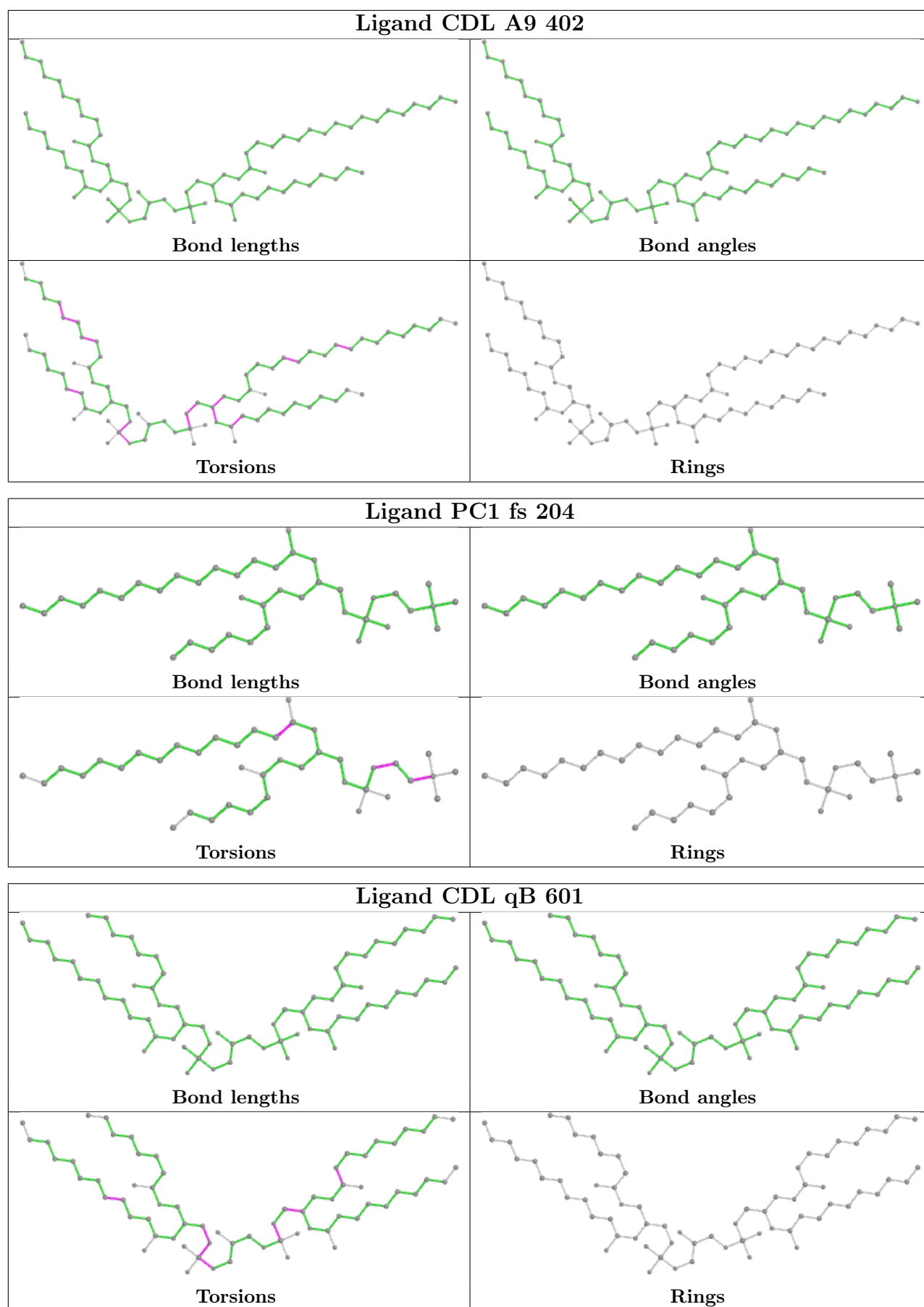


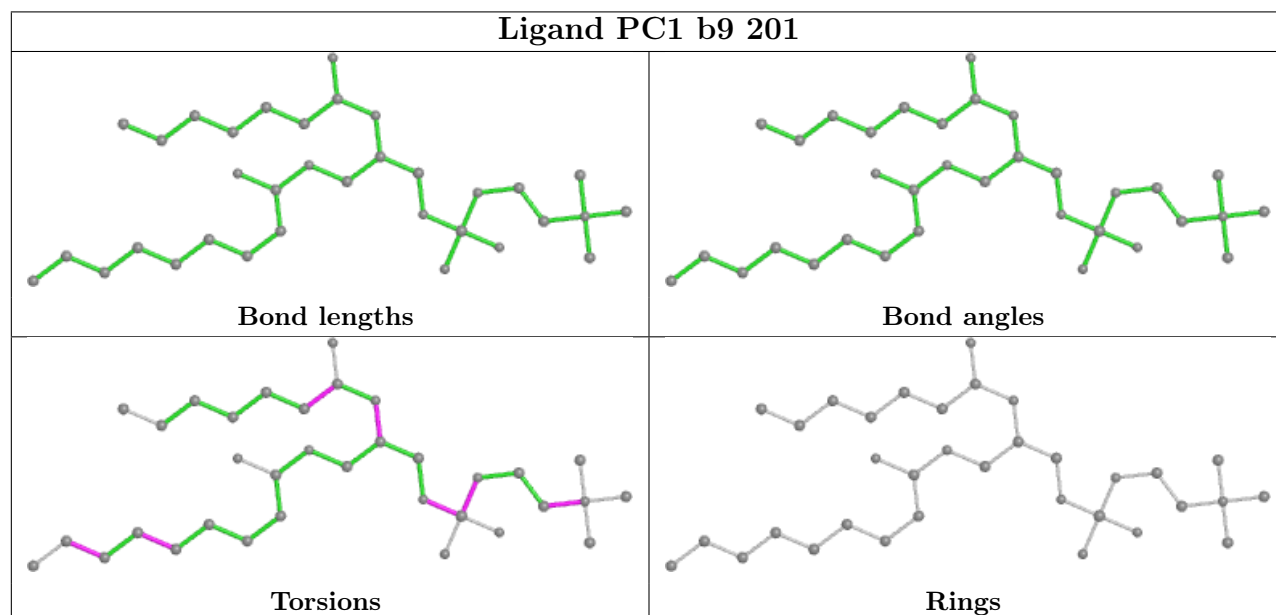
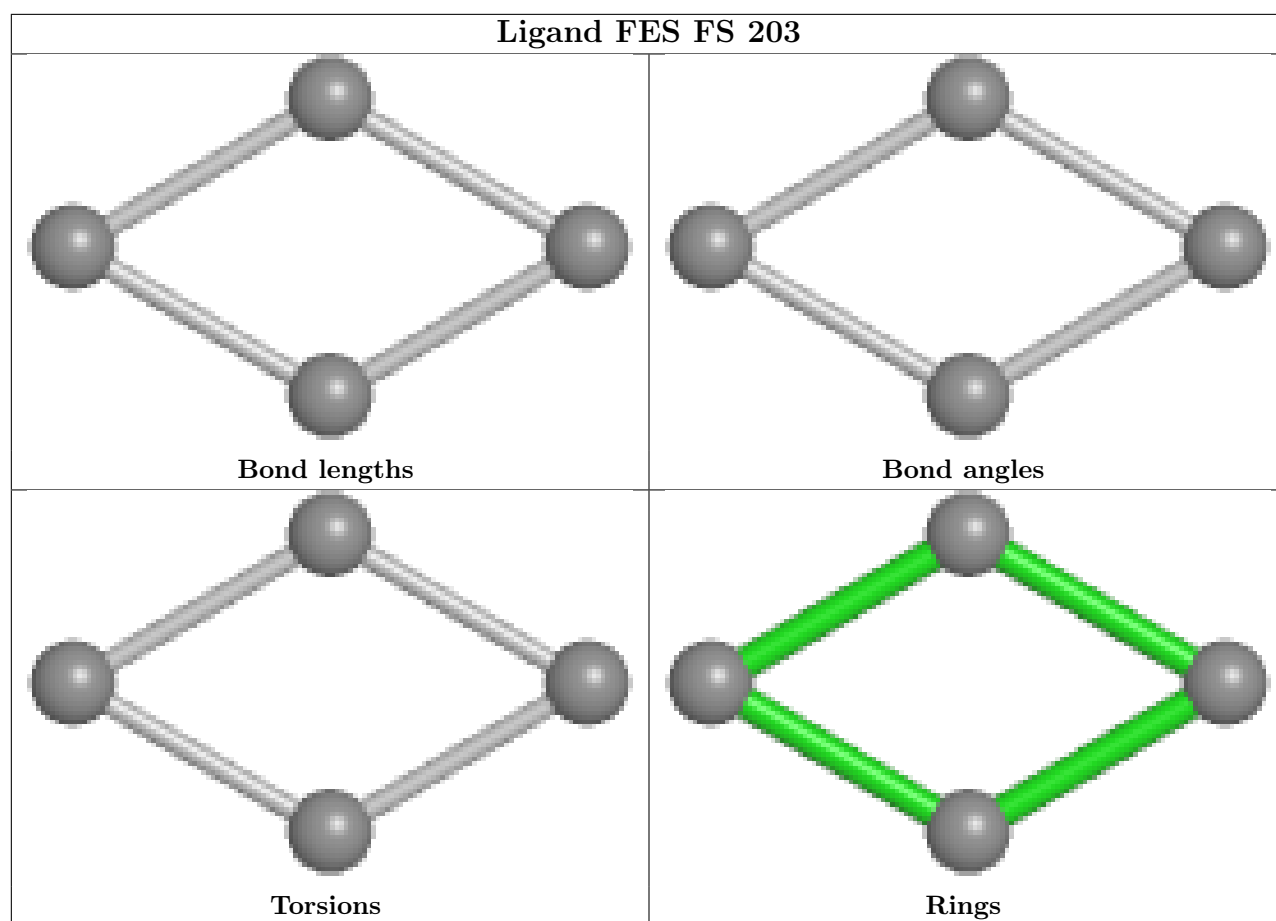


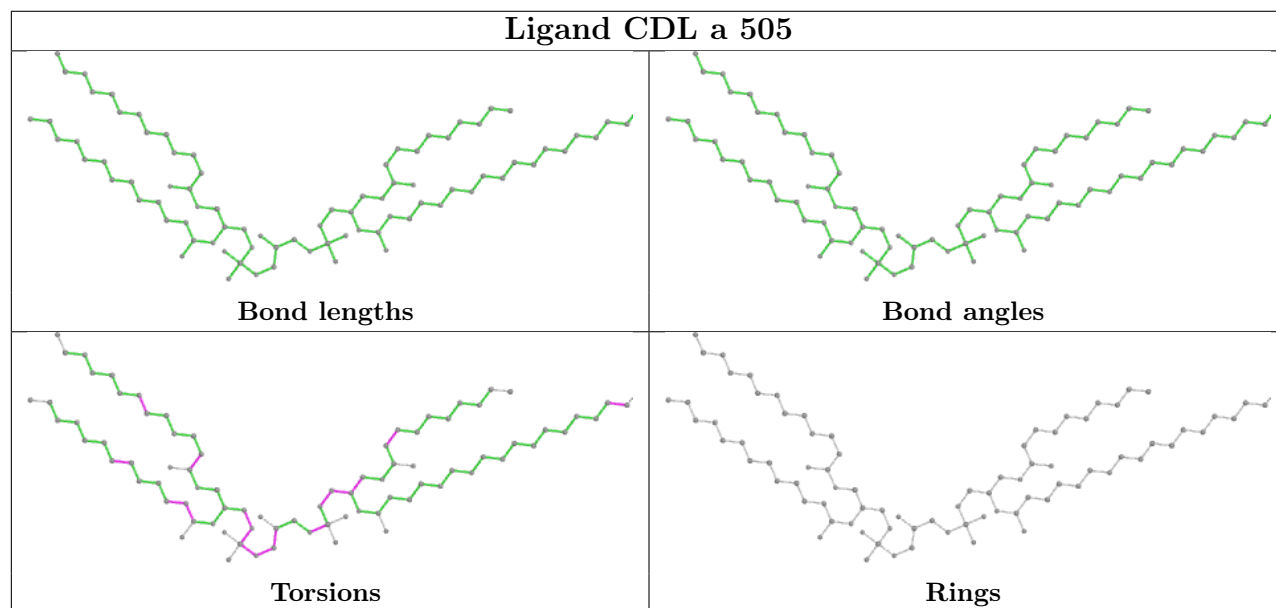
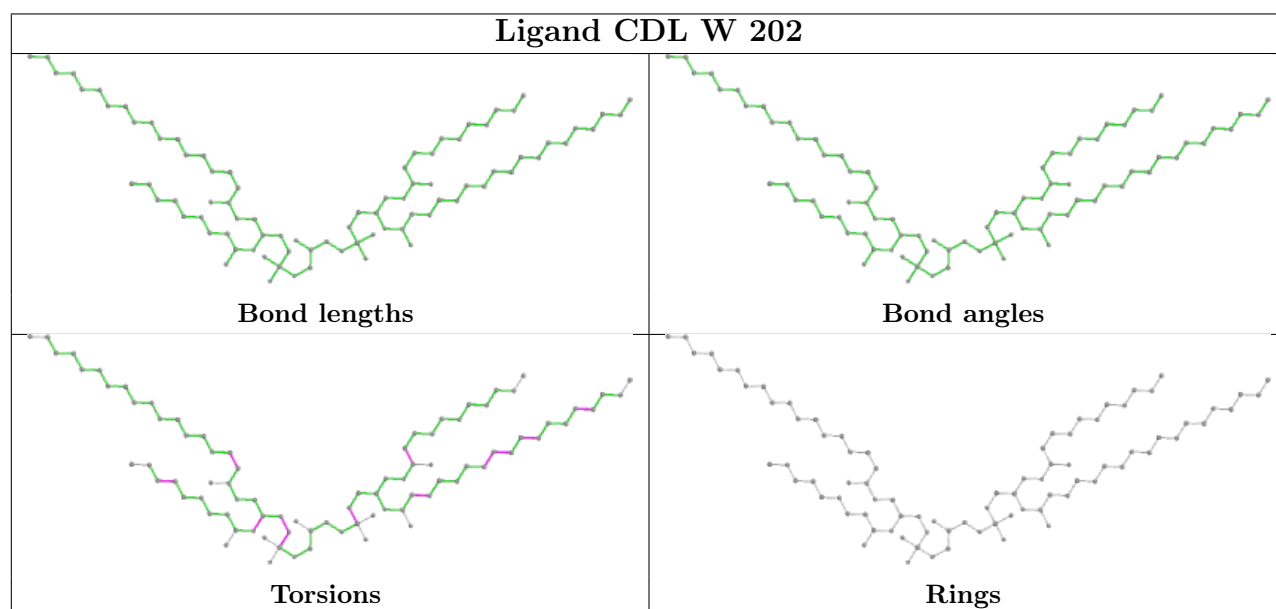
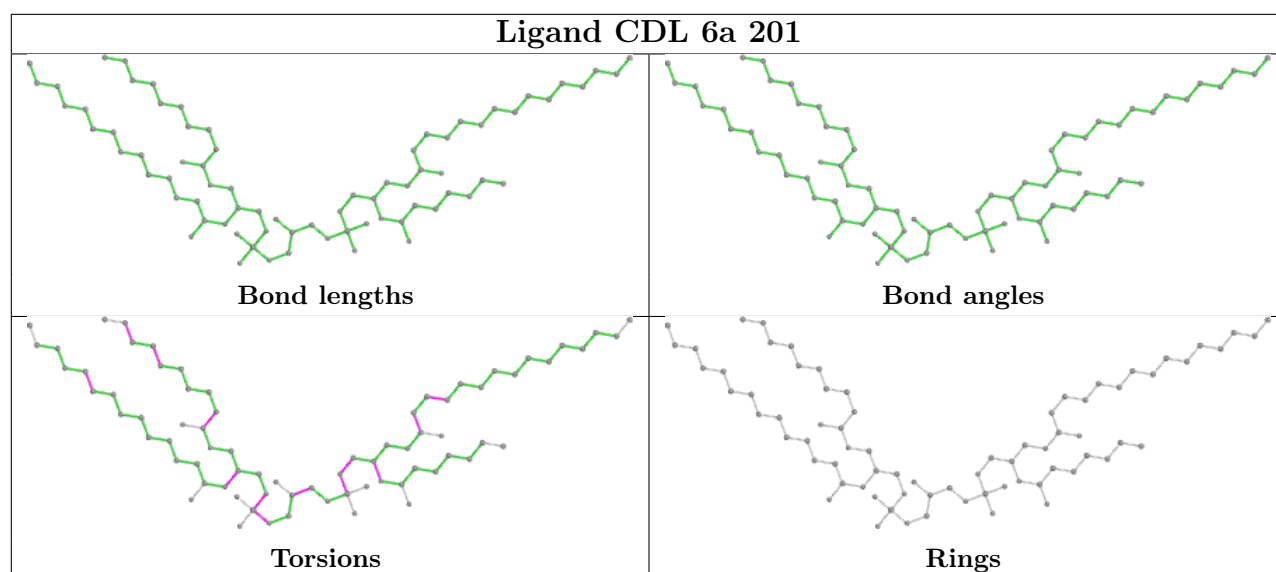


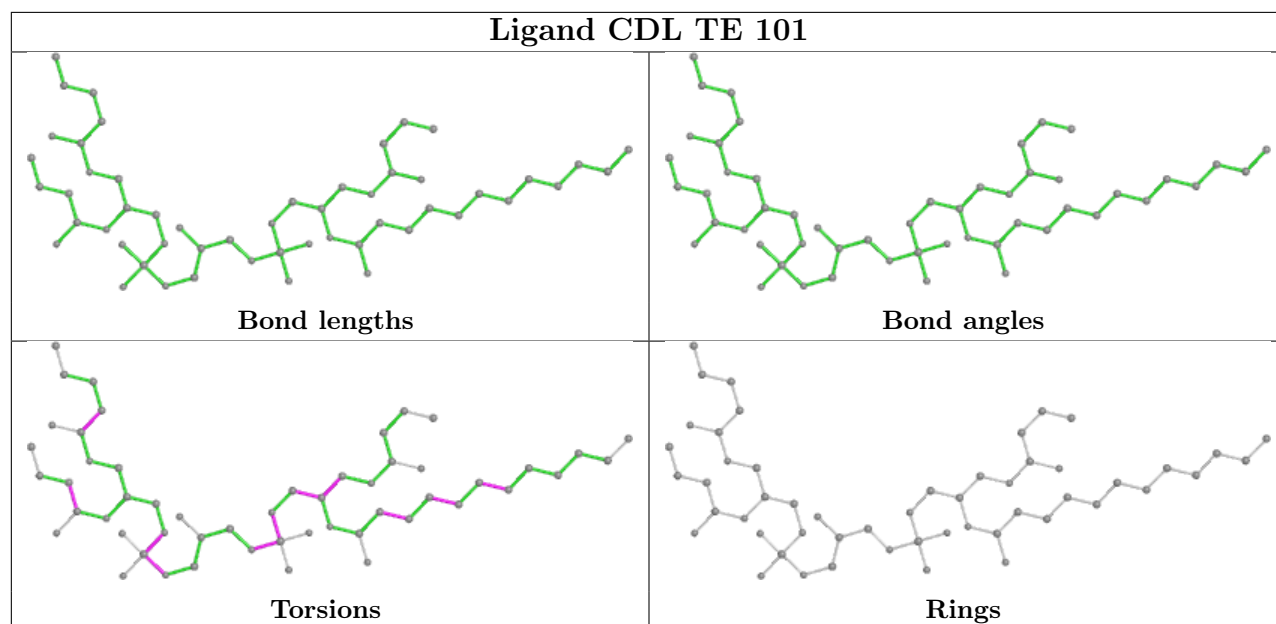
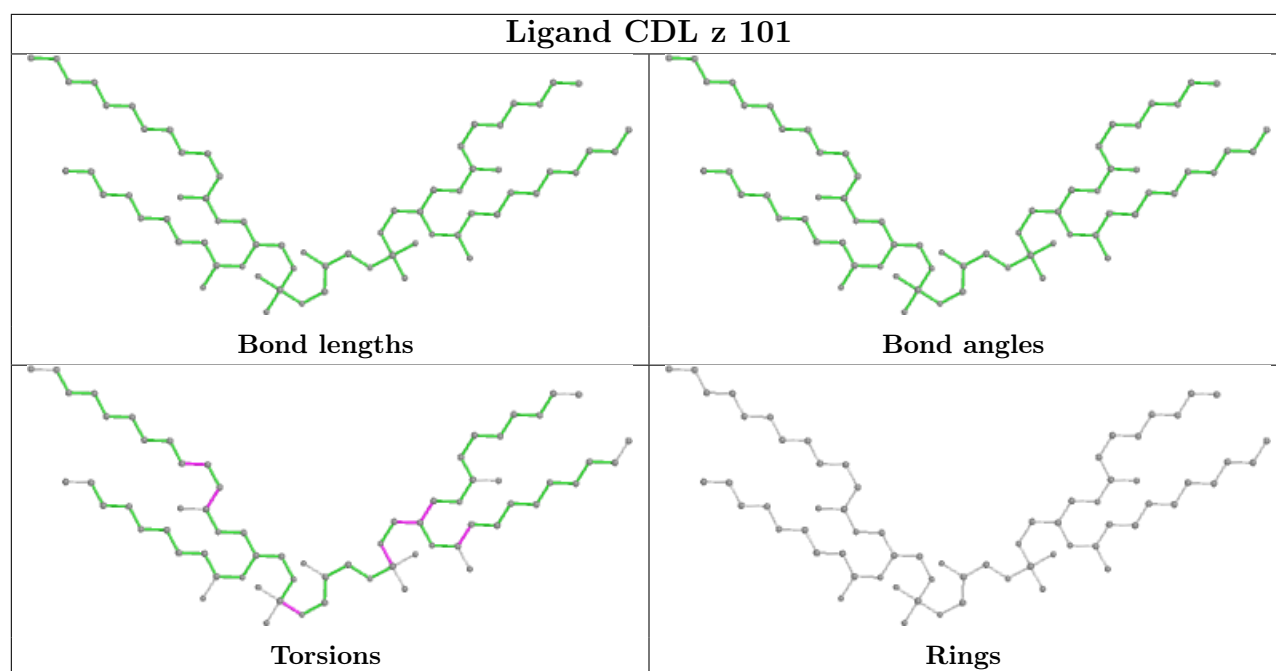


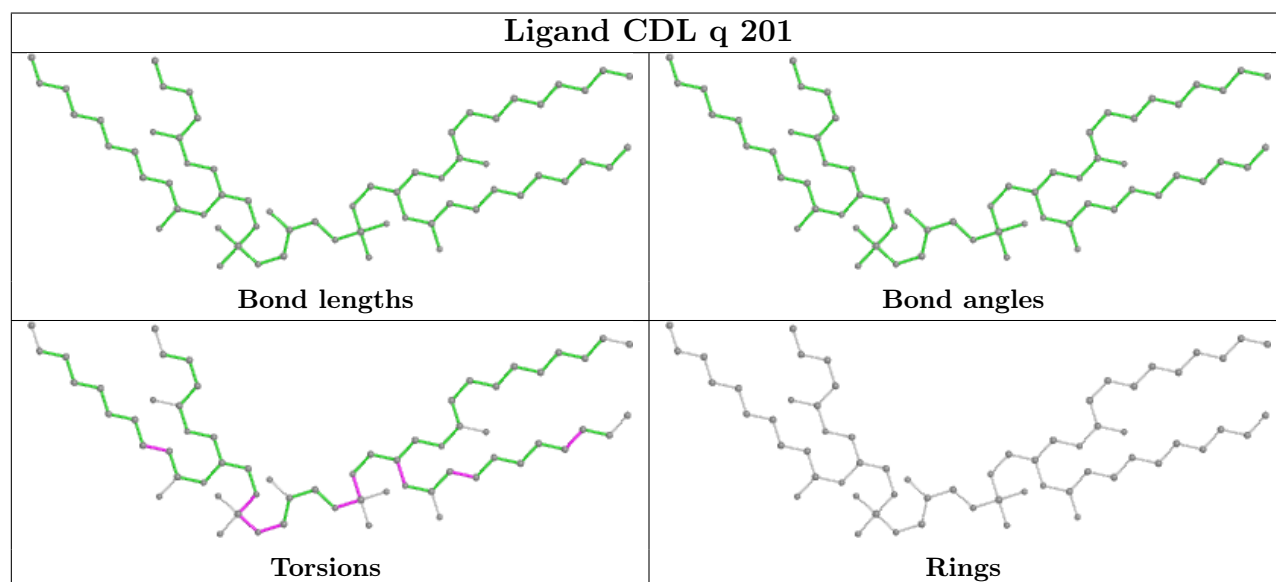
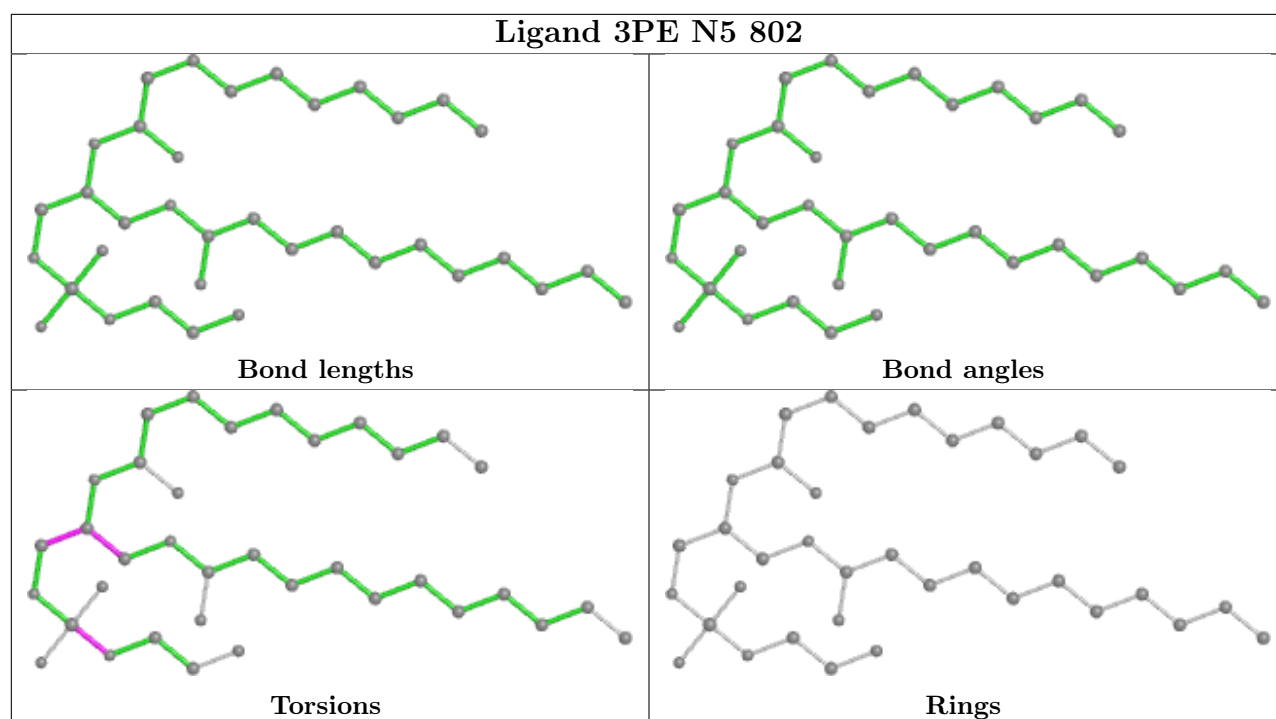


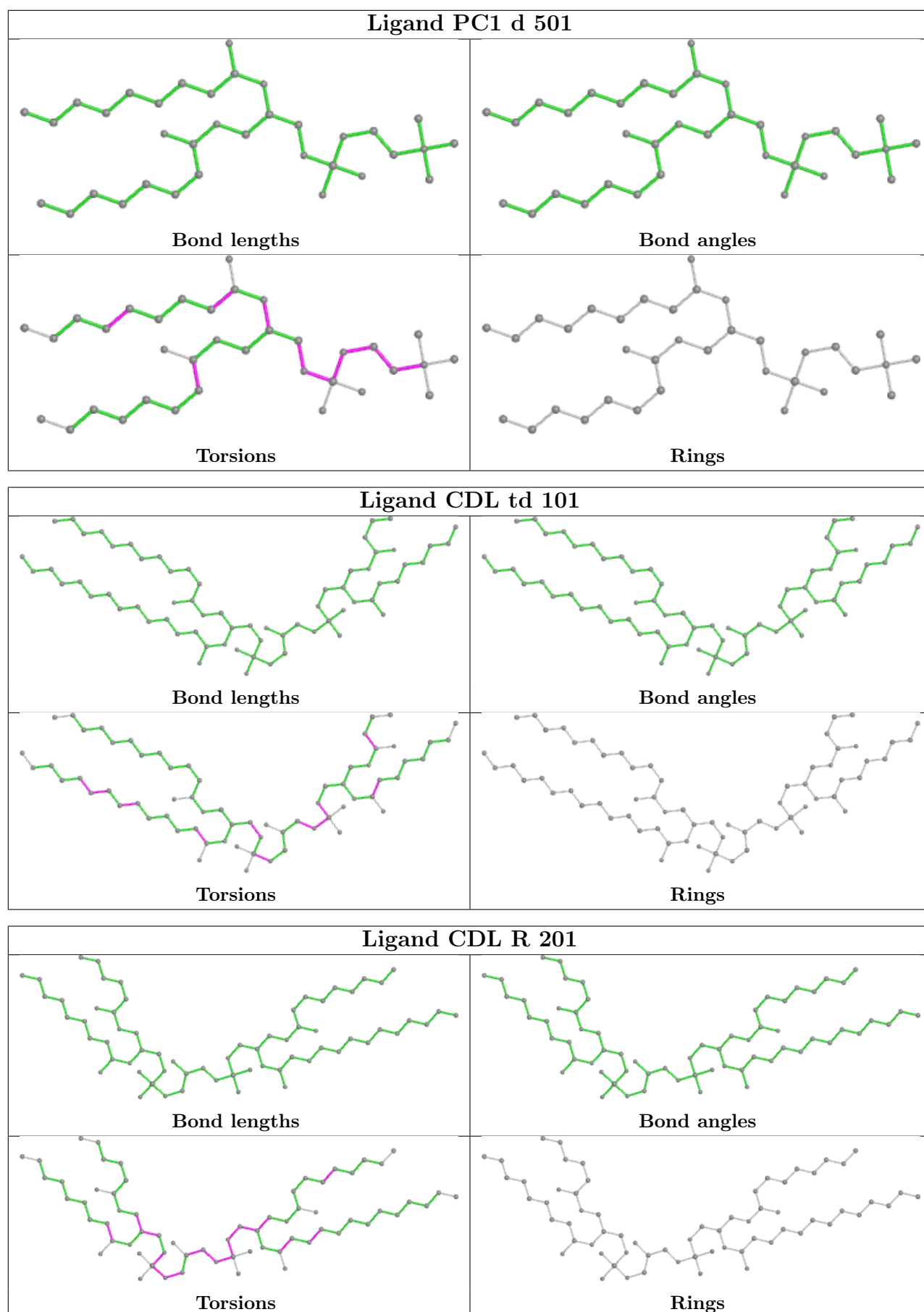


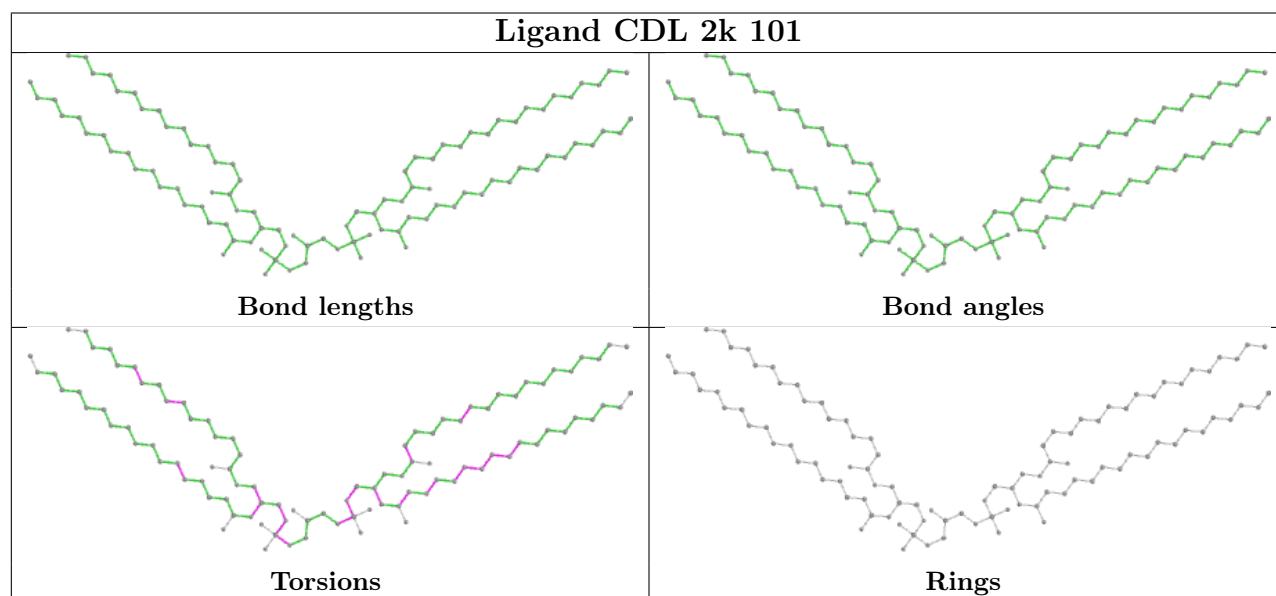
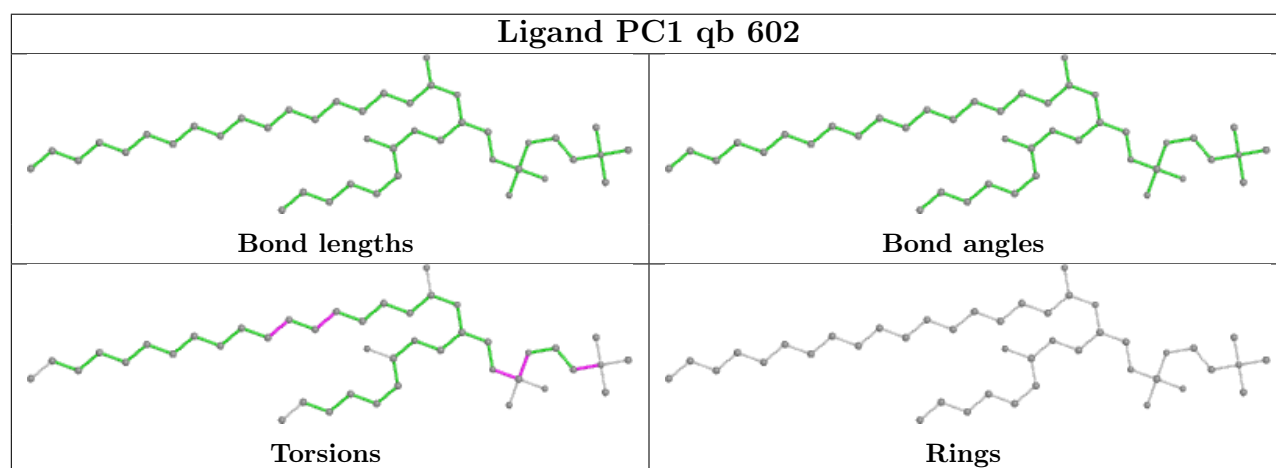
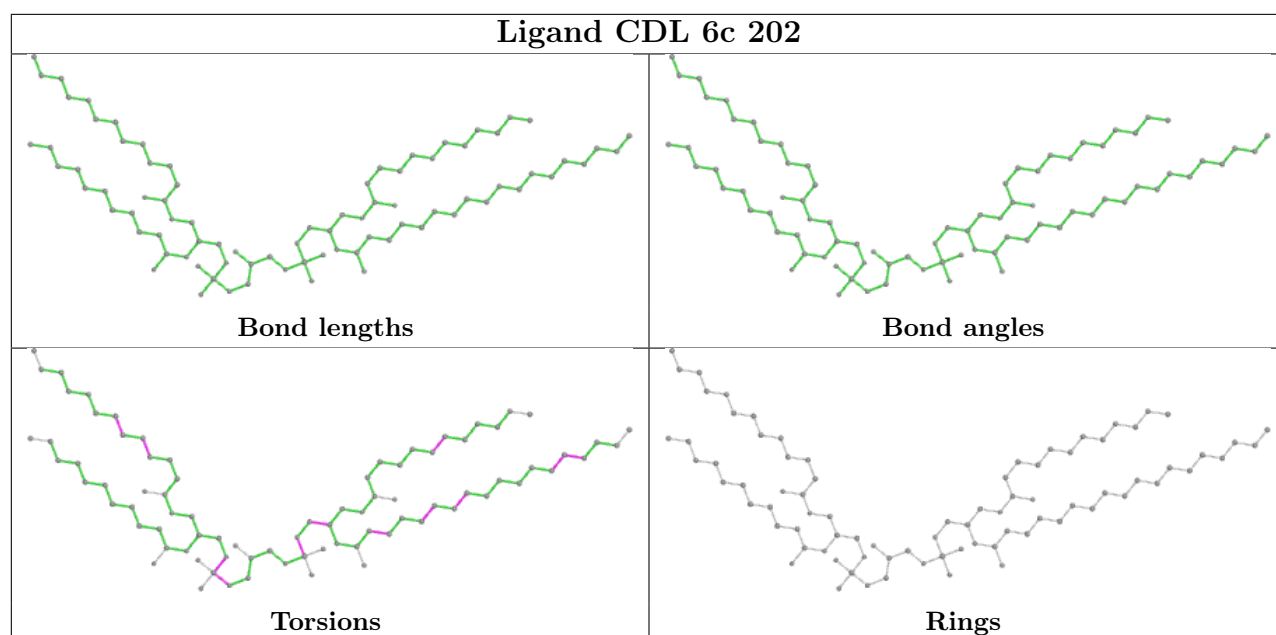


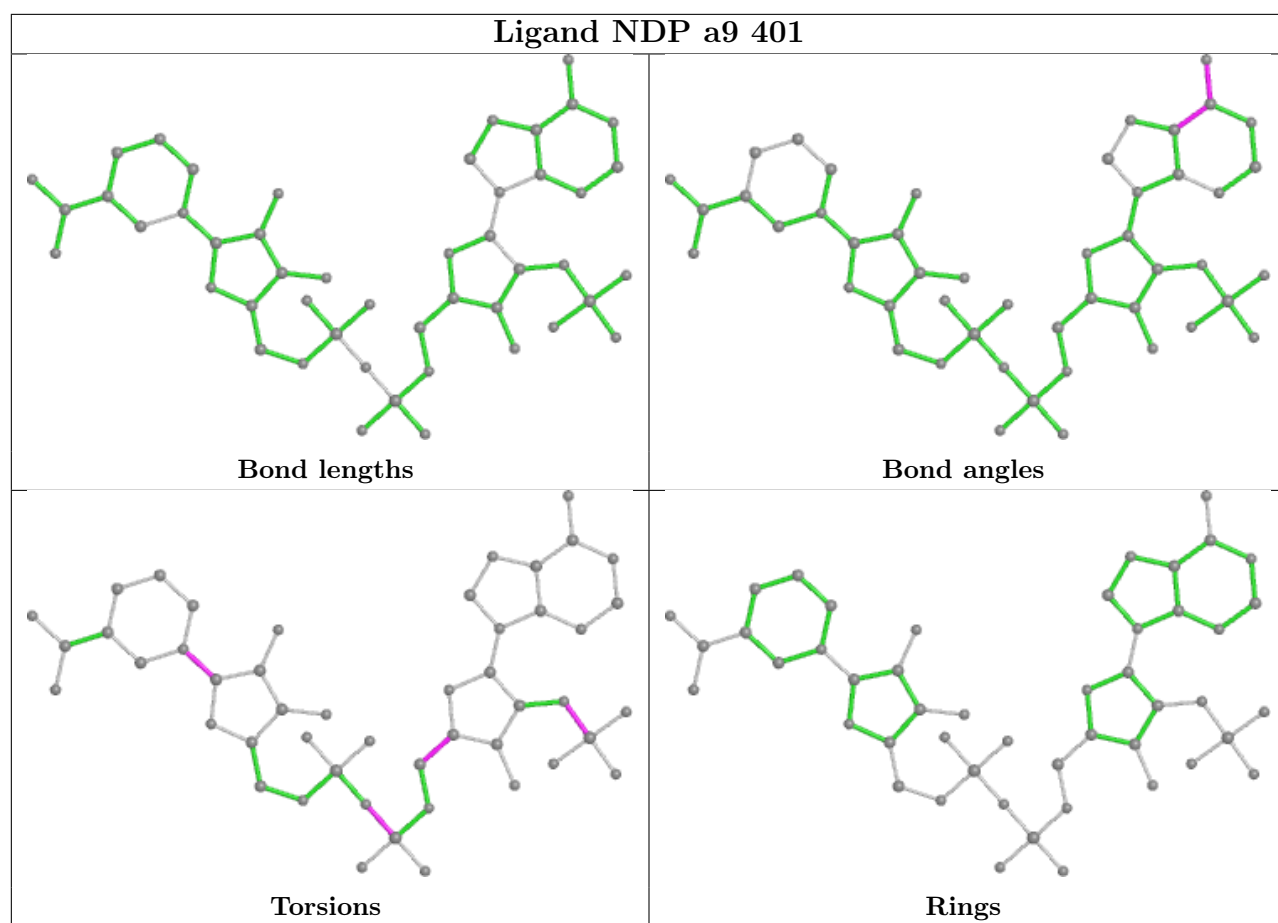




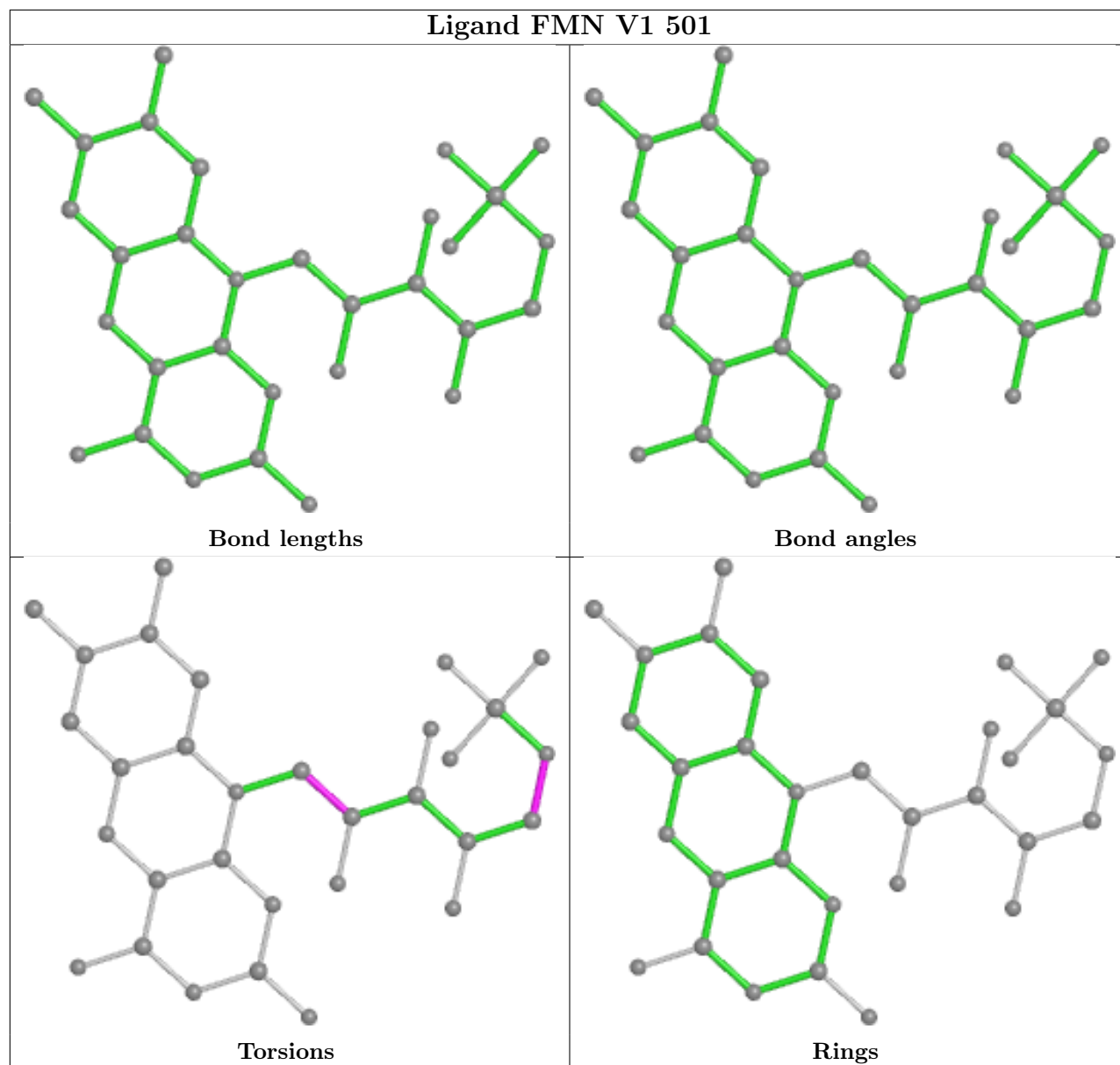


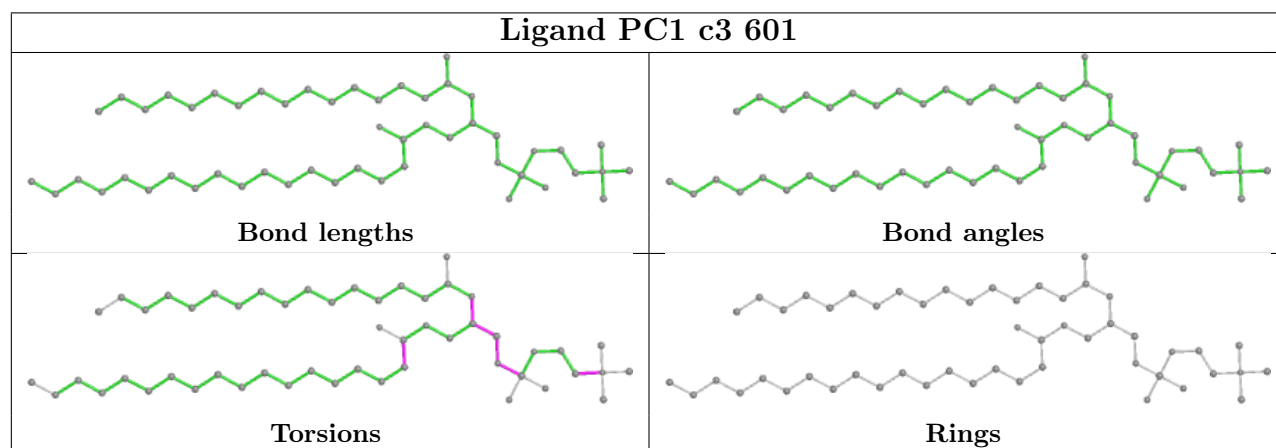
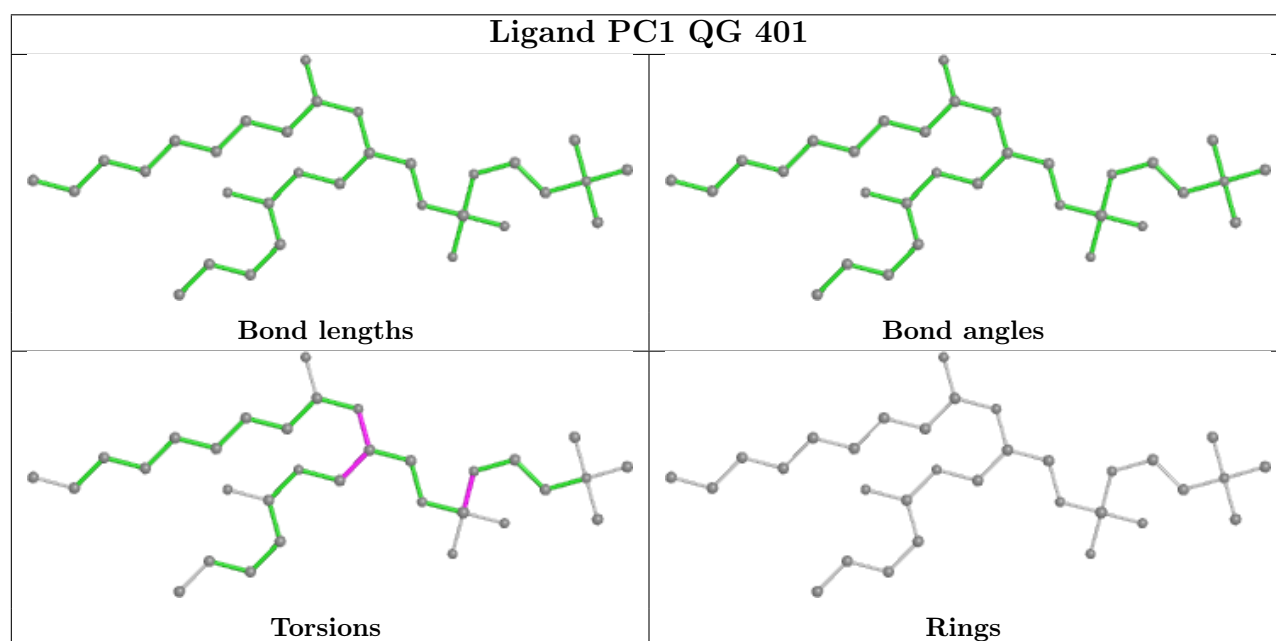
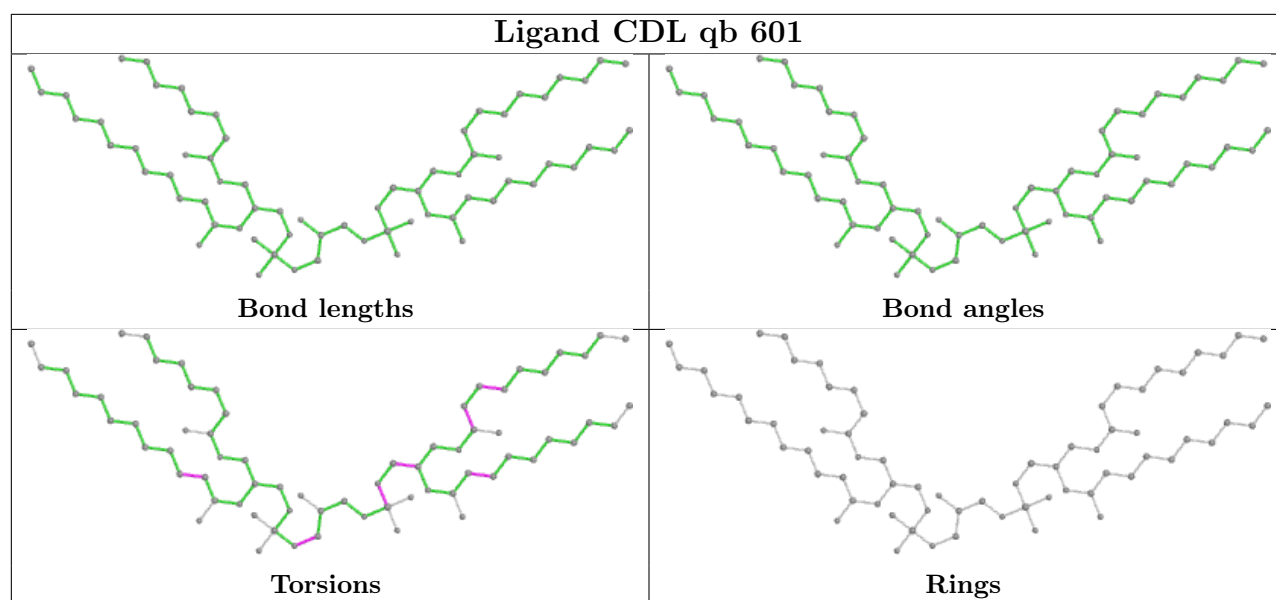


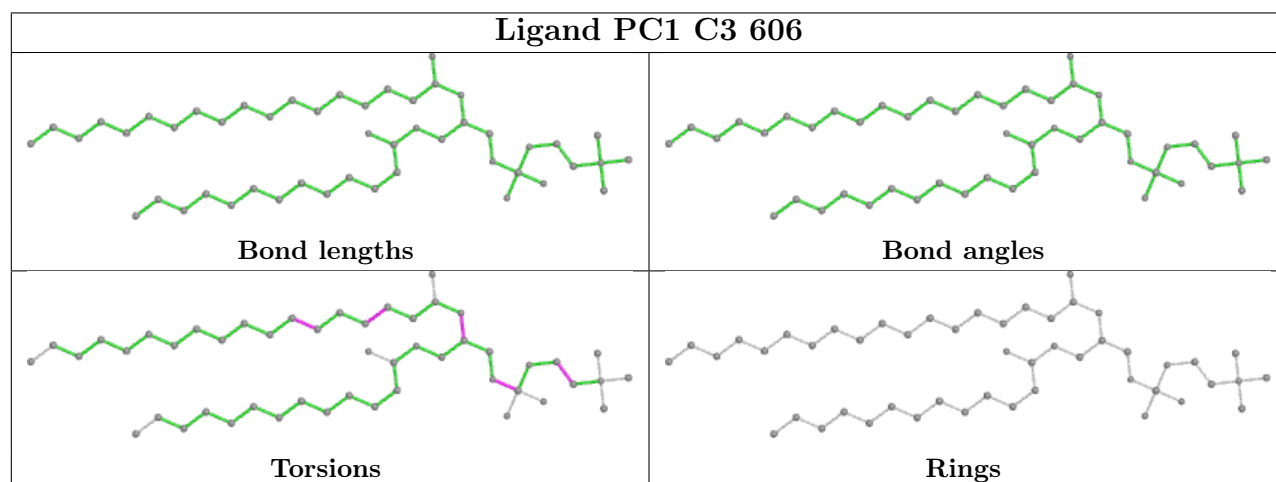
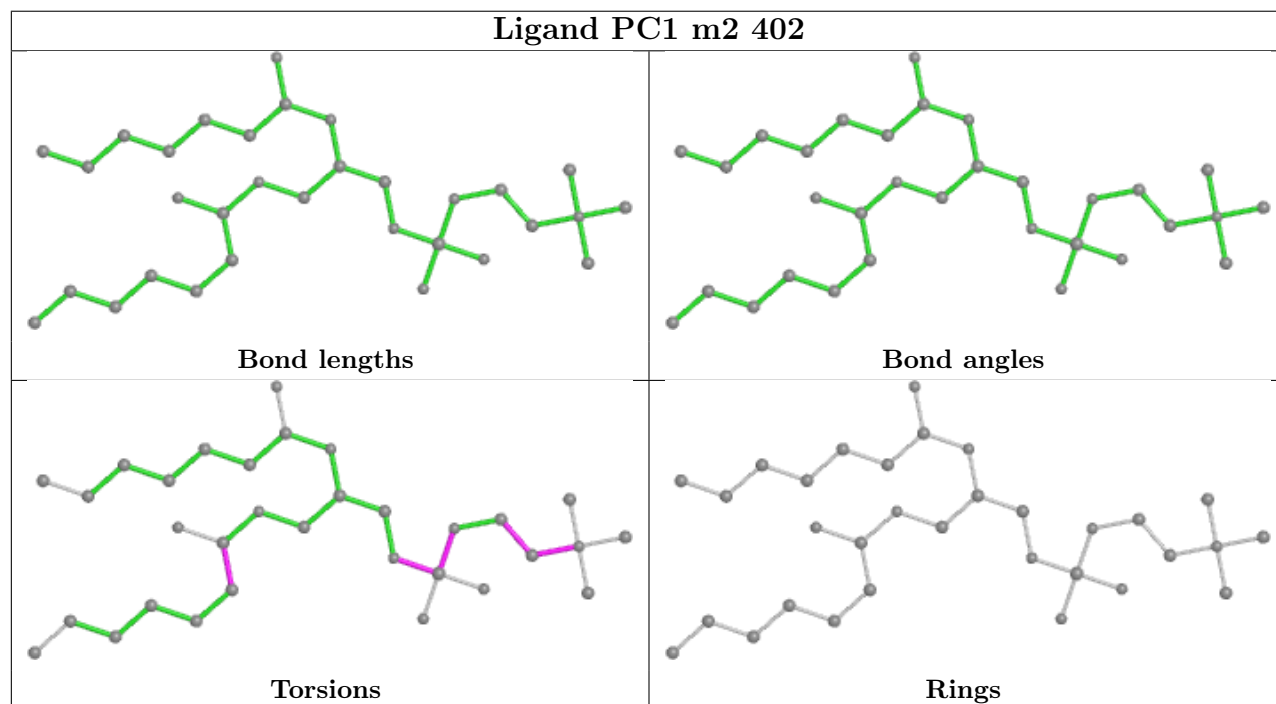
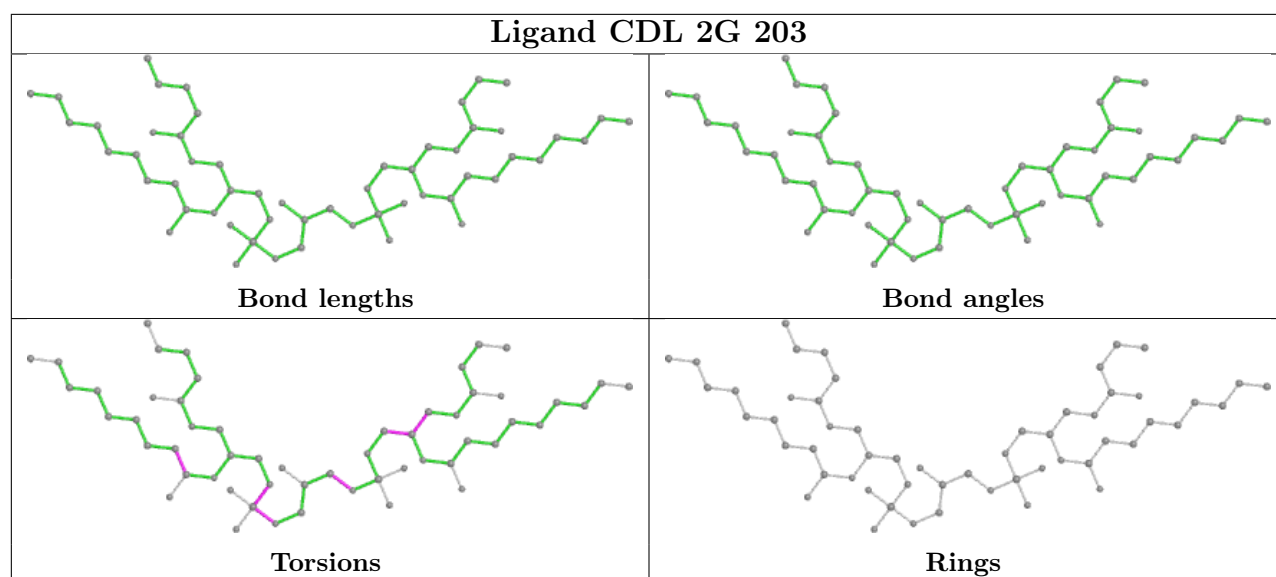


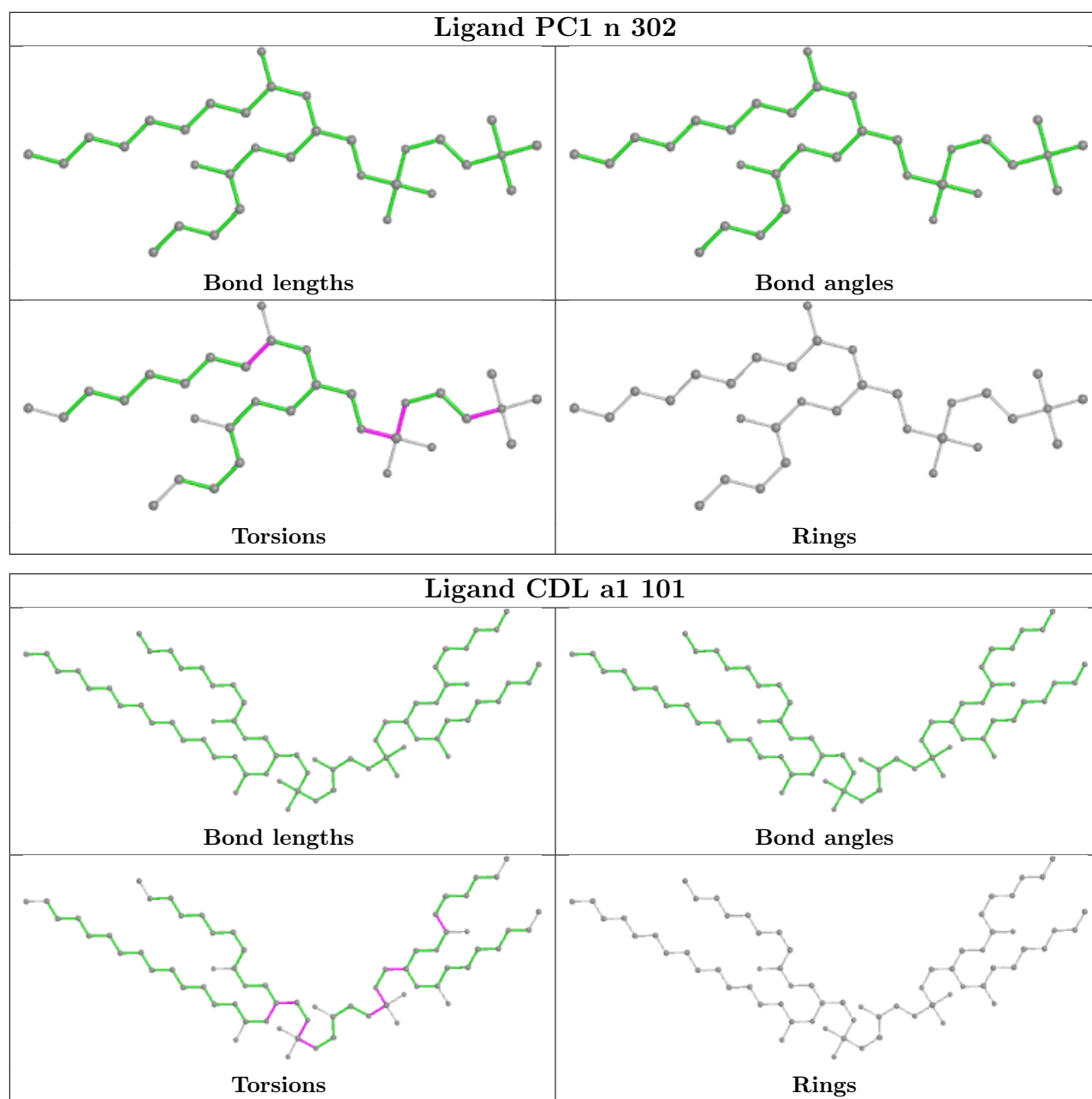


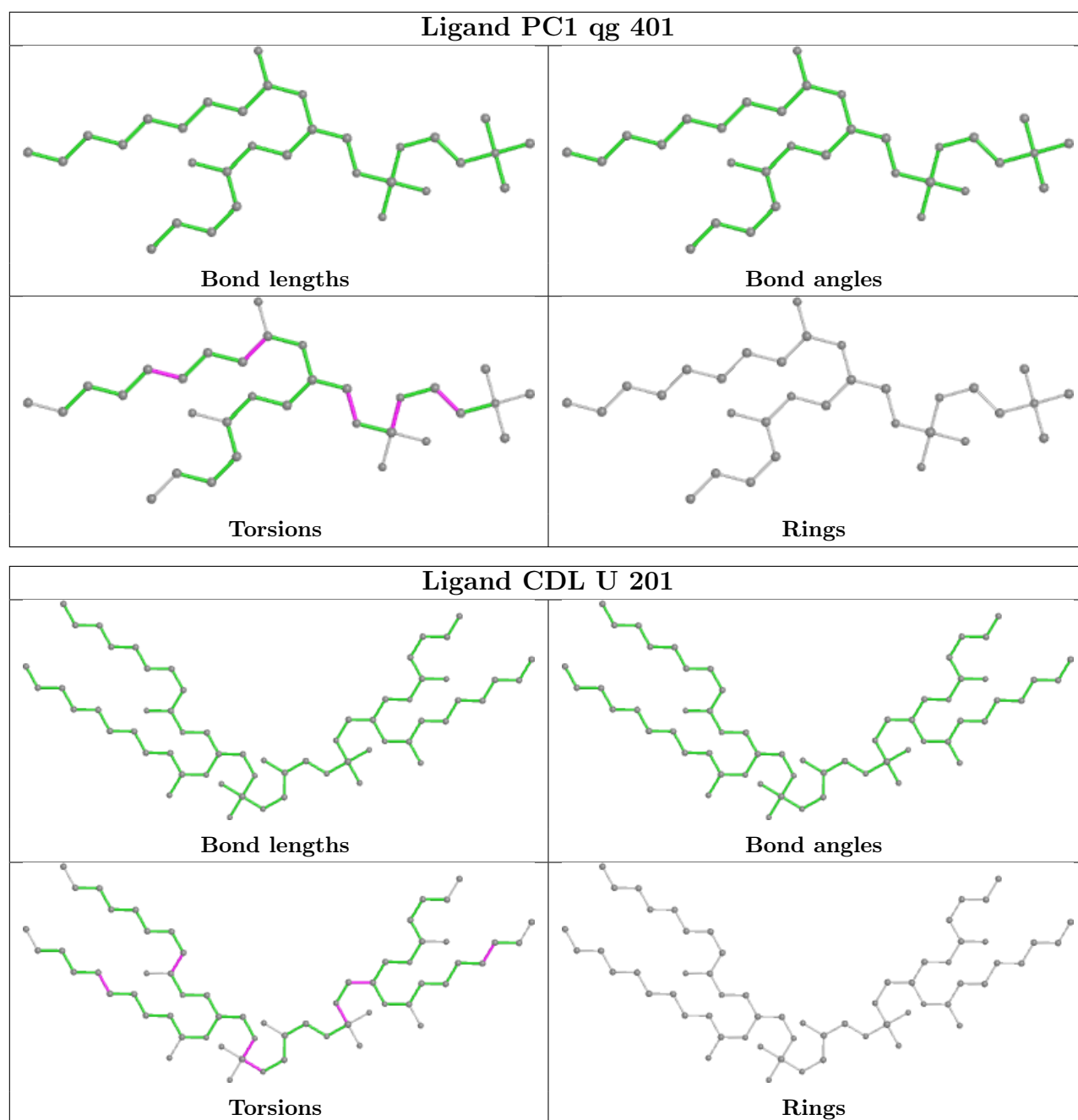
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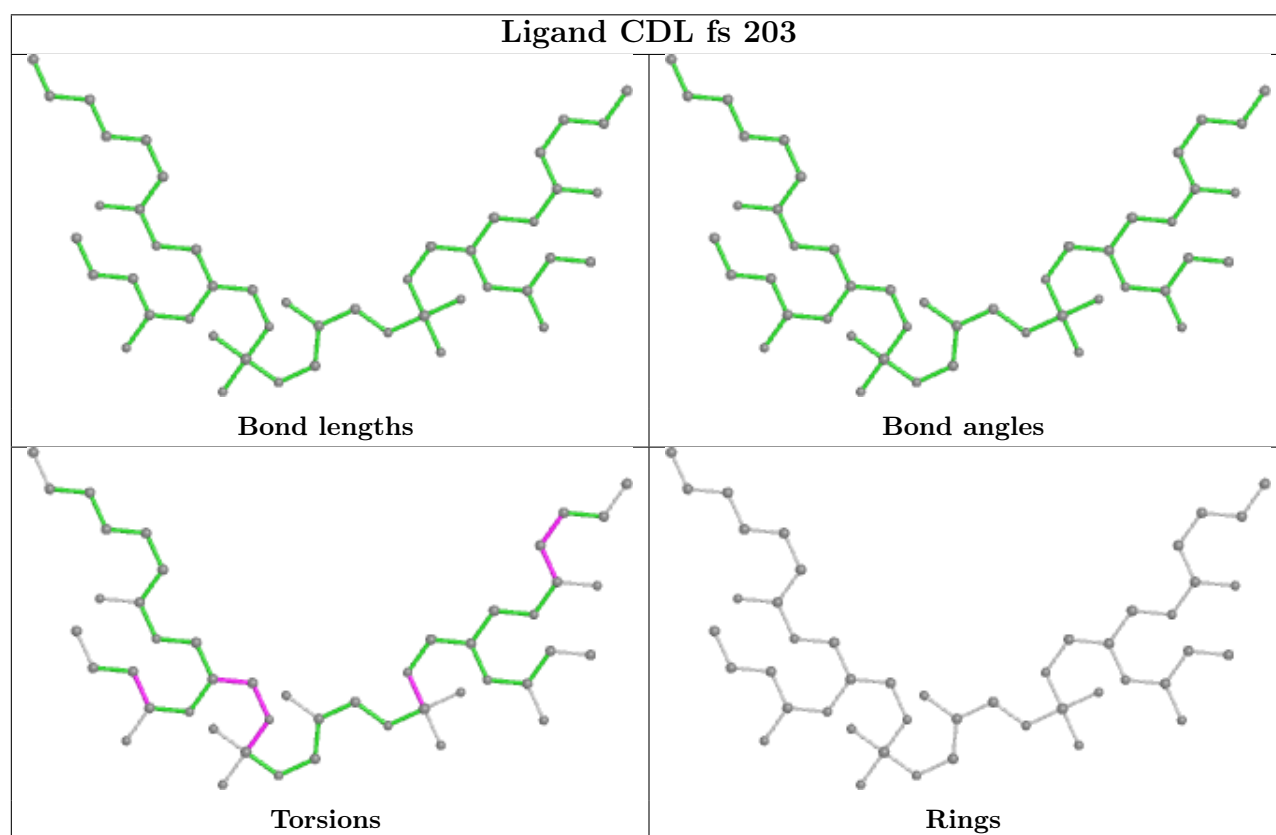
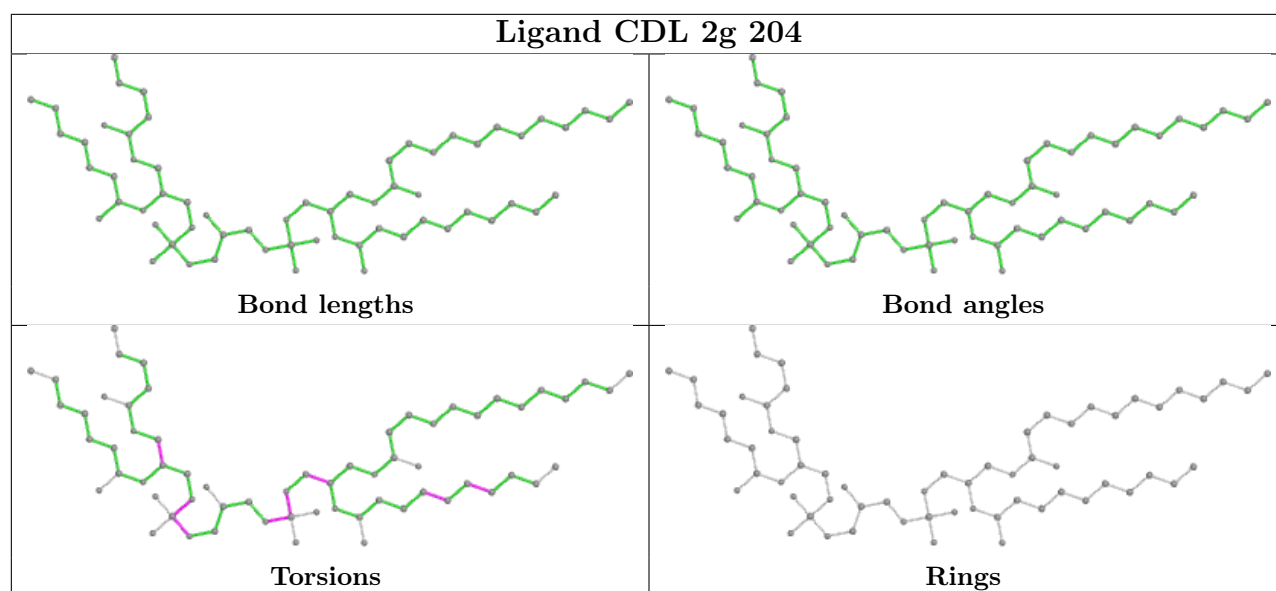


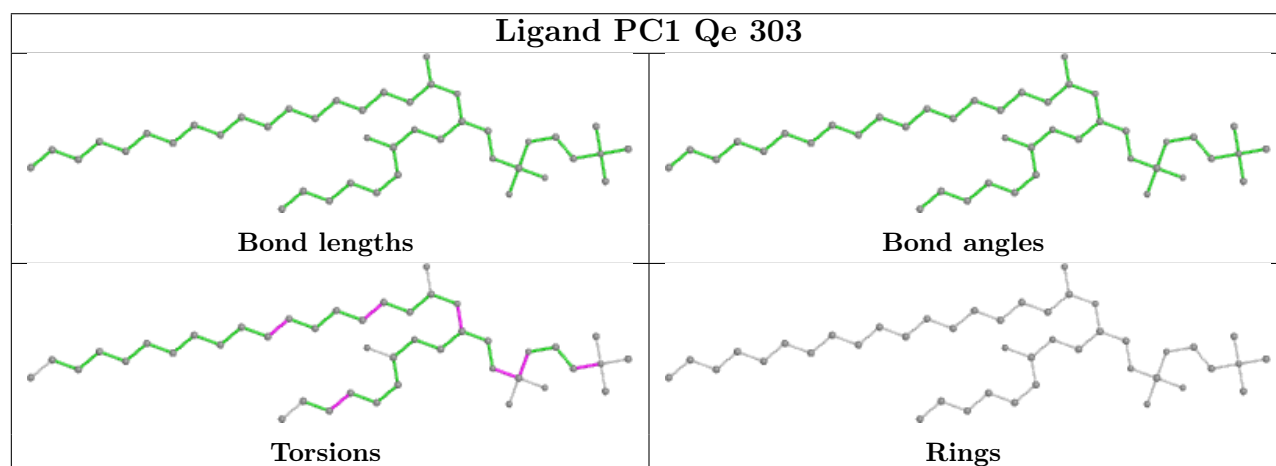
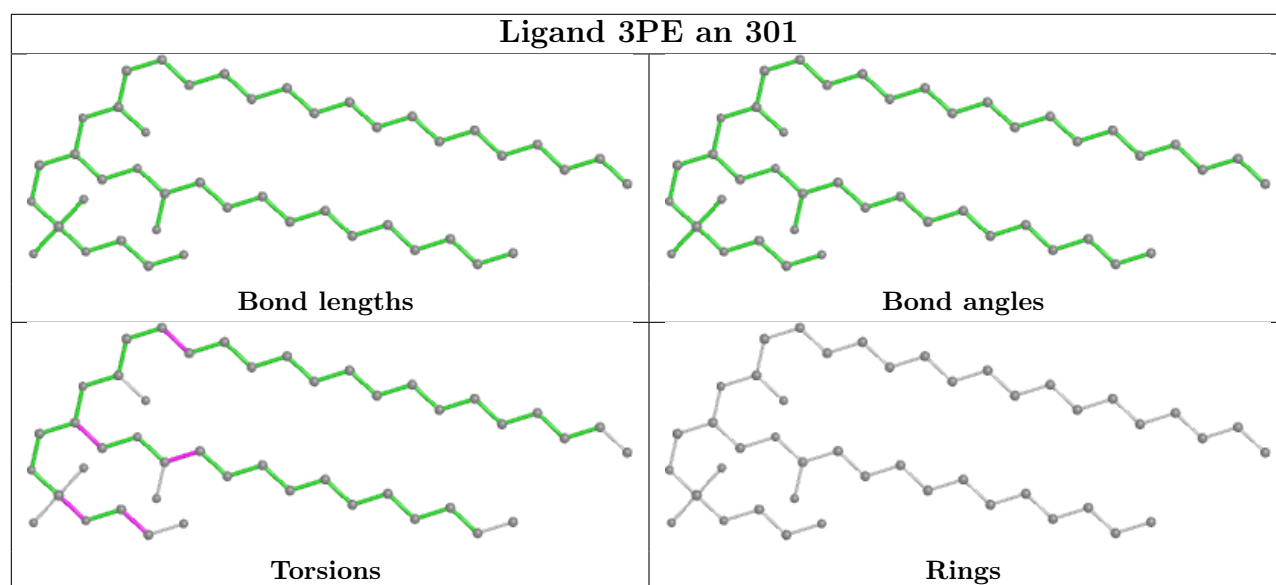
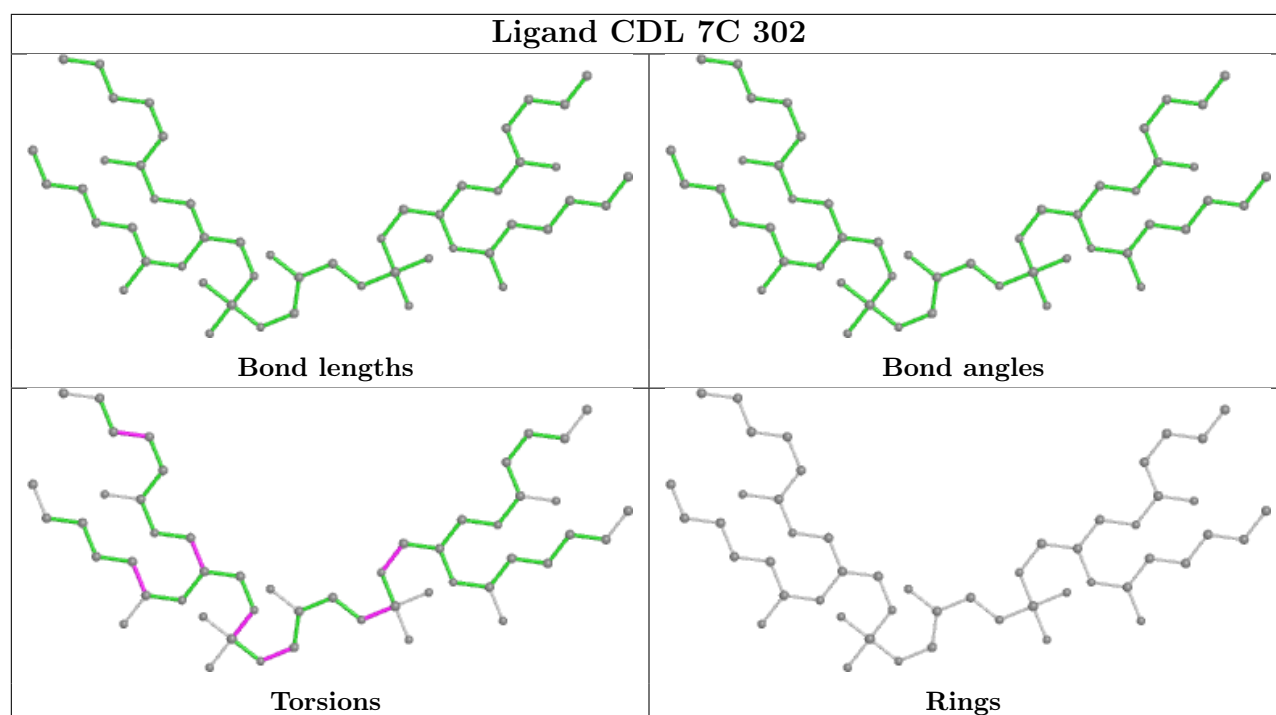


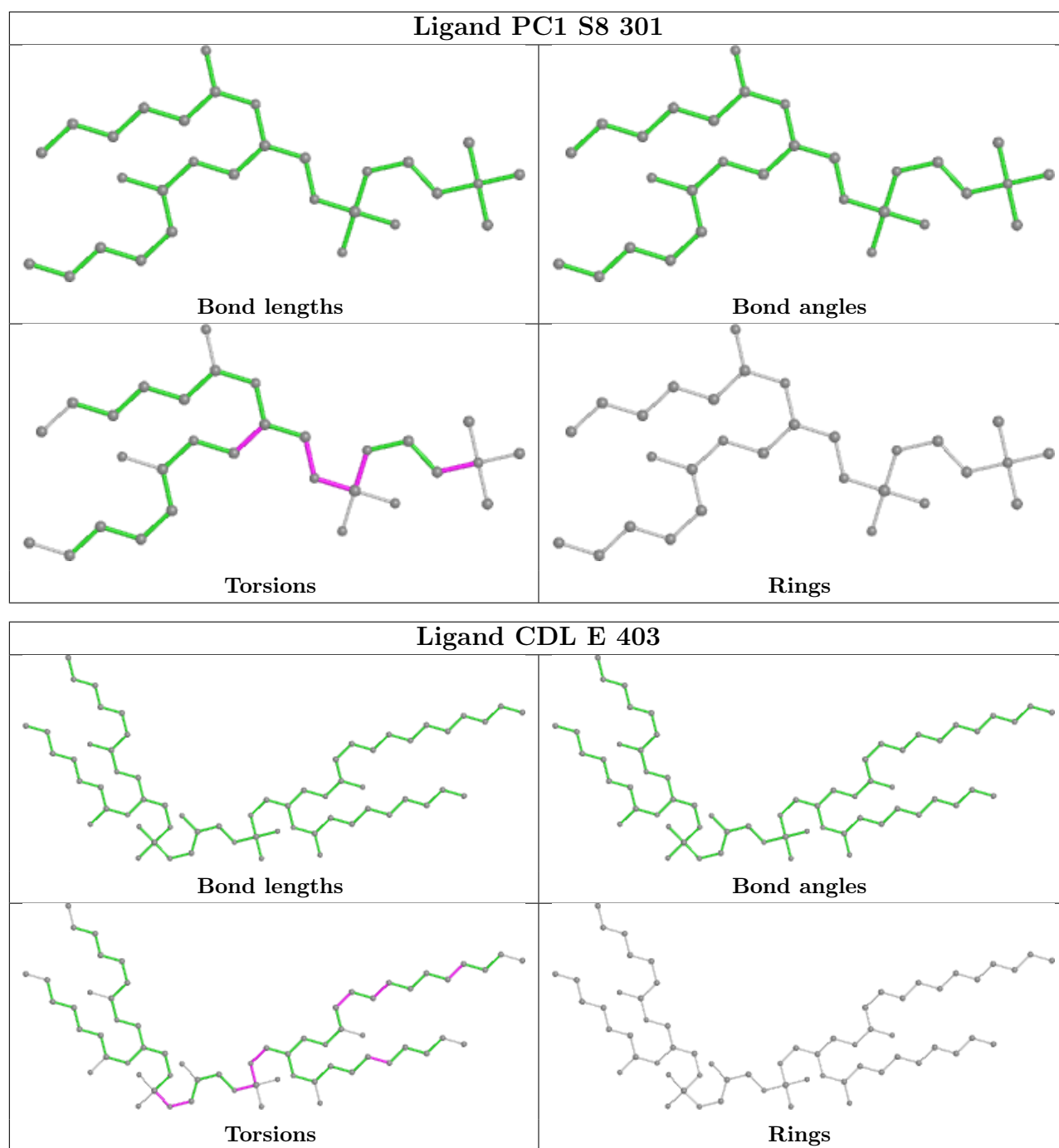


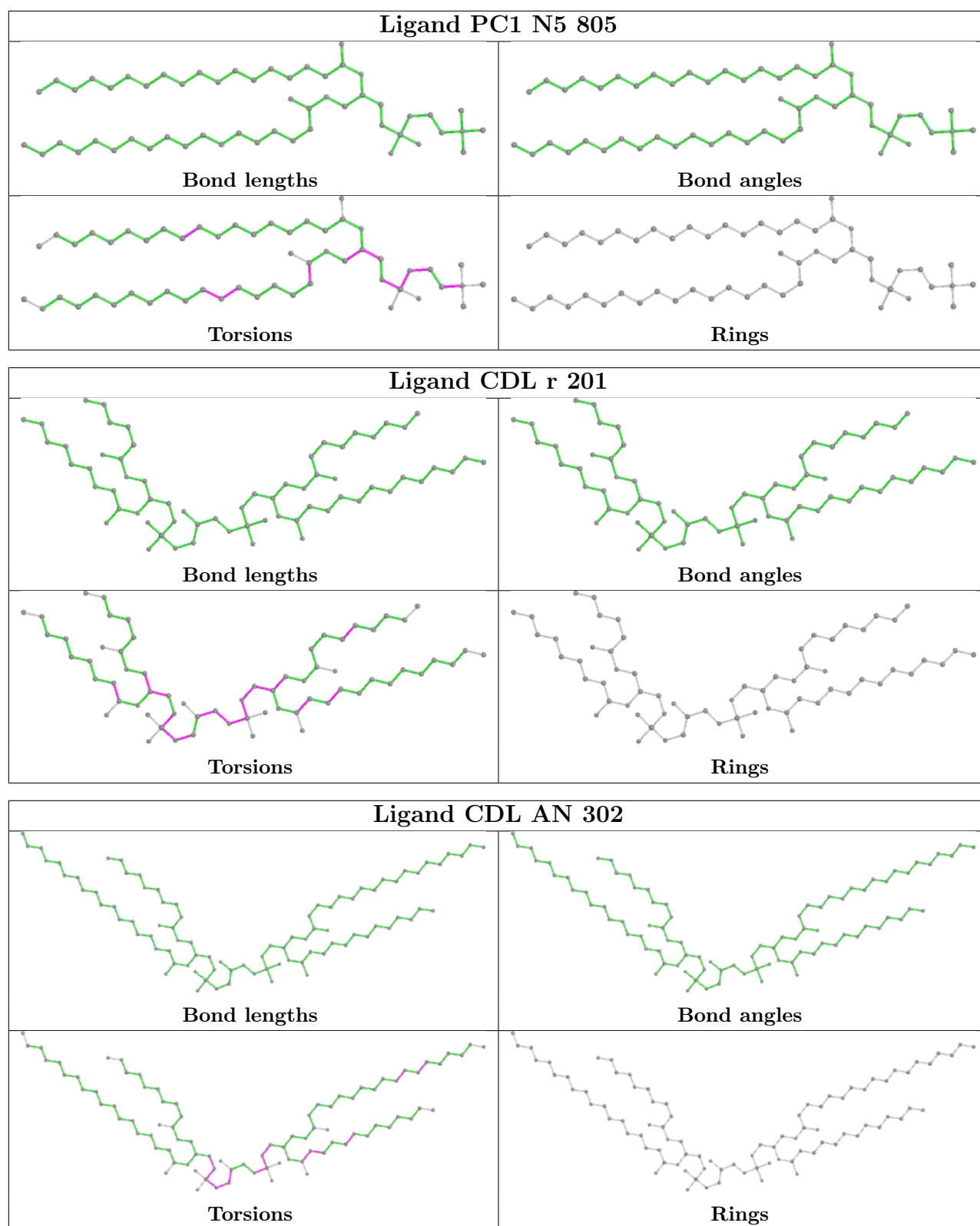


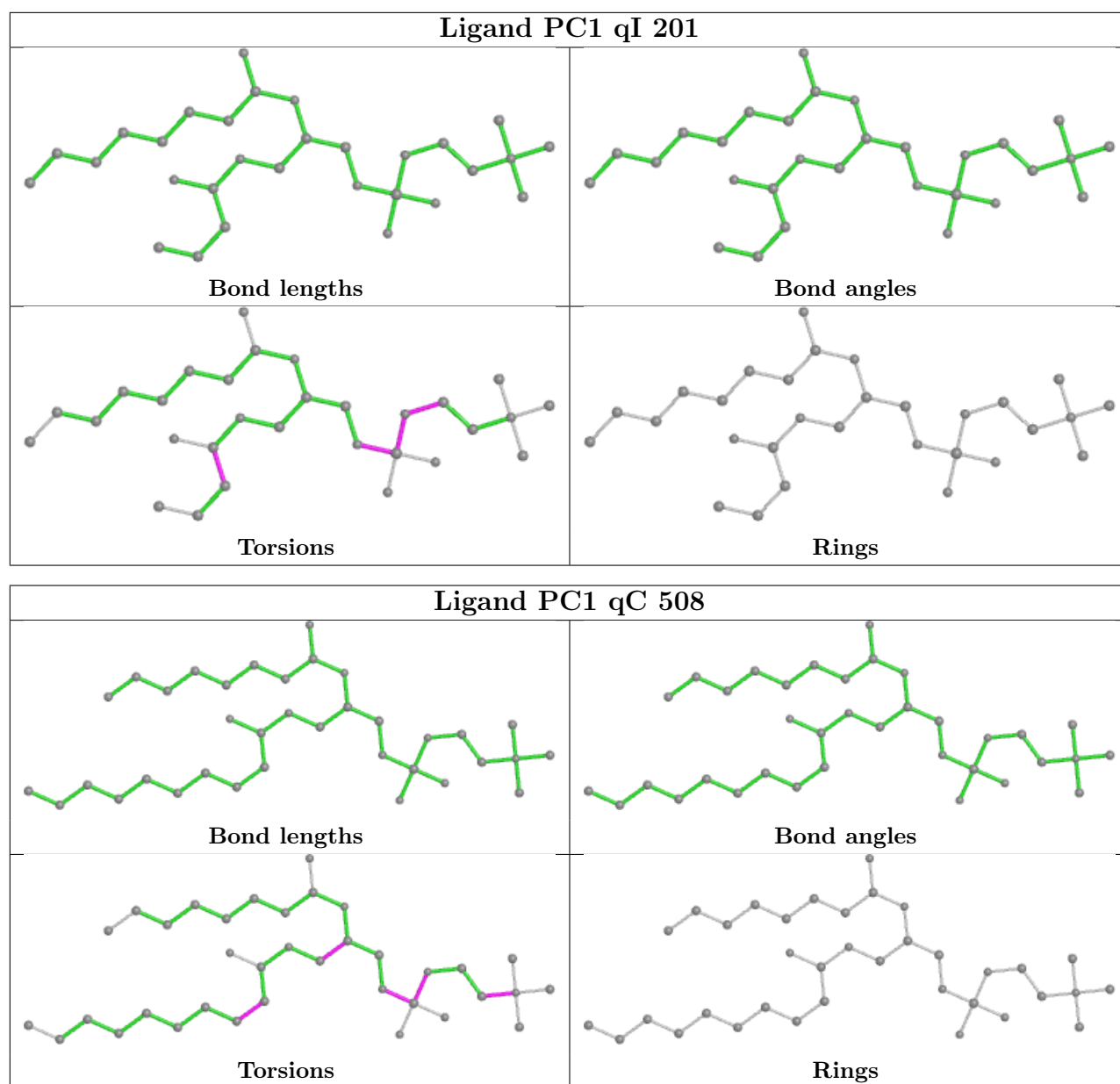


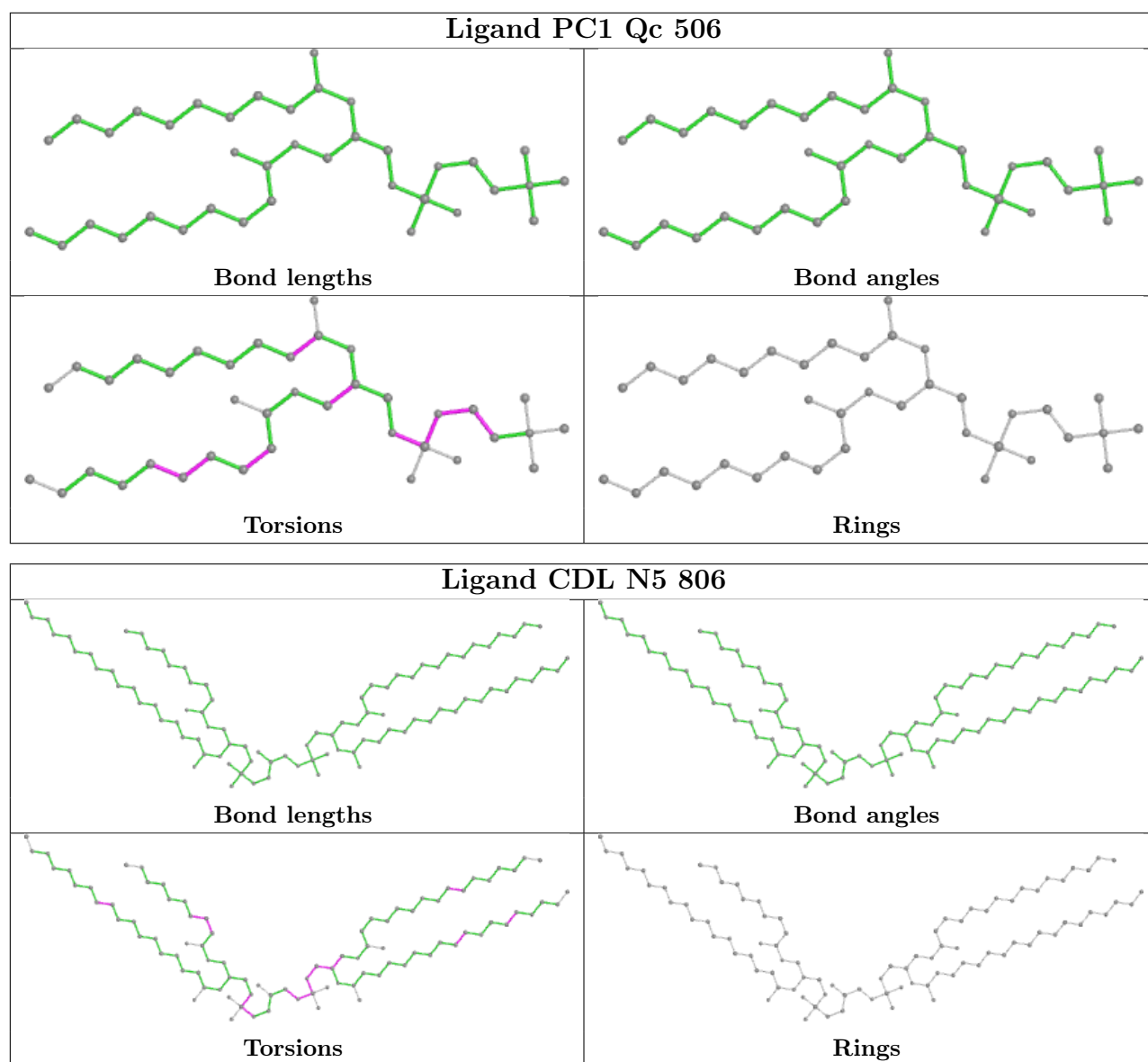


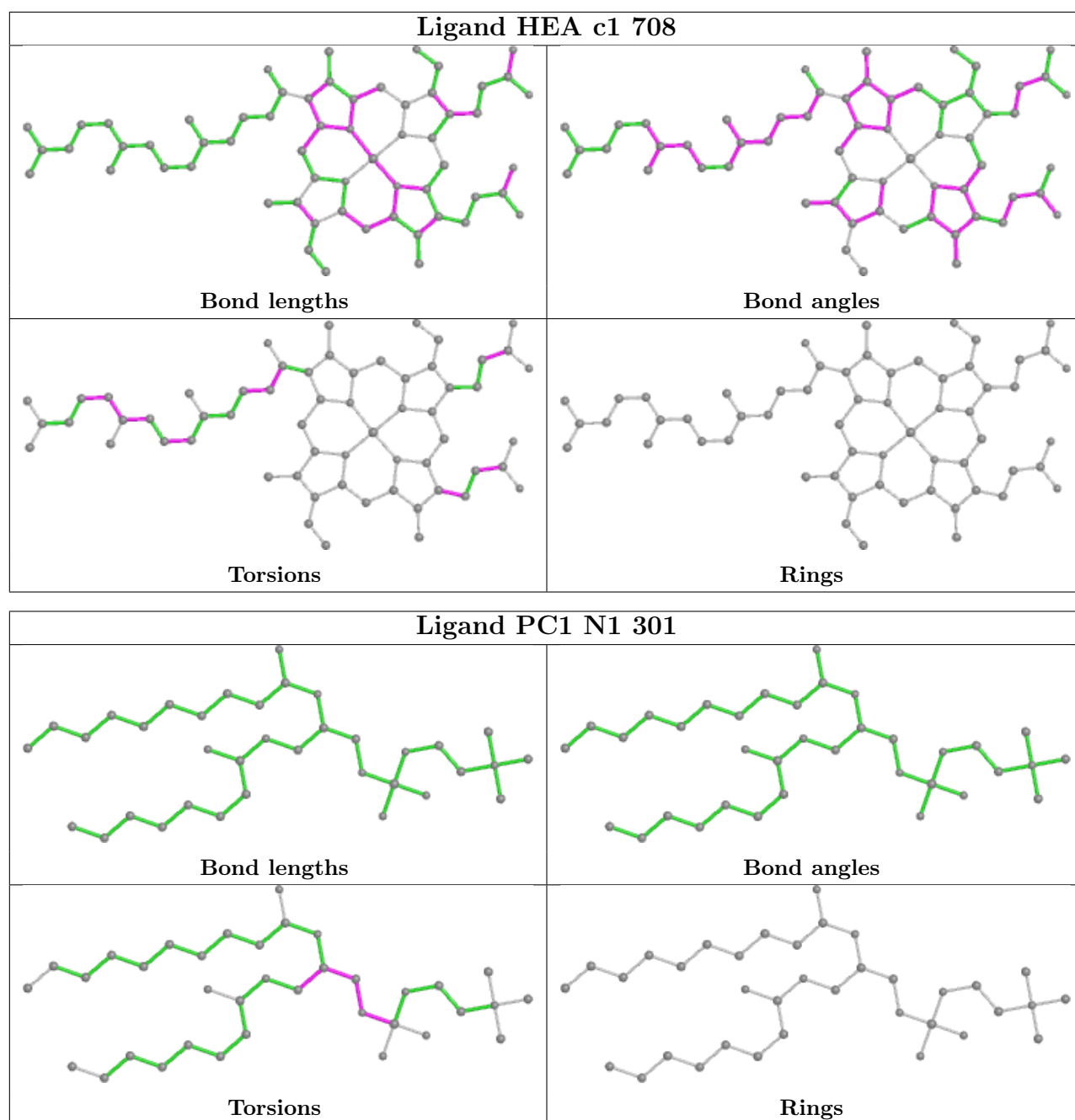


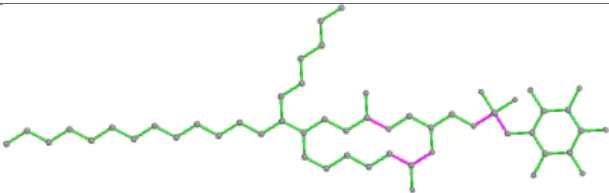
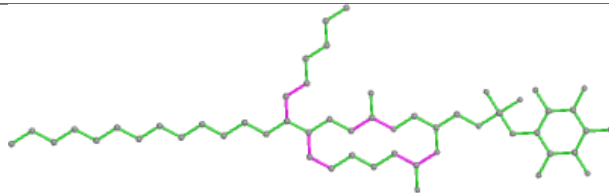
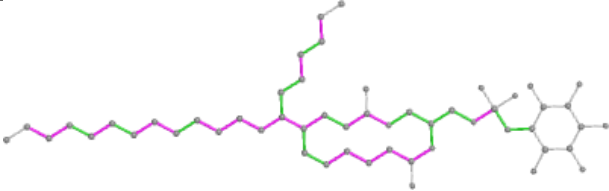
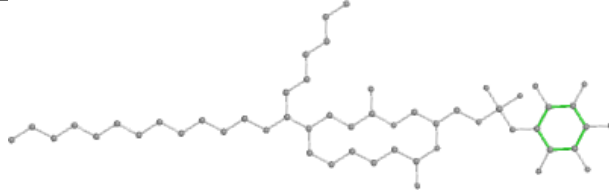


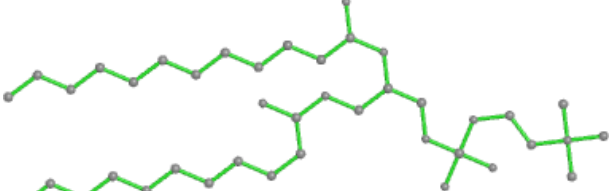
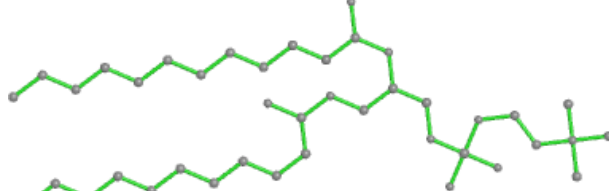
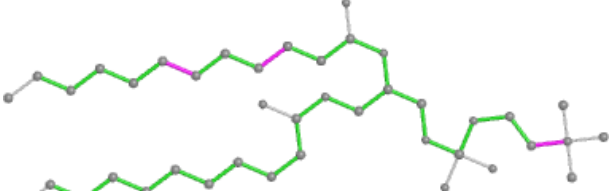
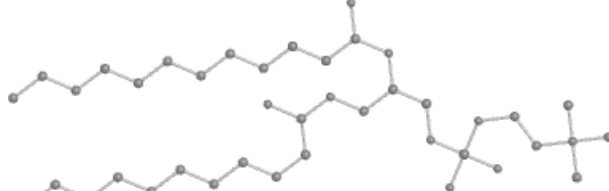


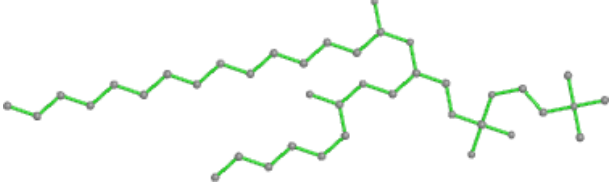
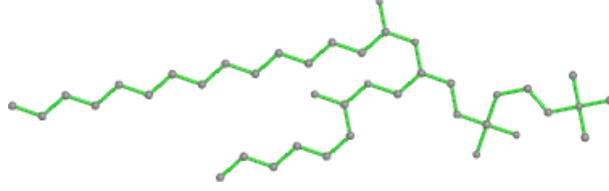
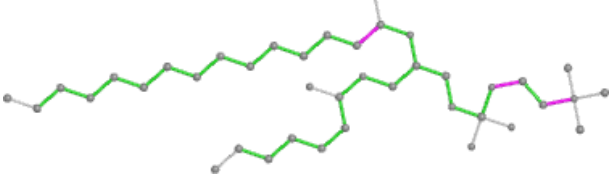
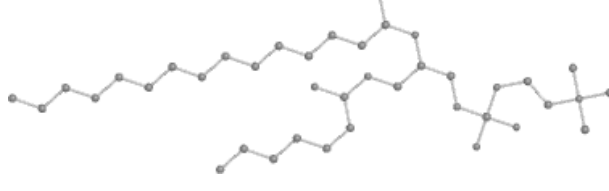


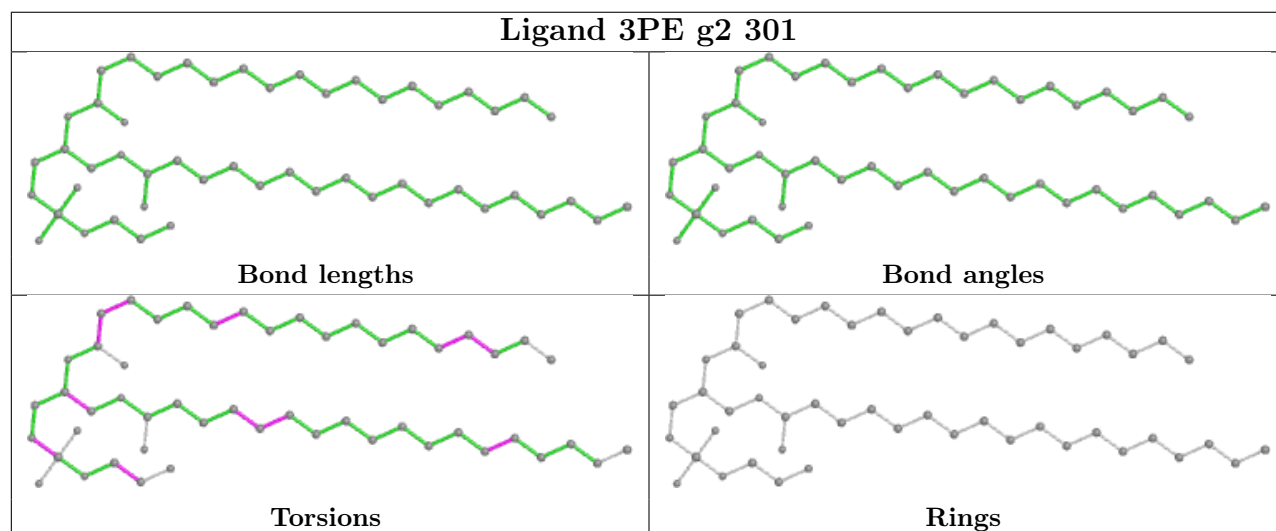
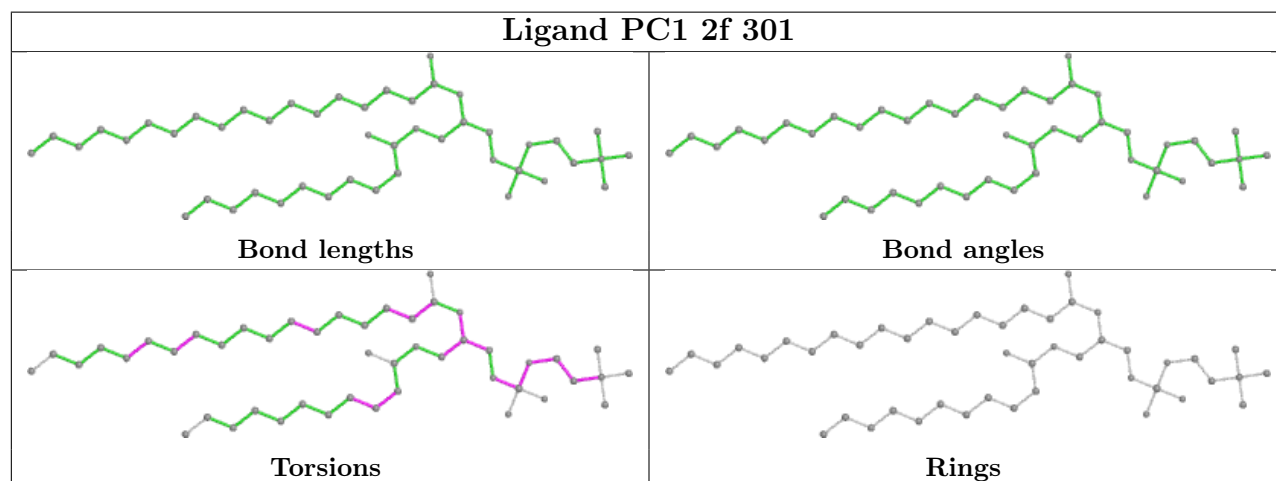
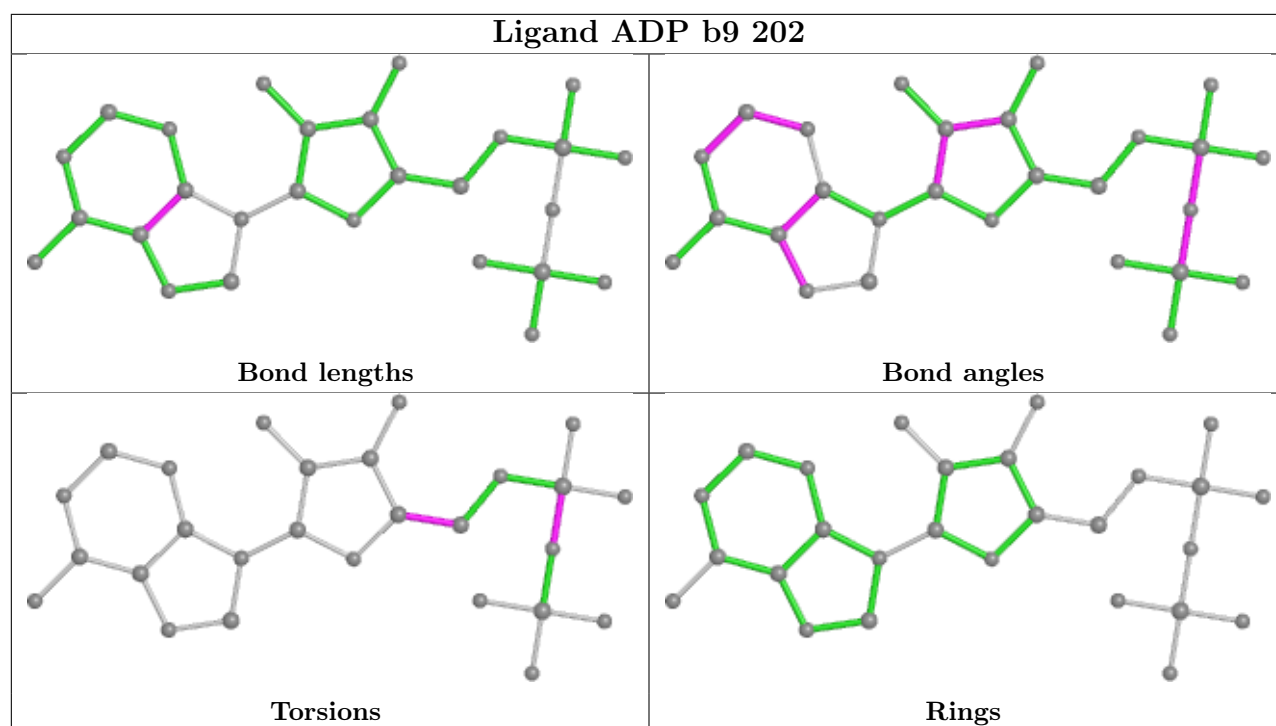


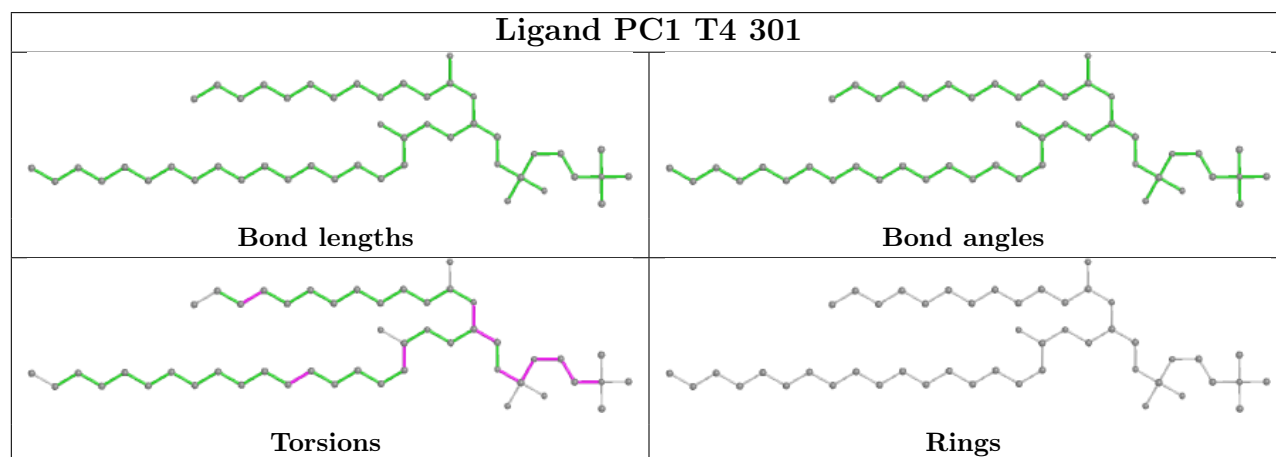
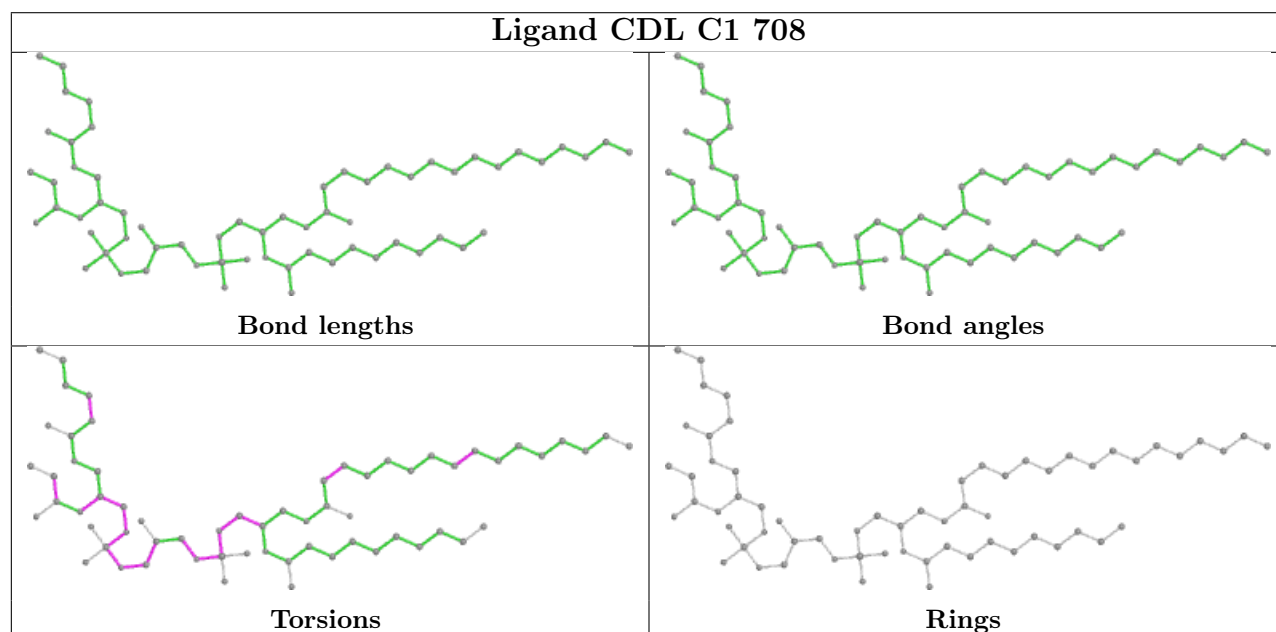
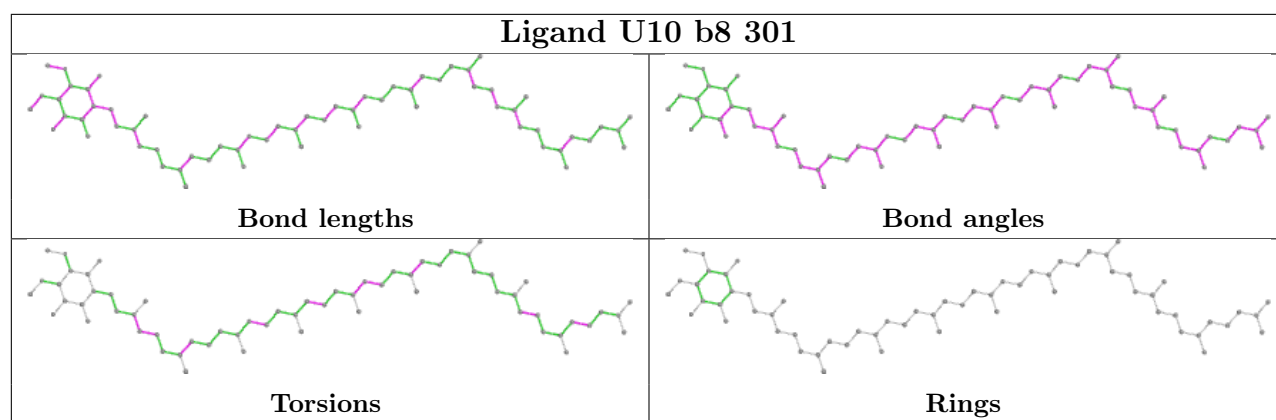


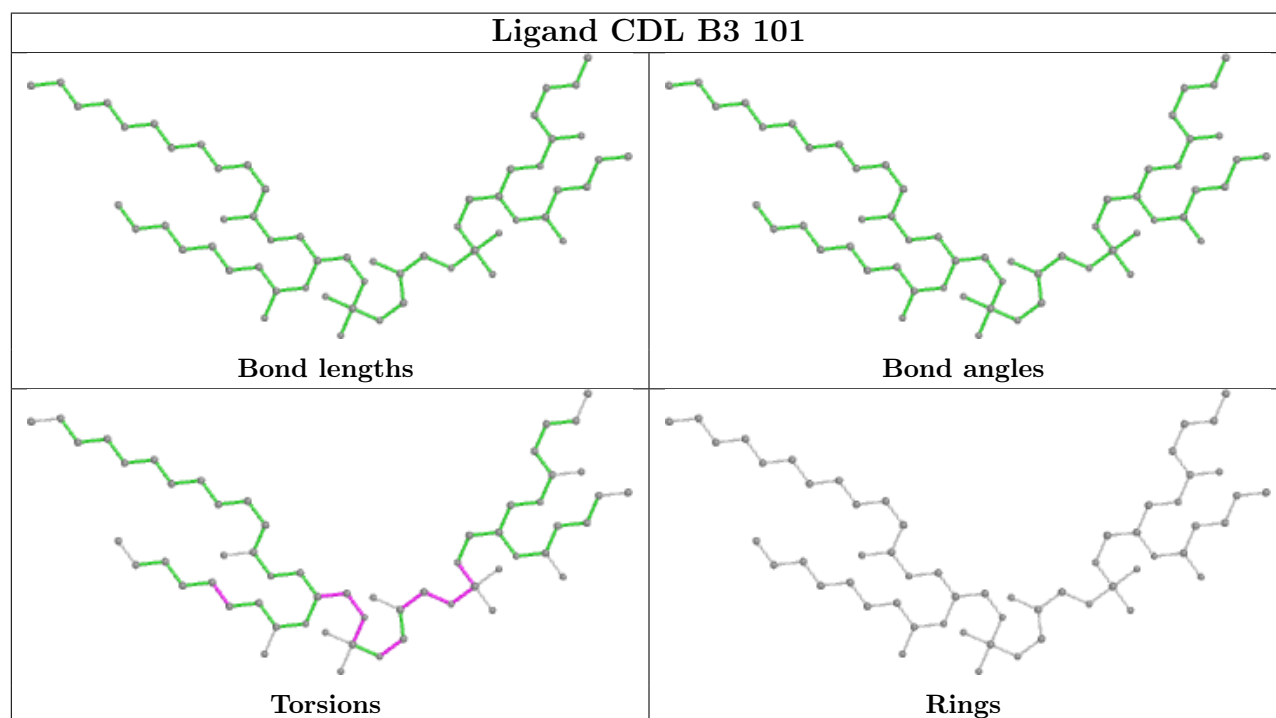
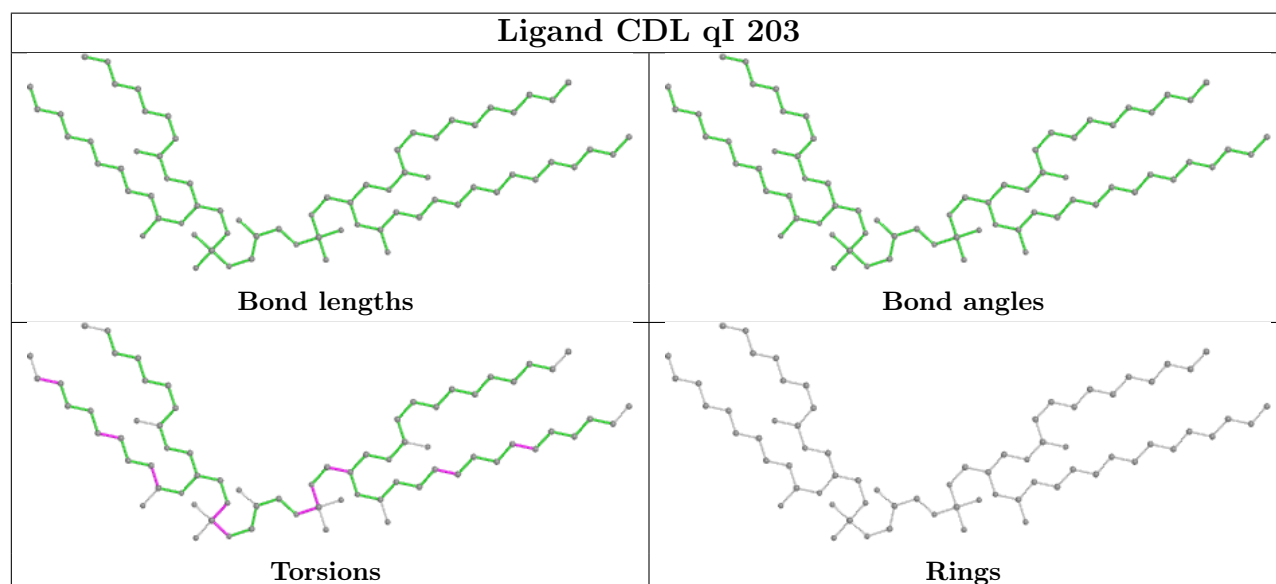
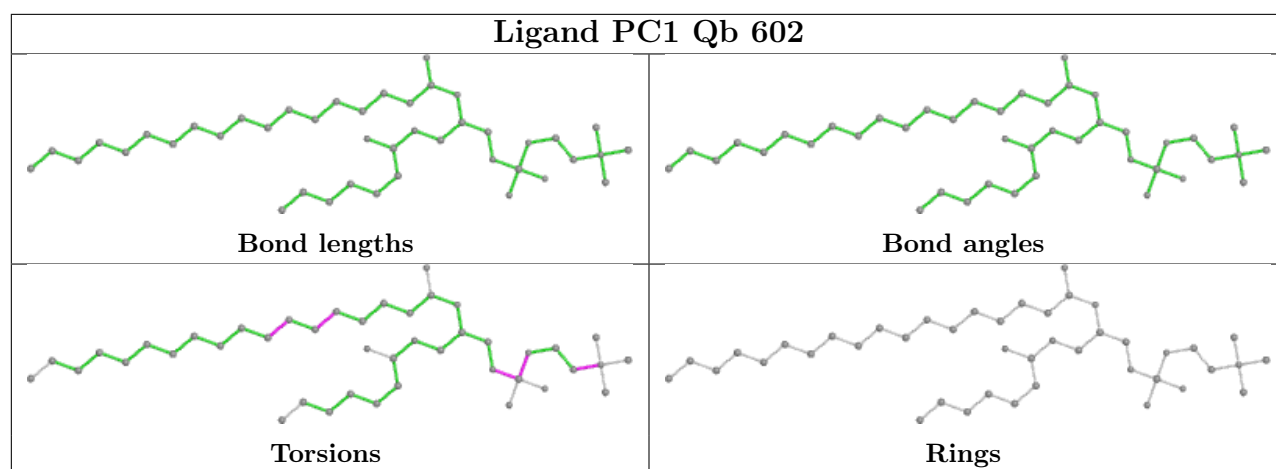
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|  |  |
| Torsions | Rings |

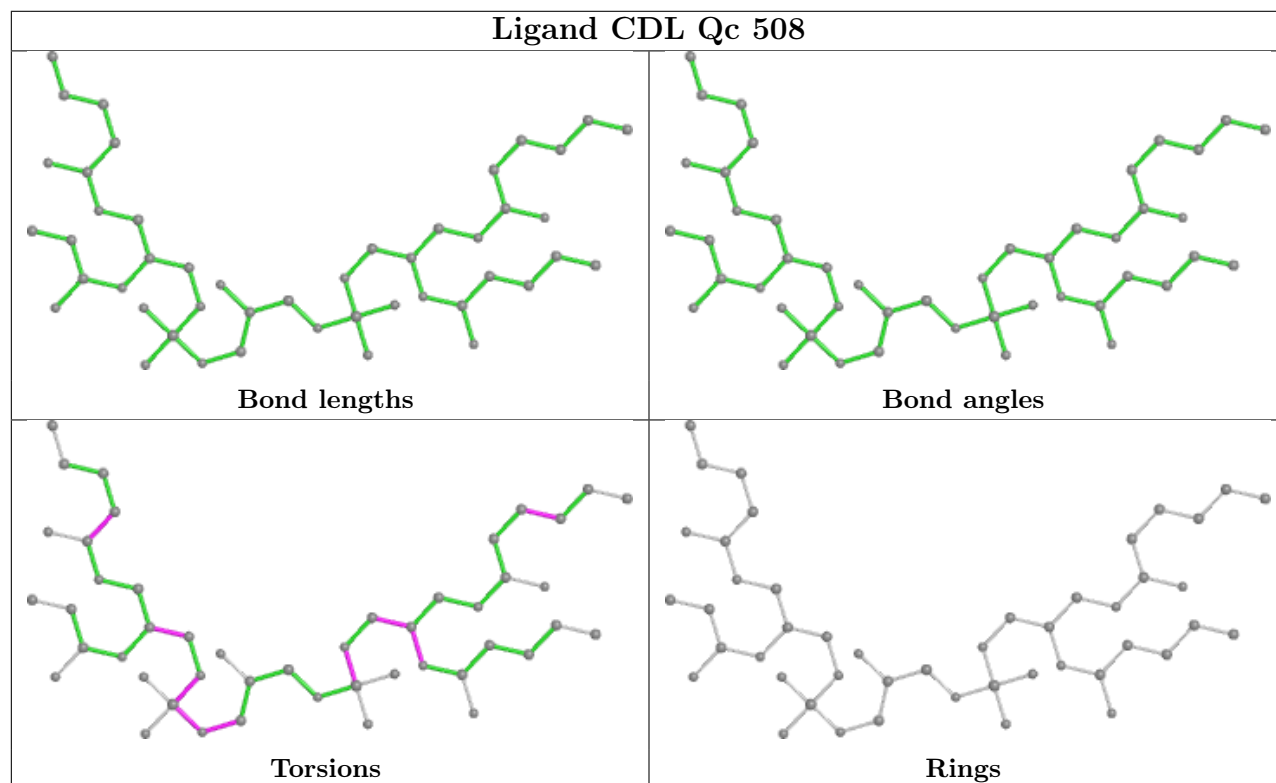
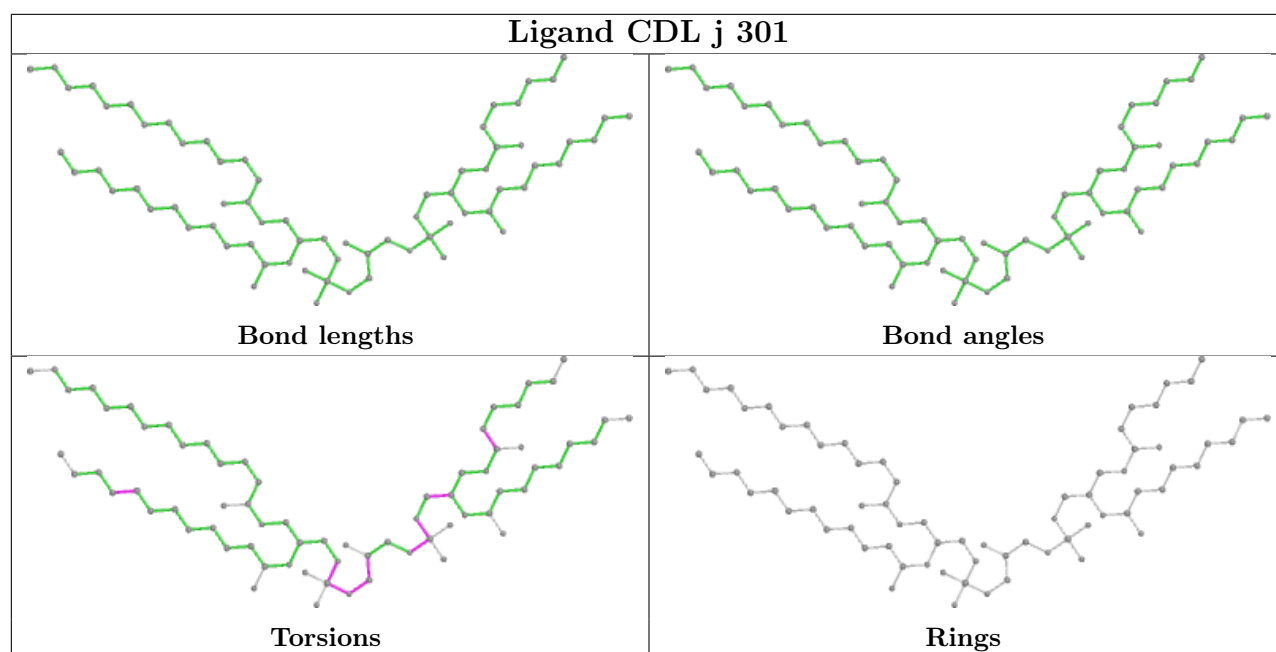
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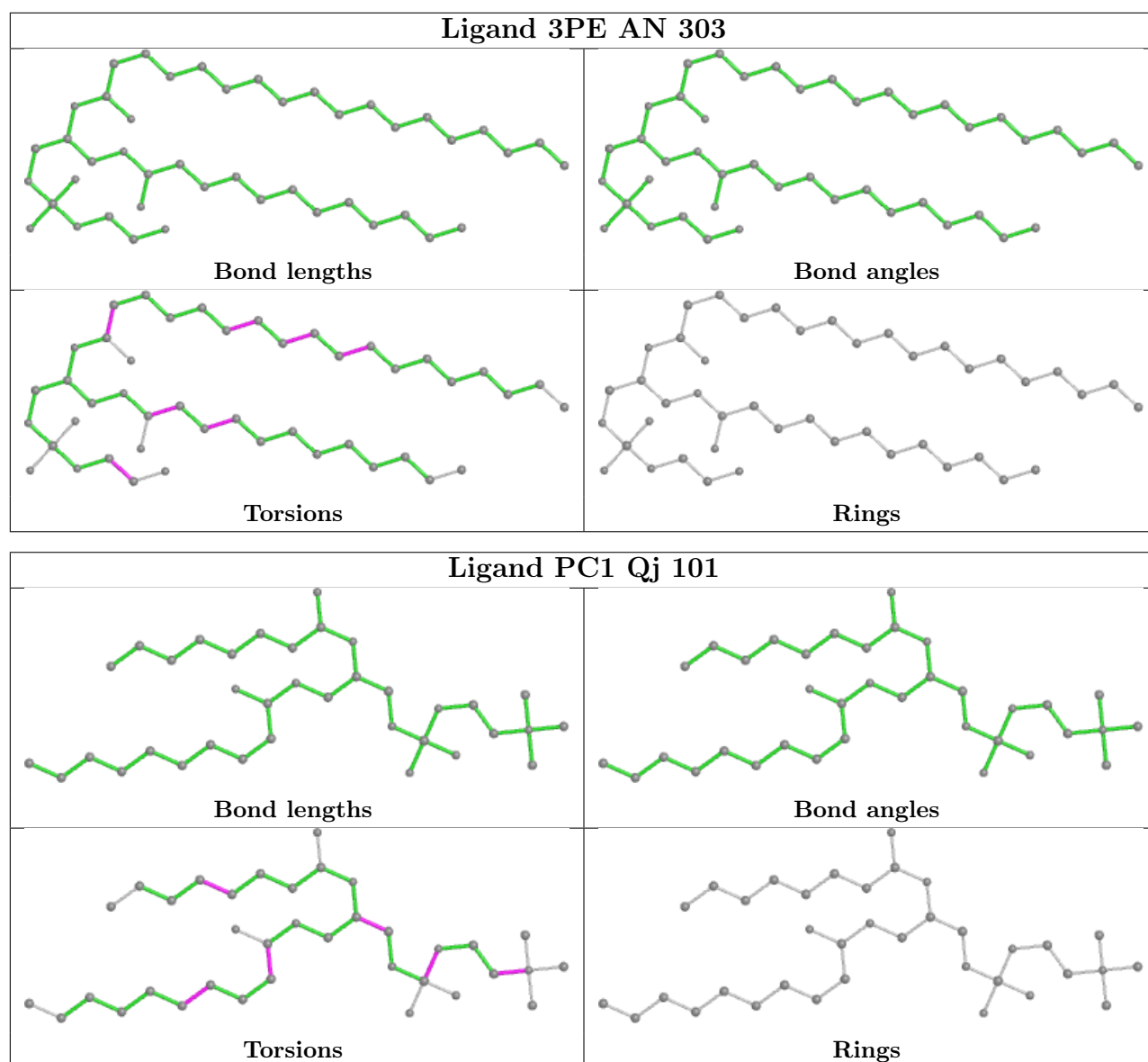
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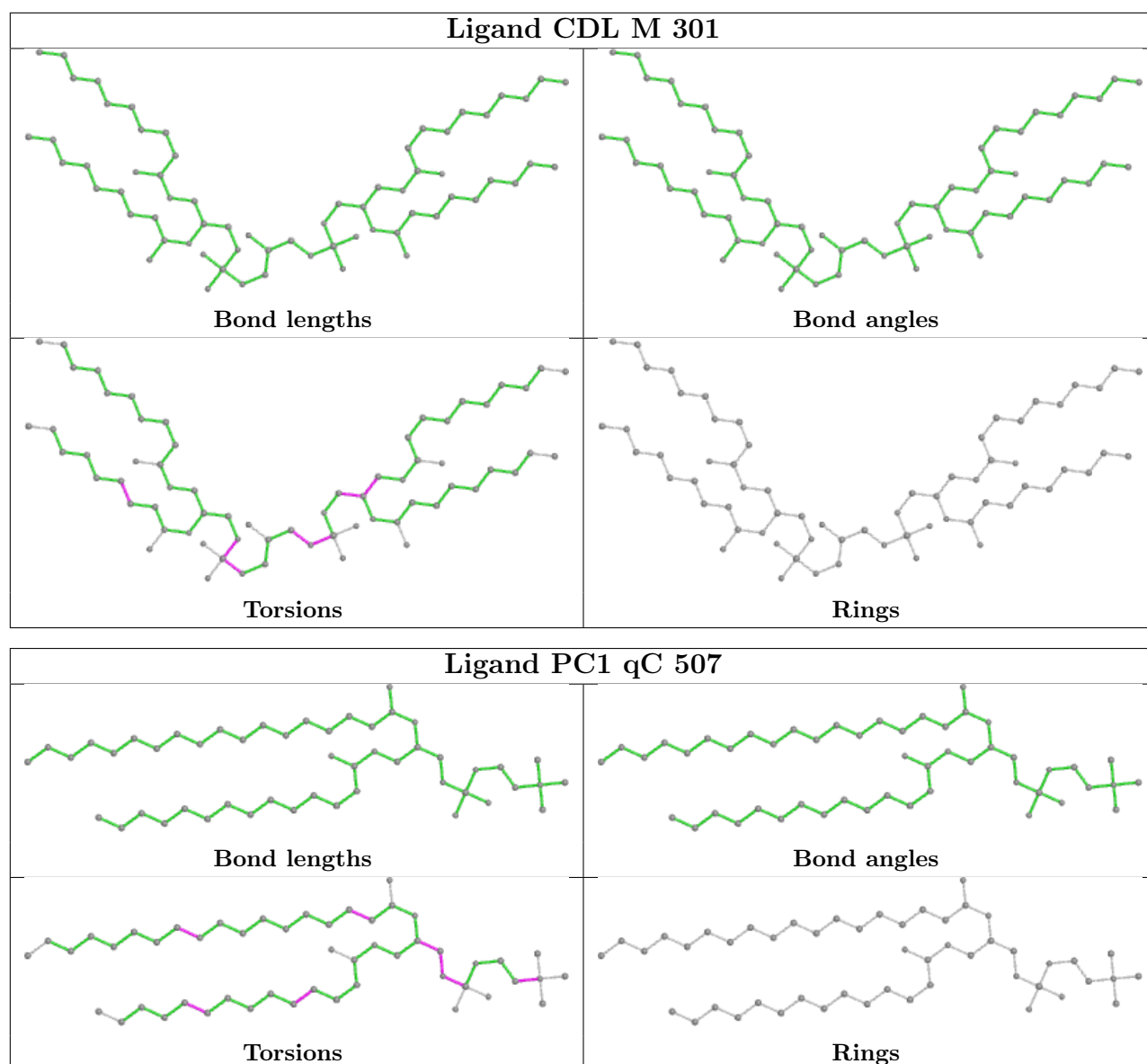


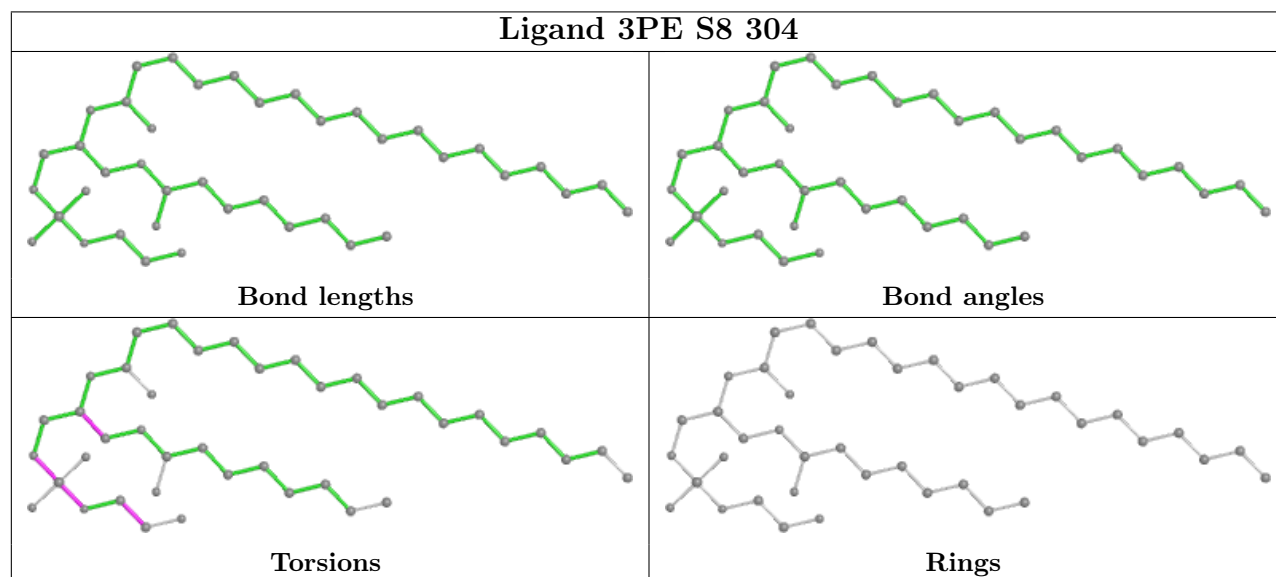
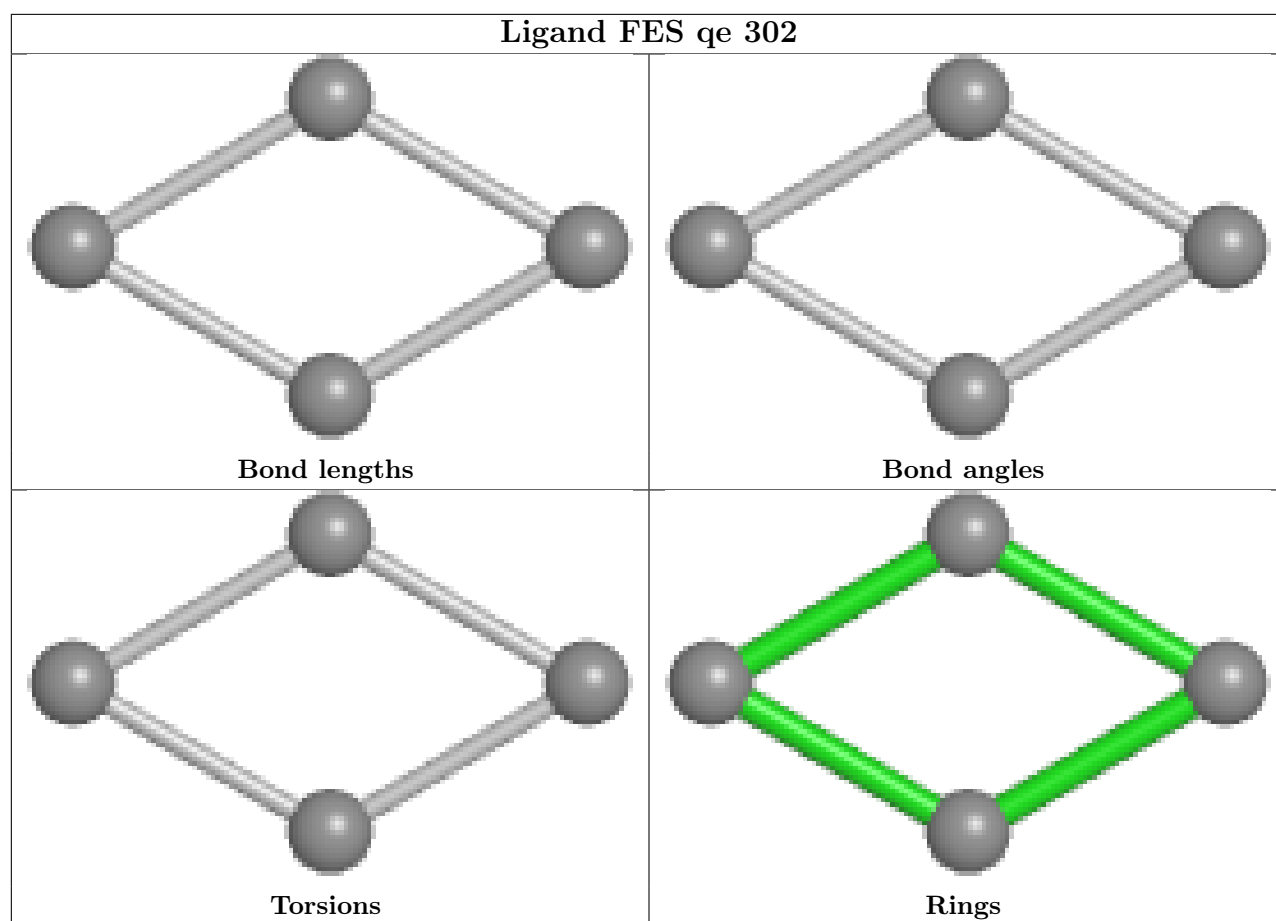


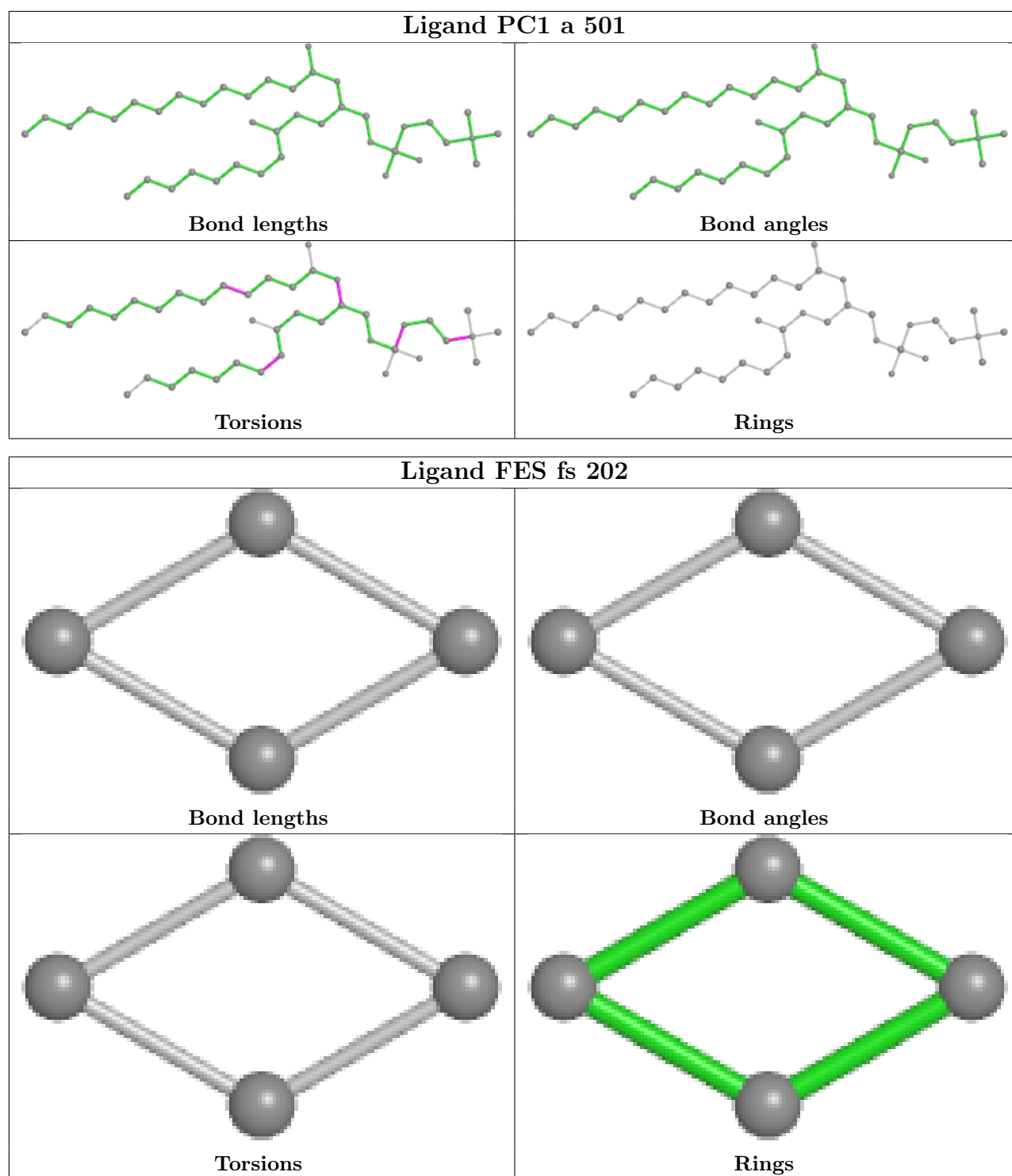


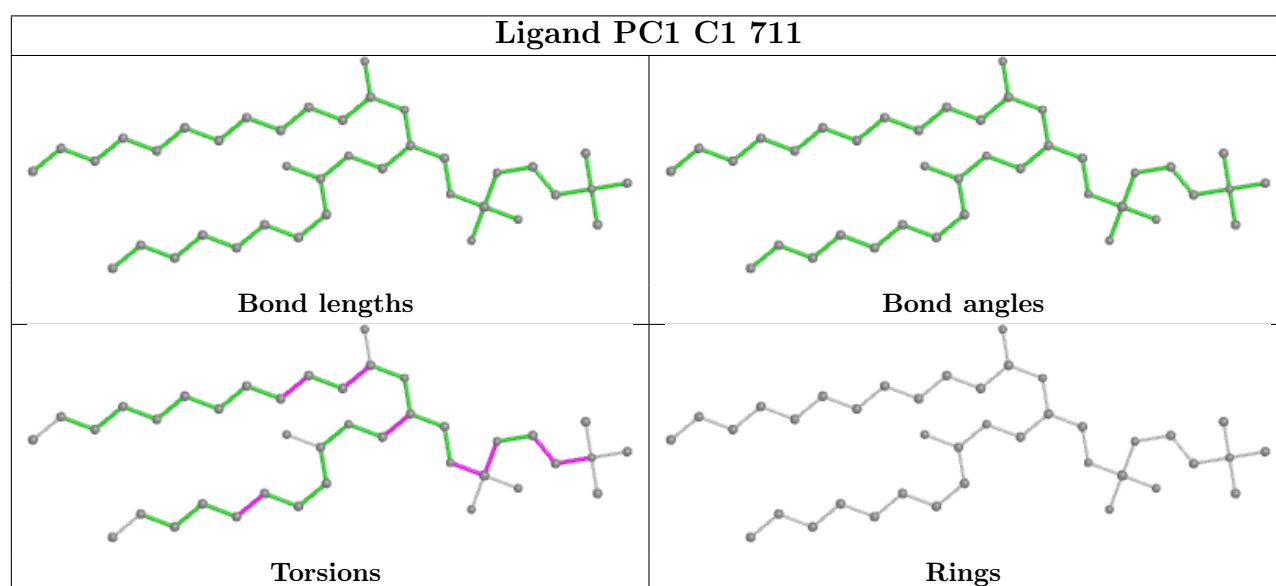
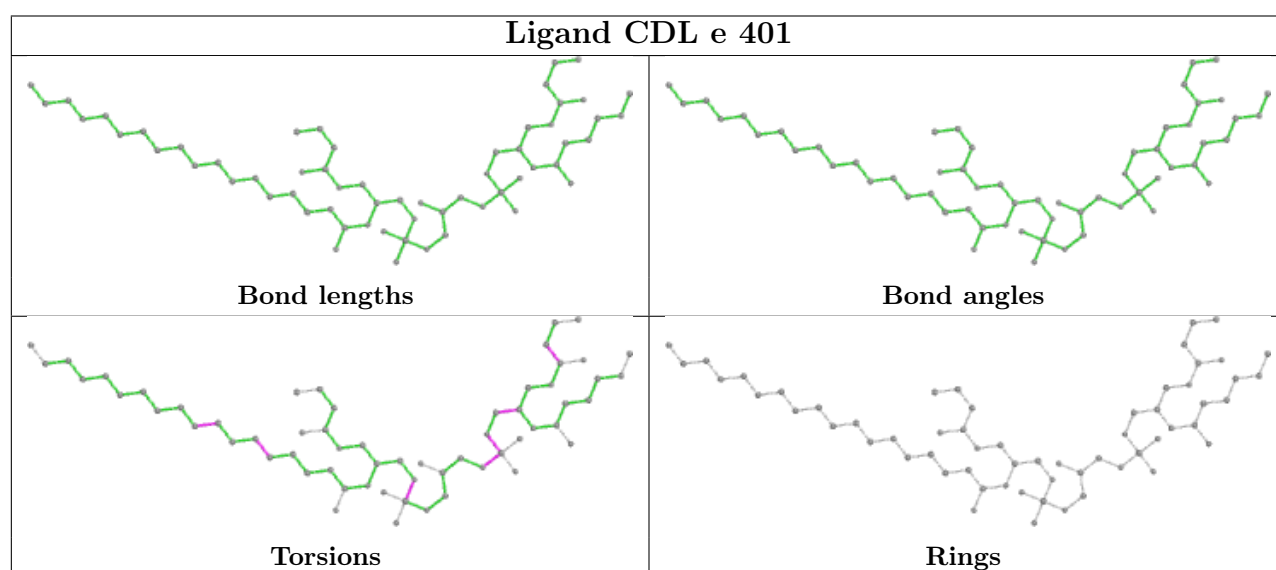
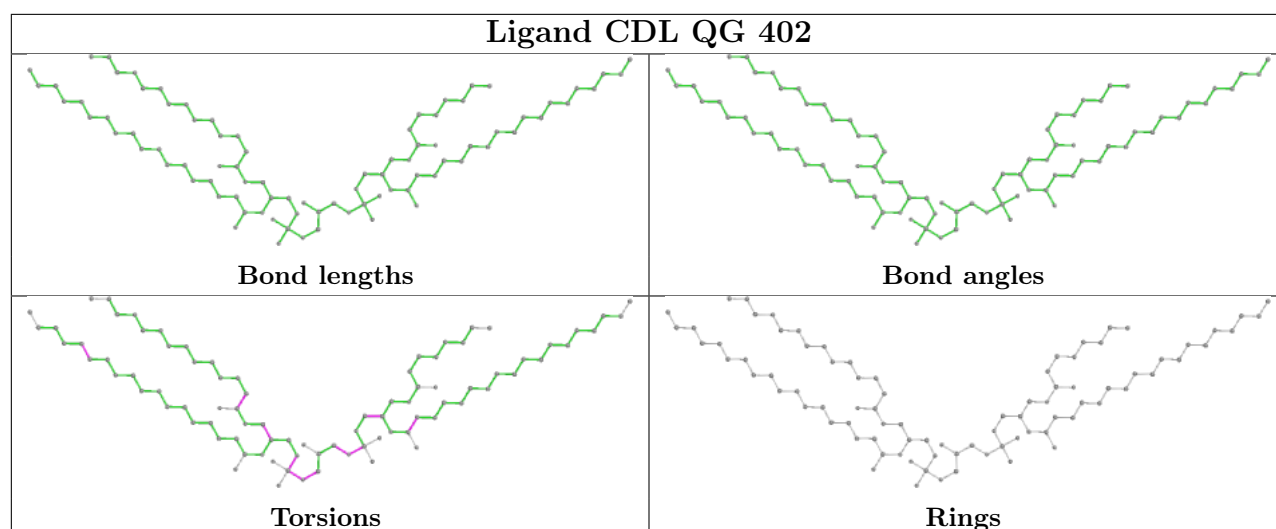


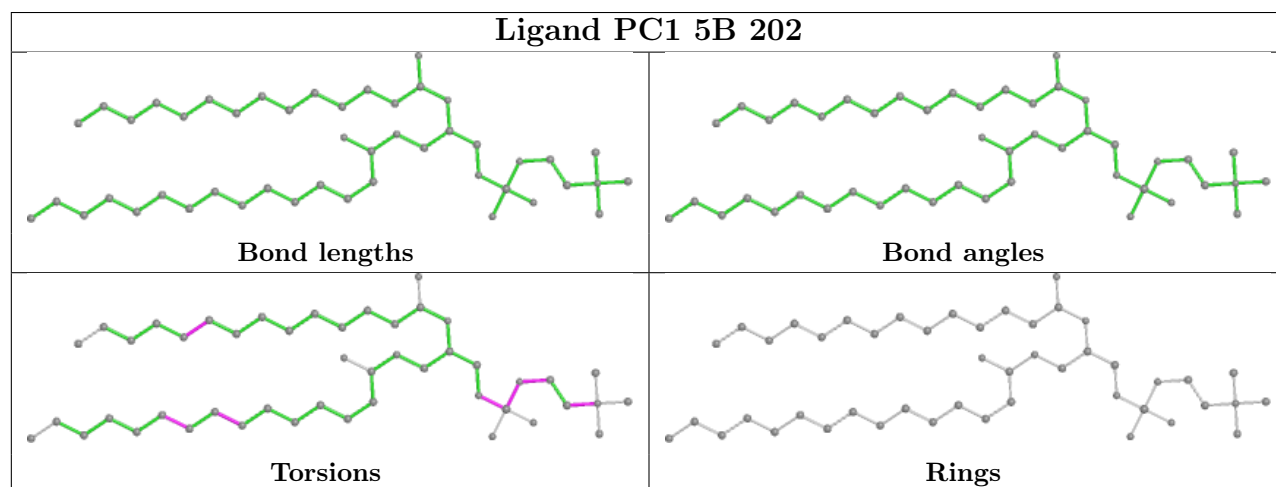
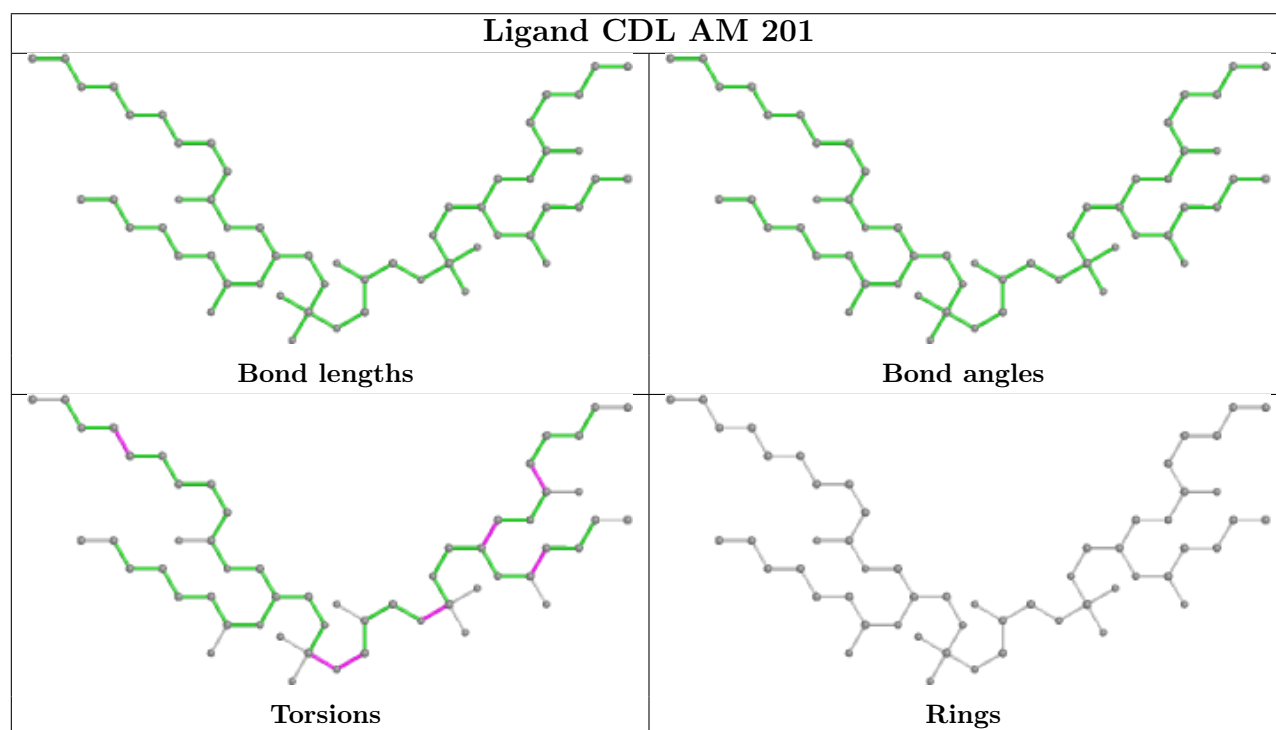
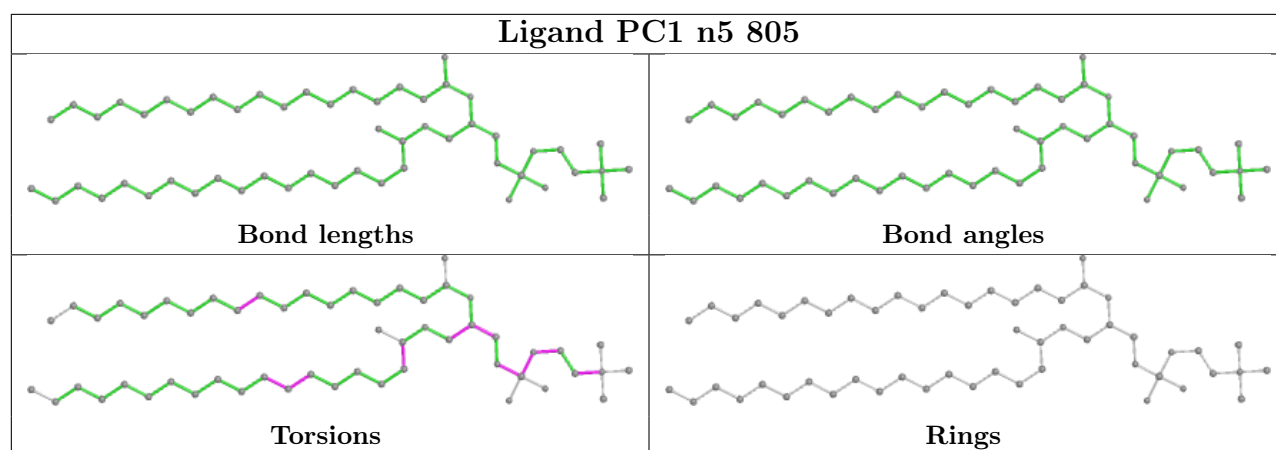


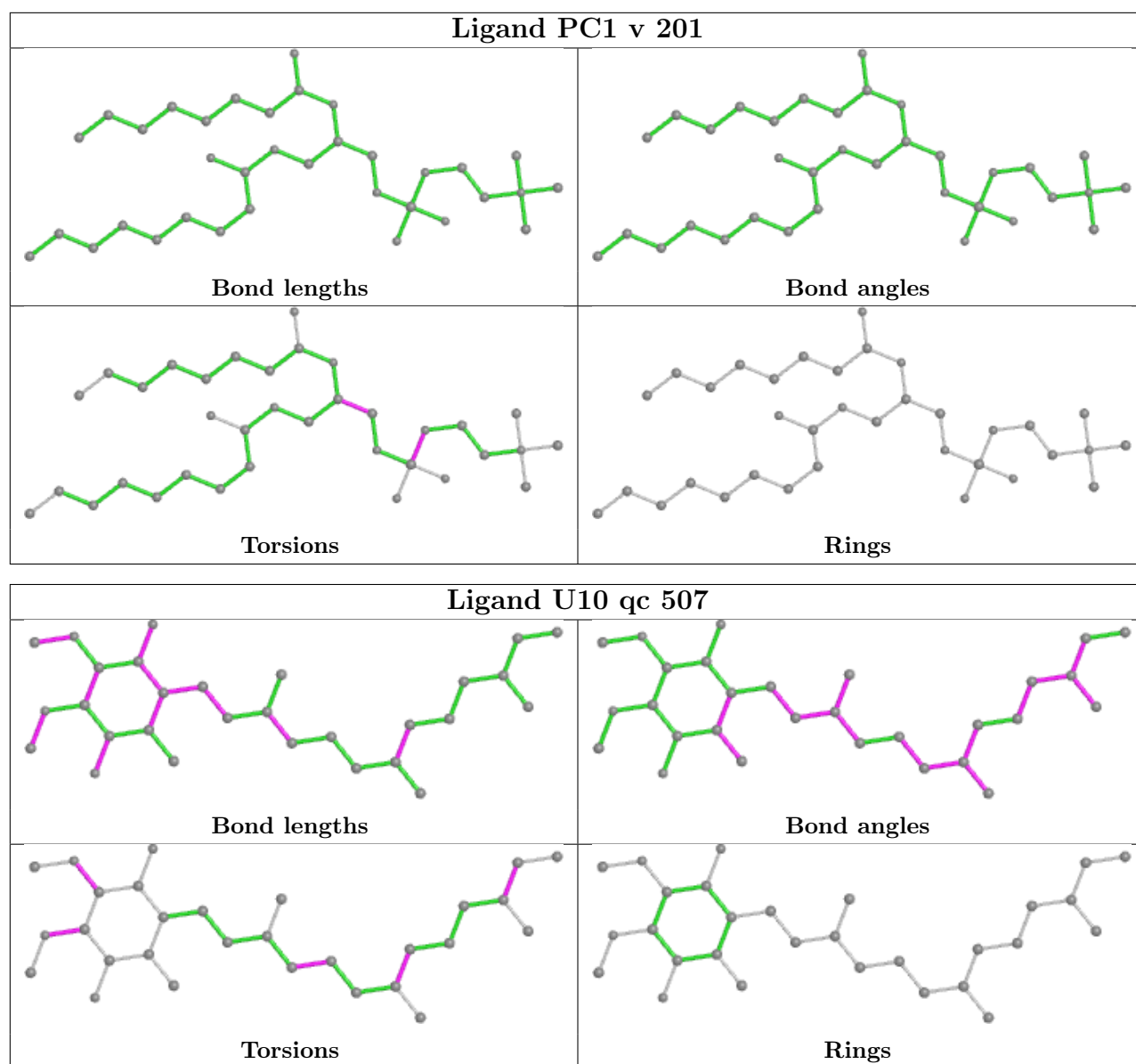


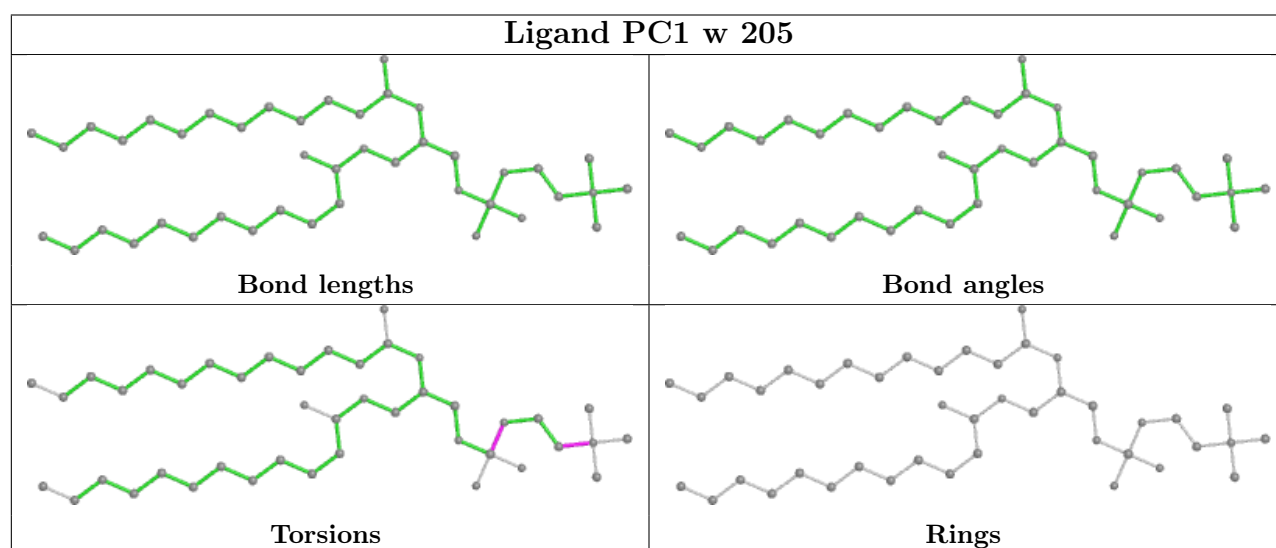
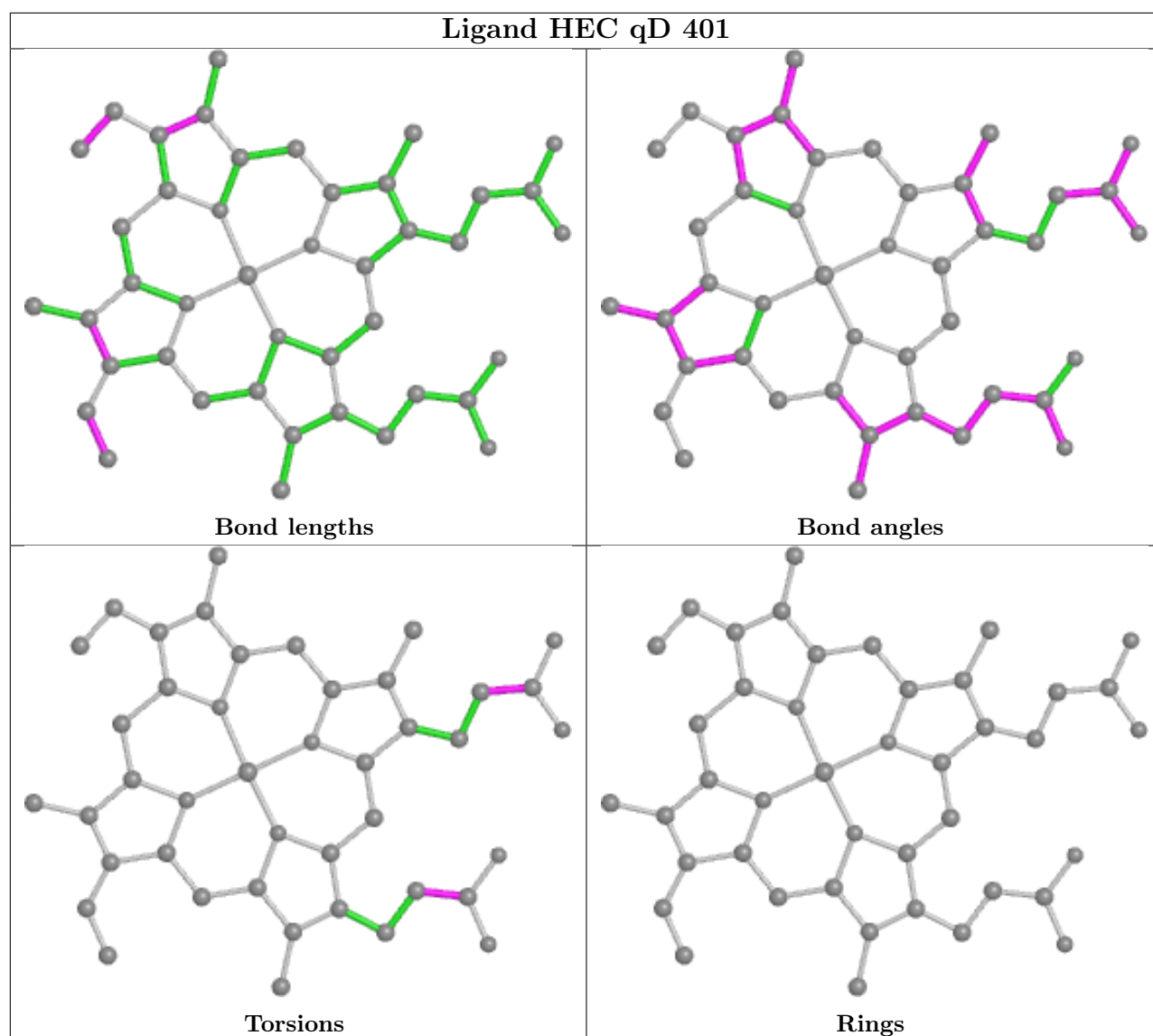


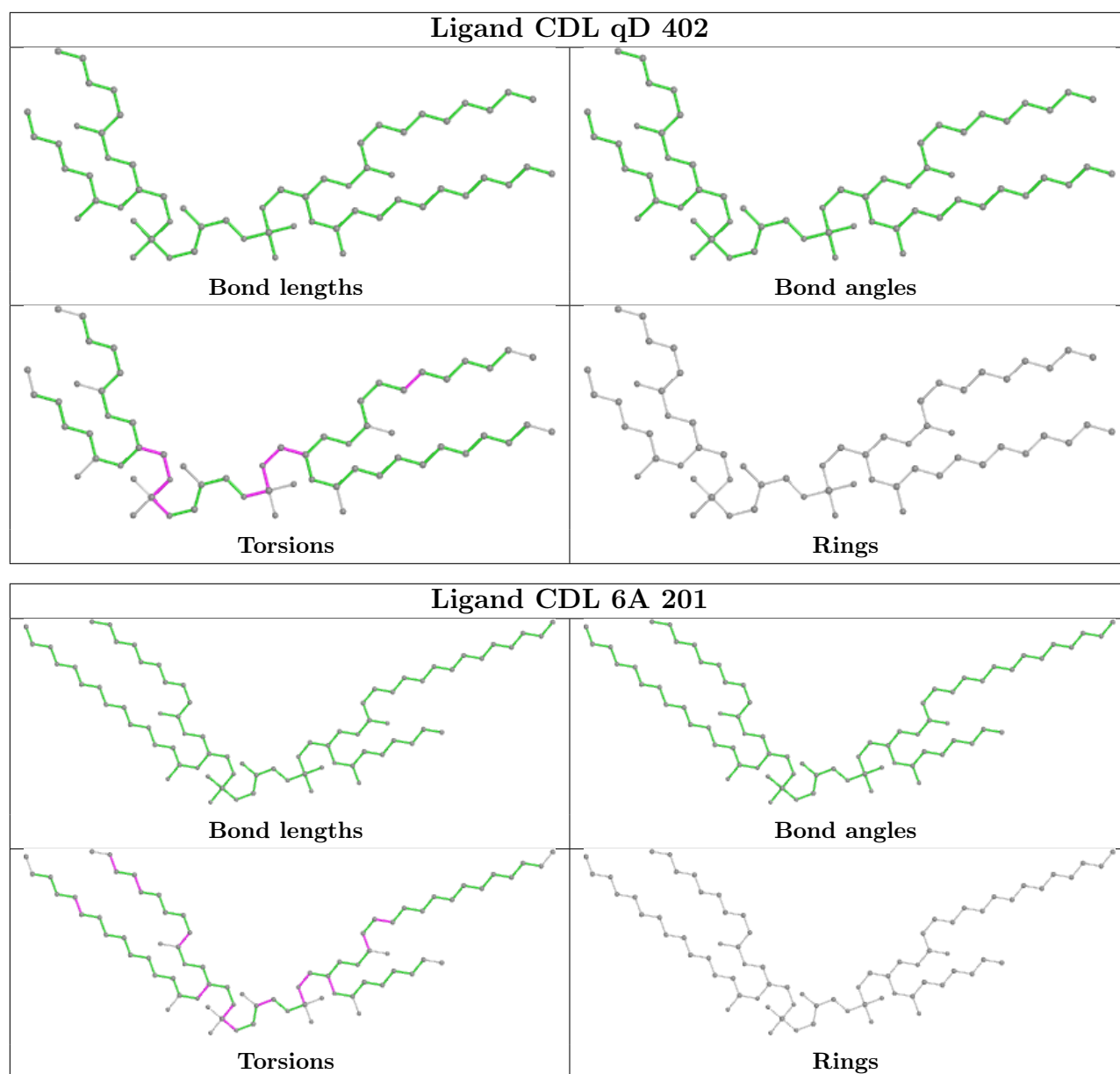


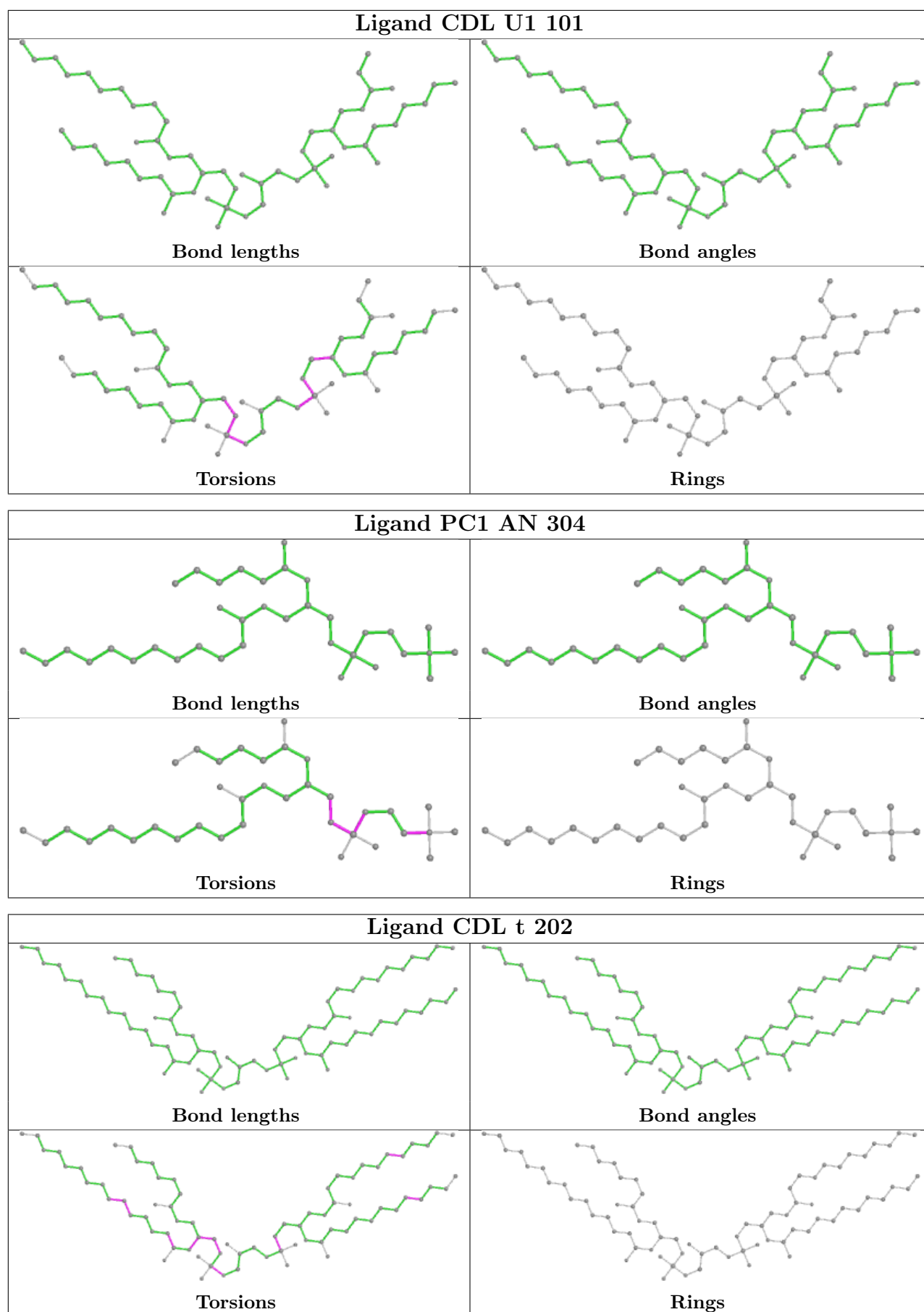


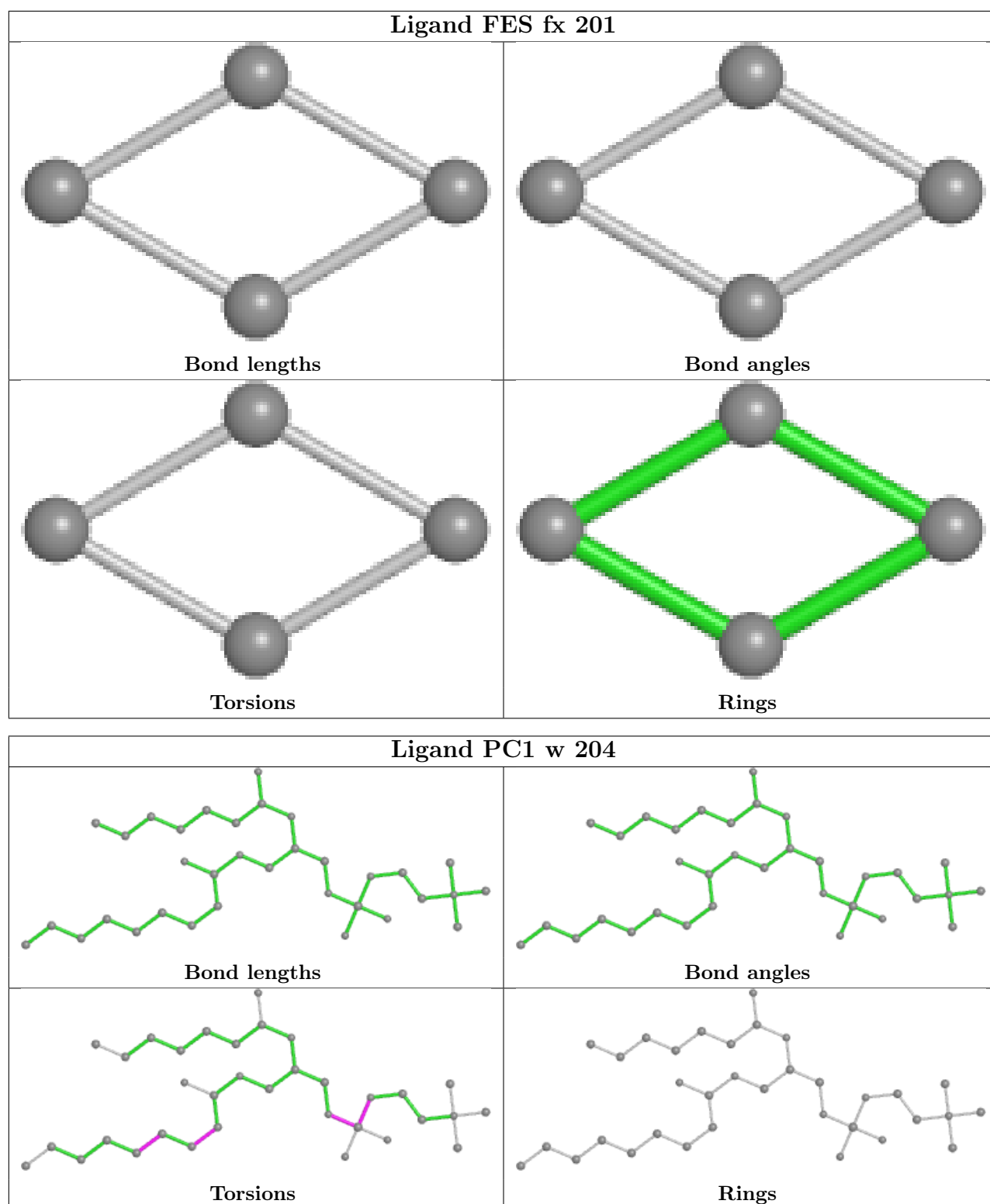


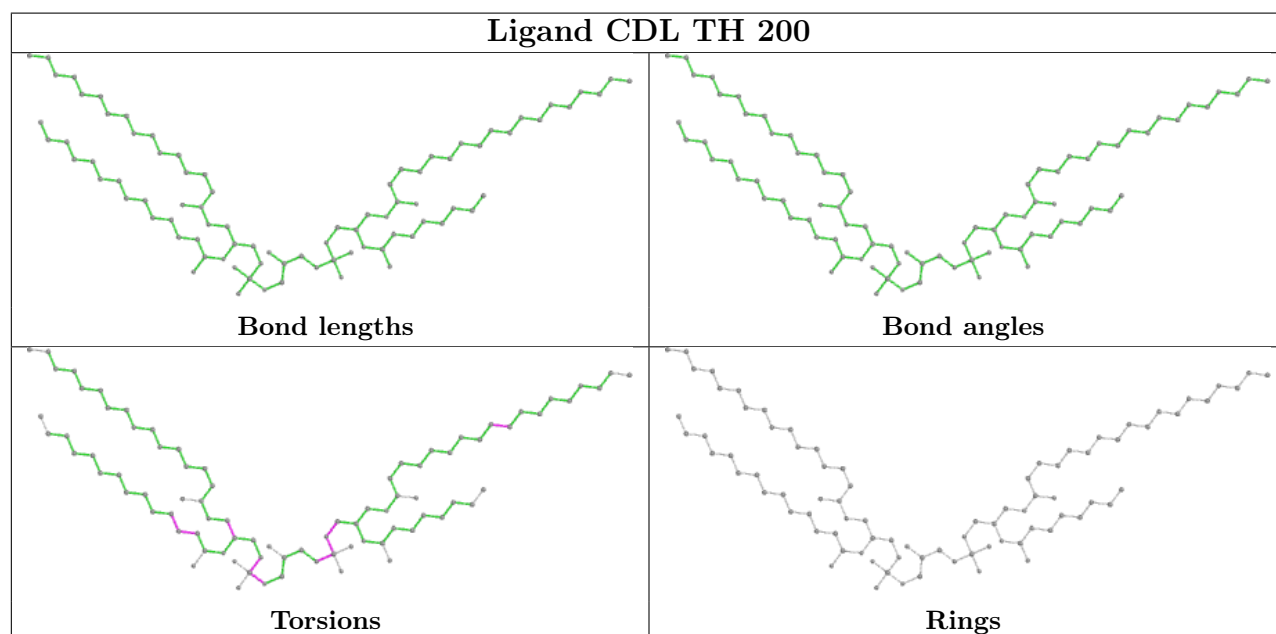
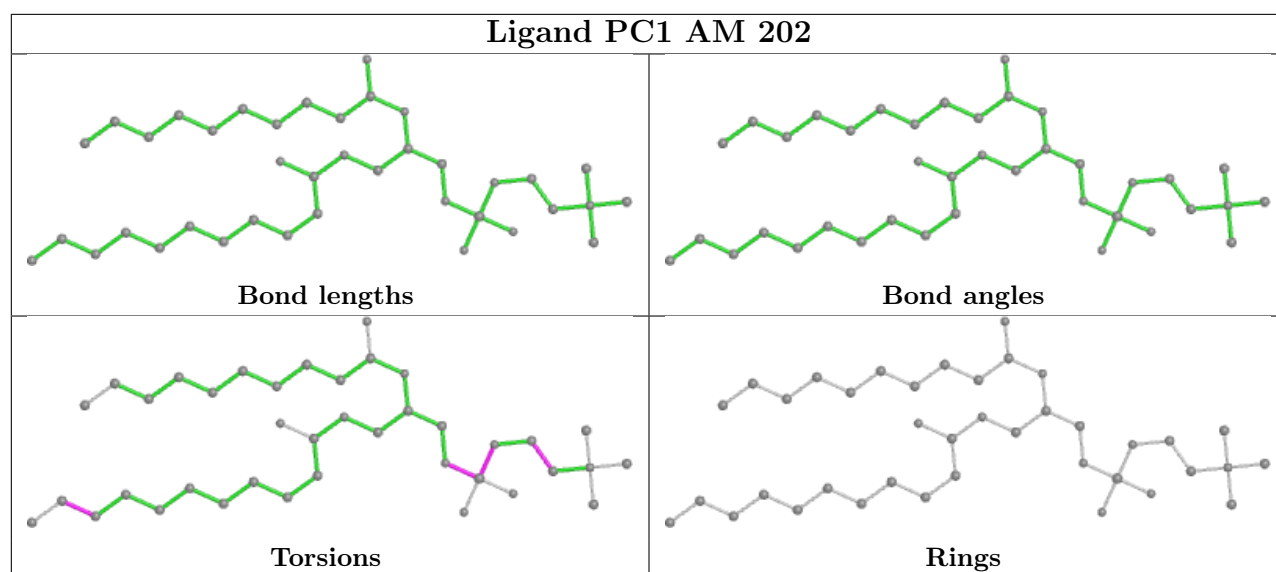


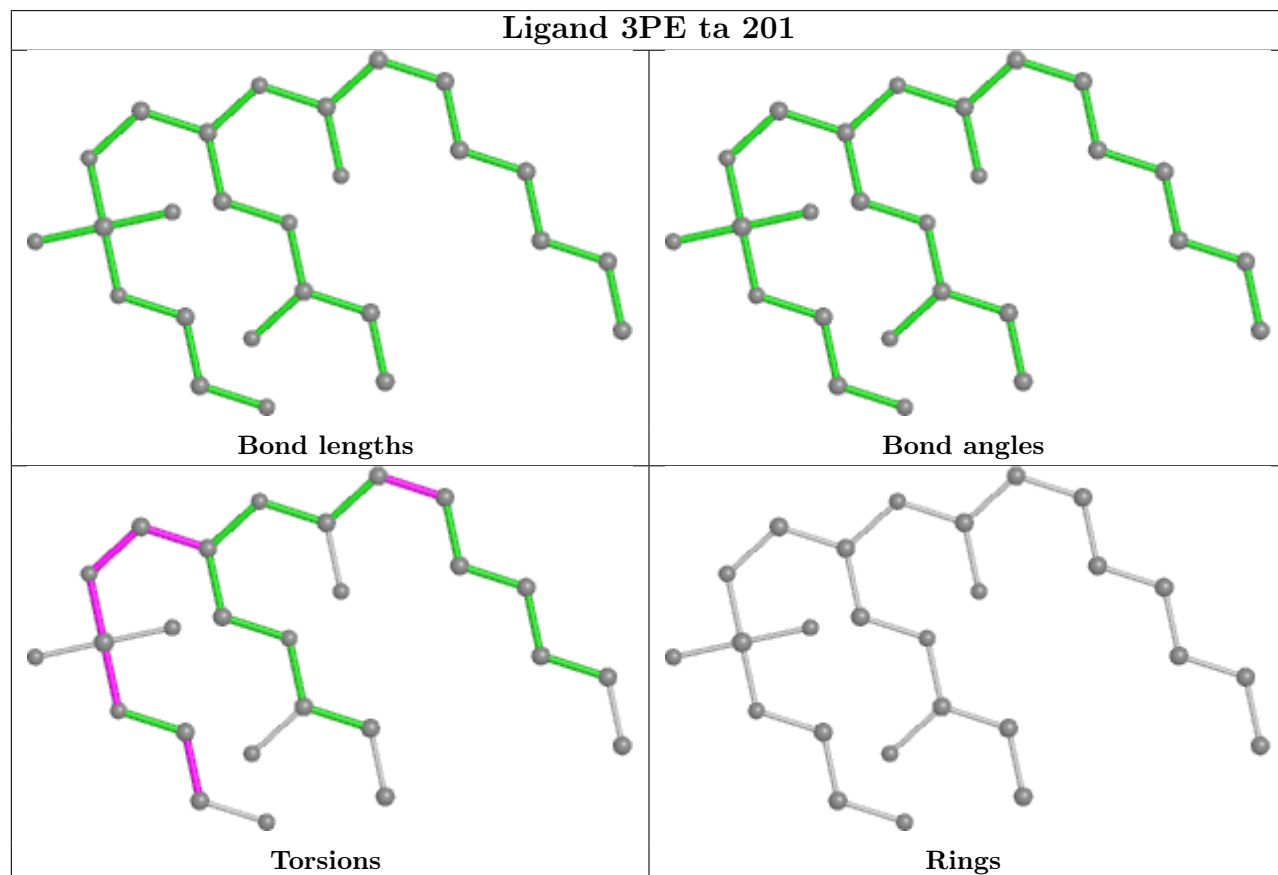
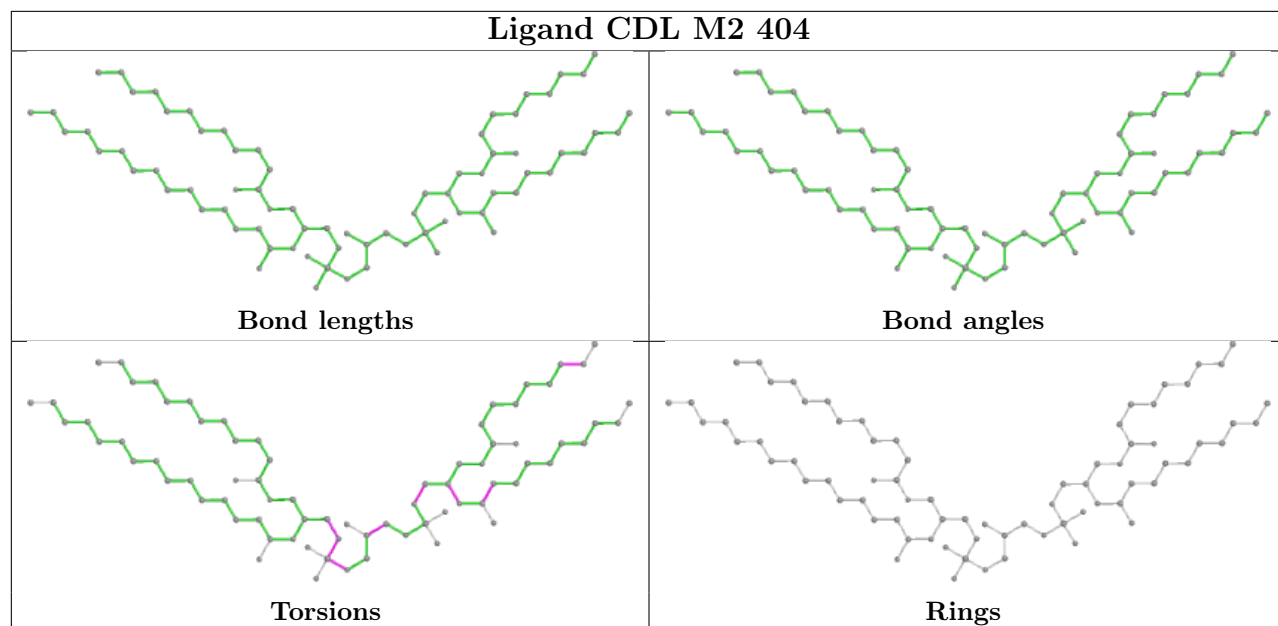


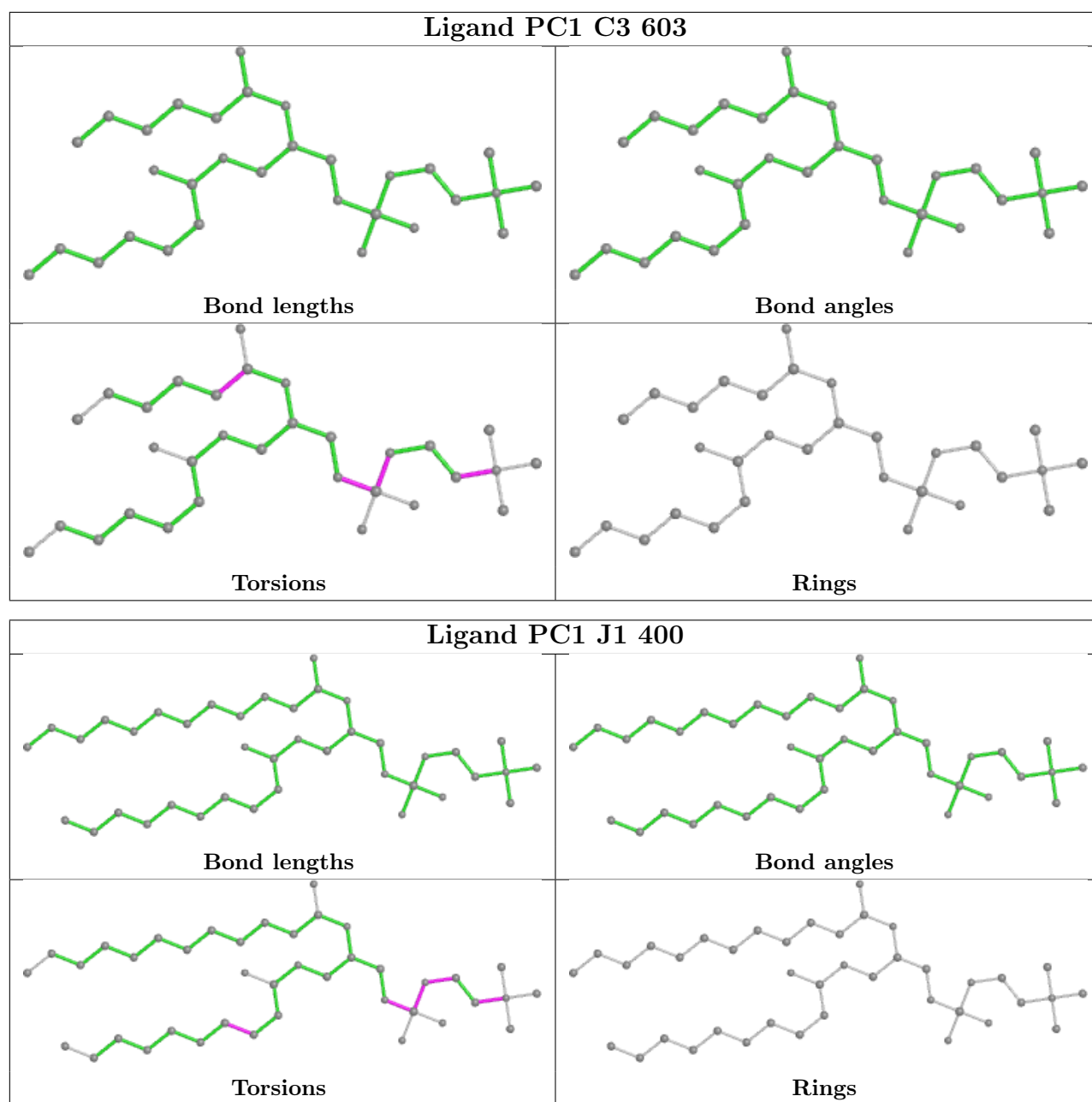


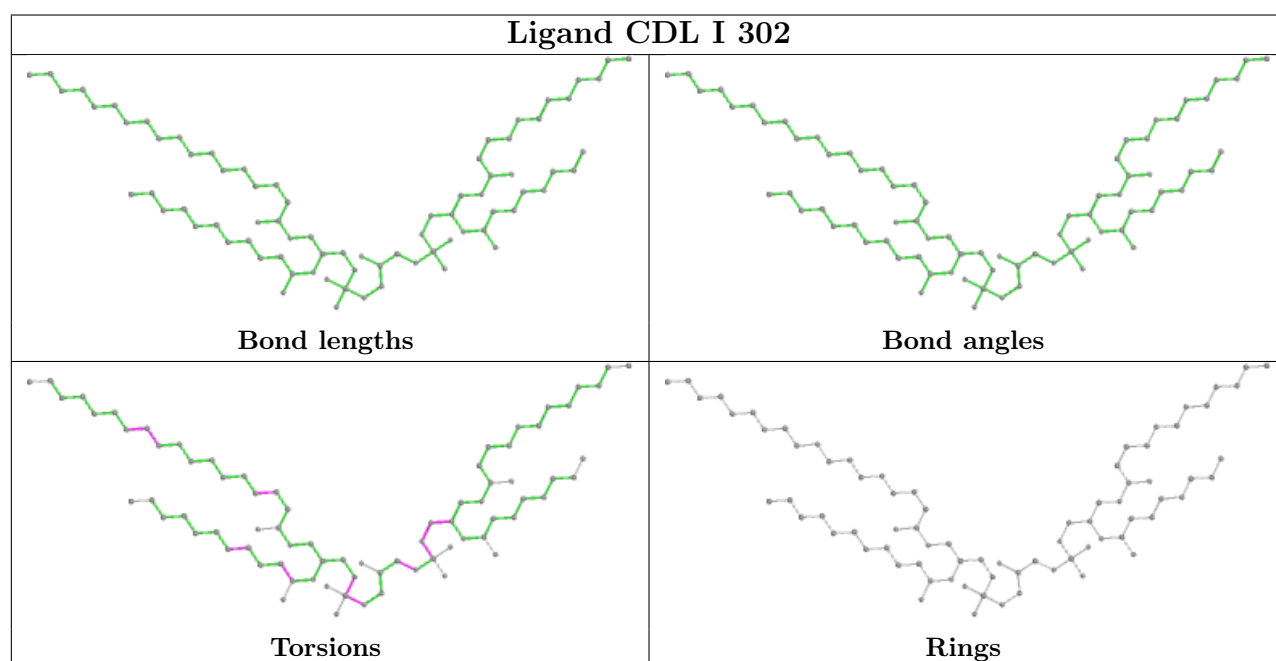
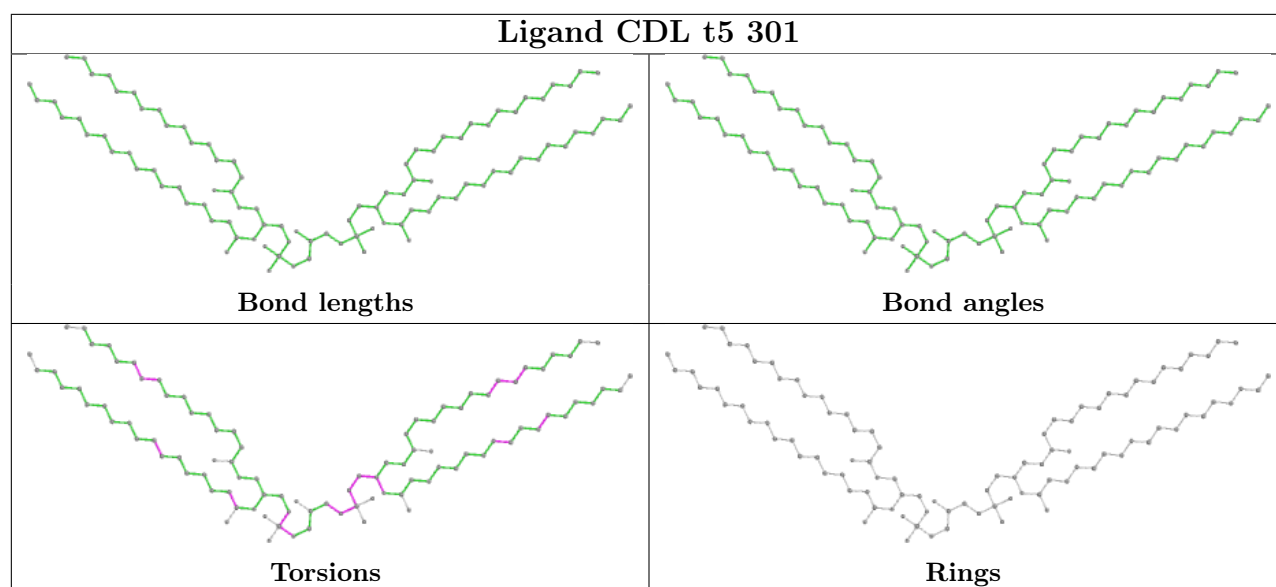




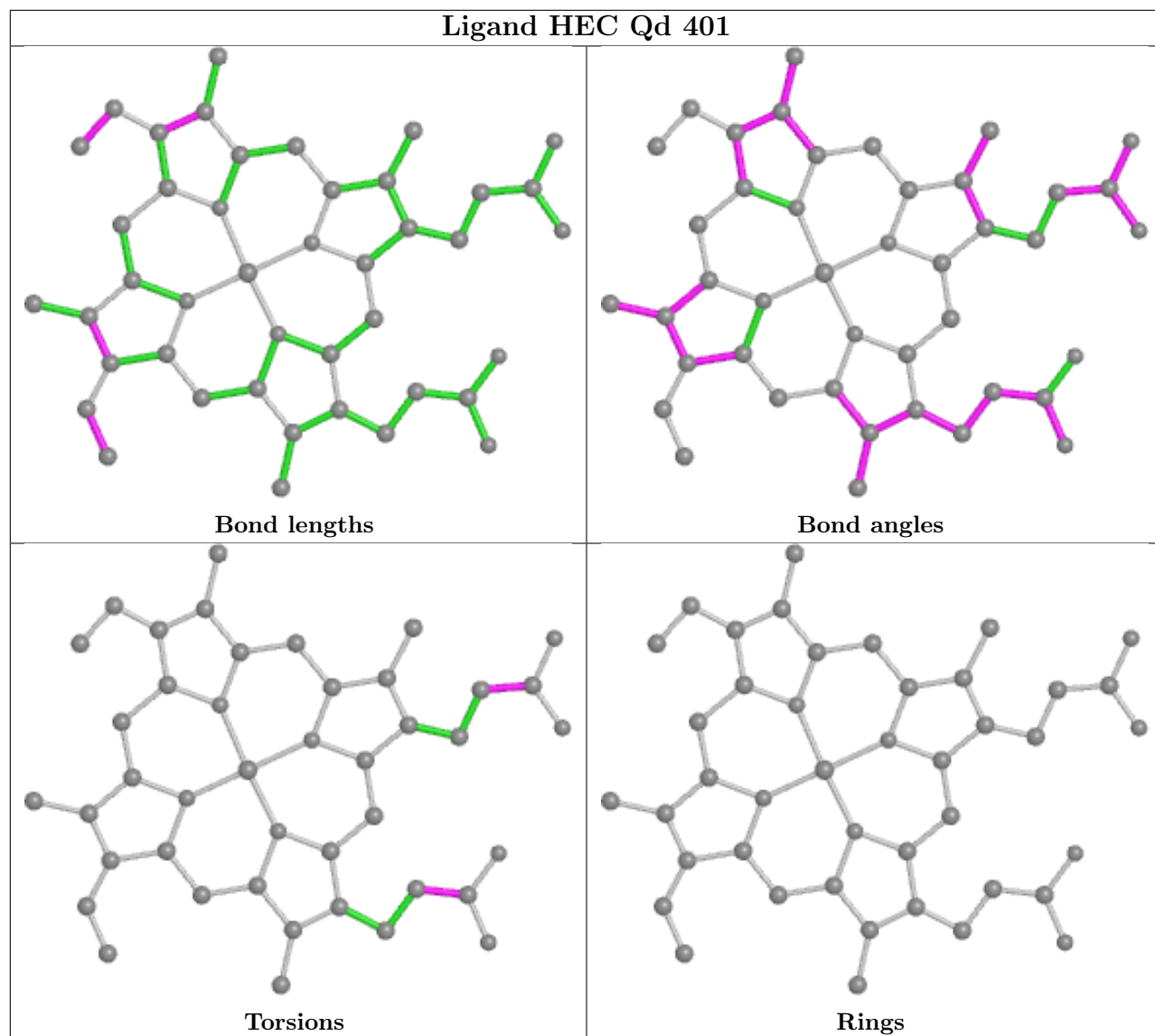


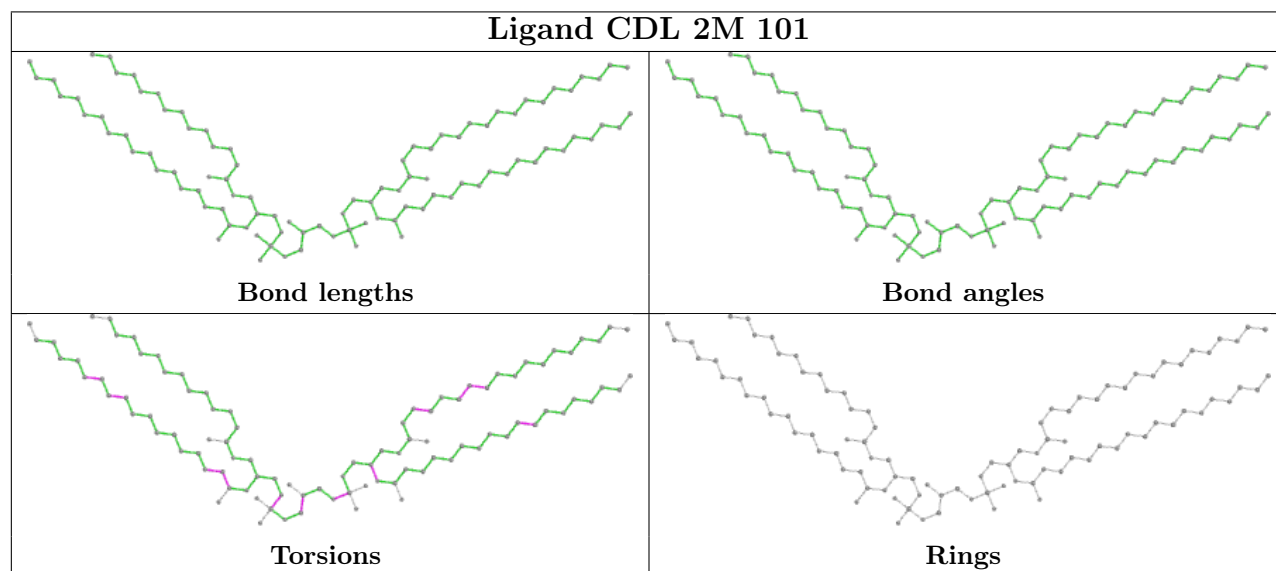
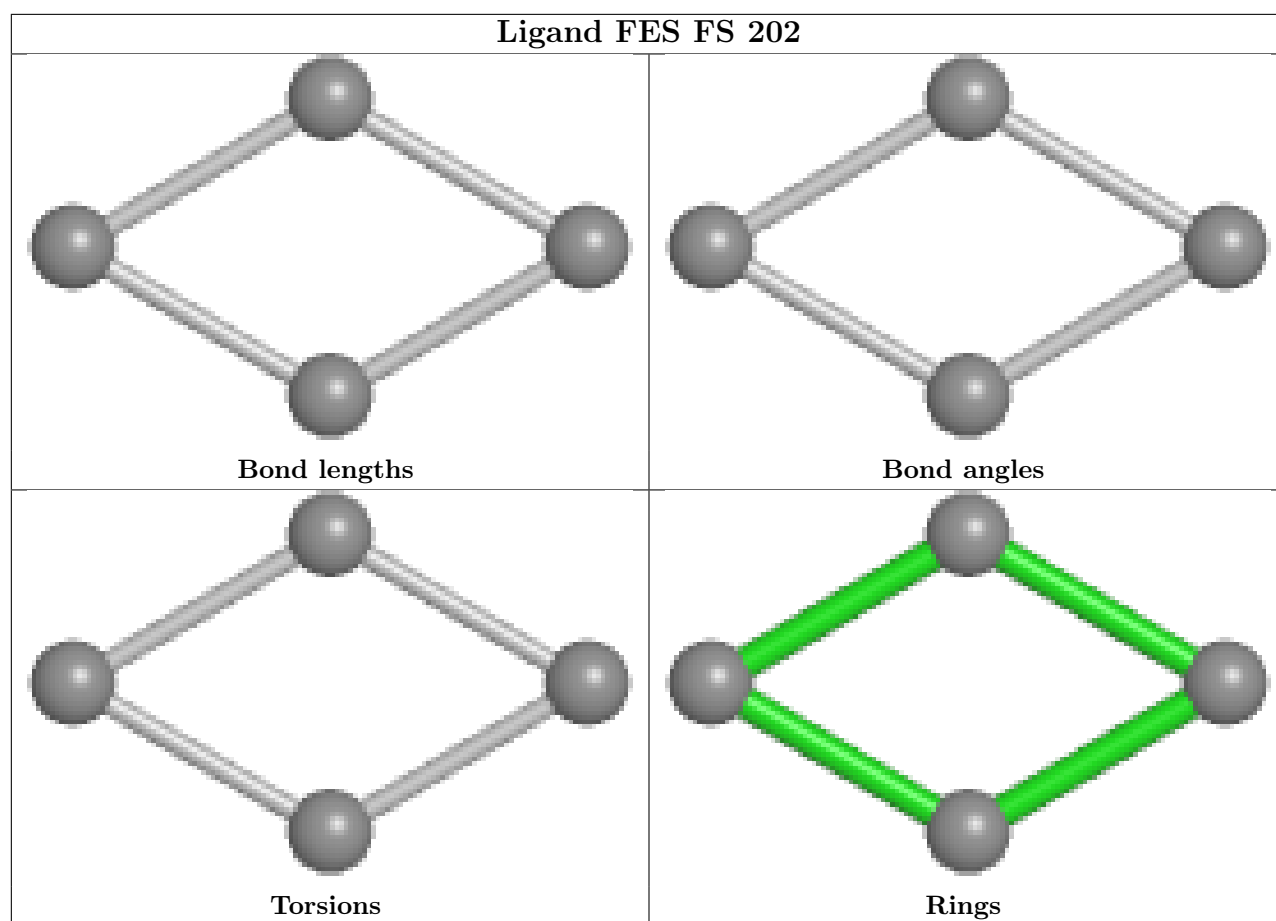


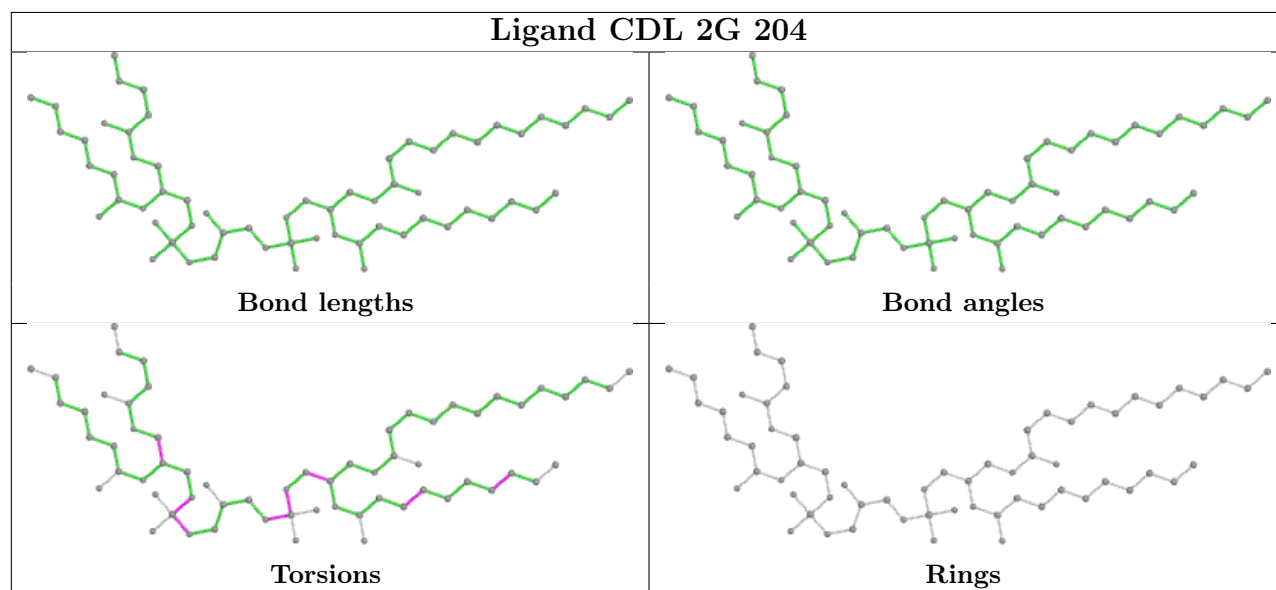
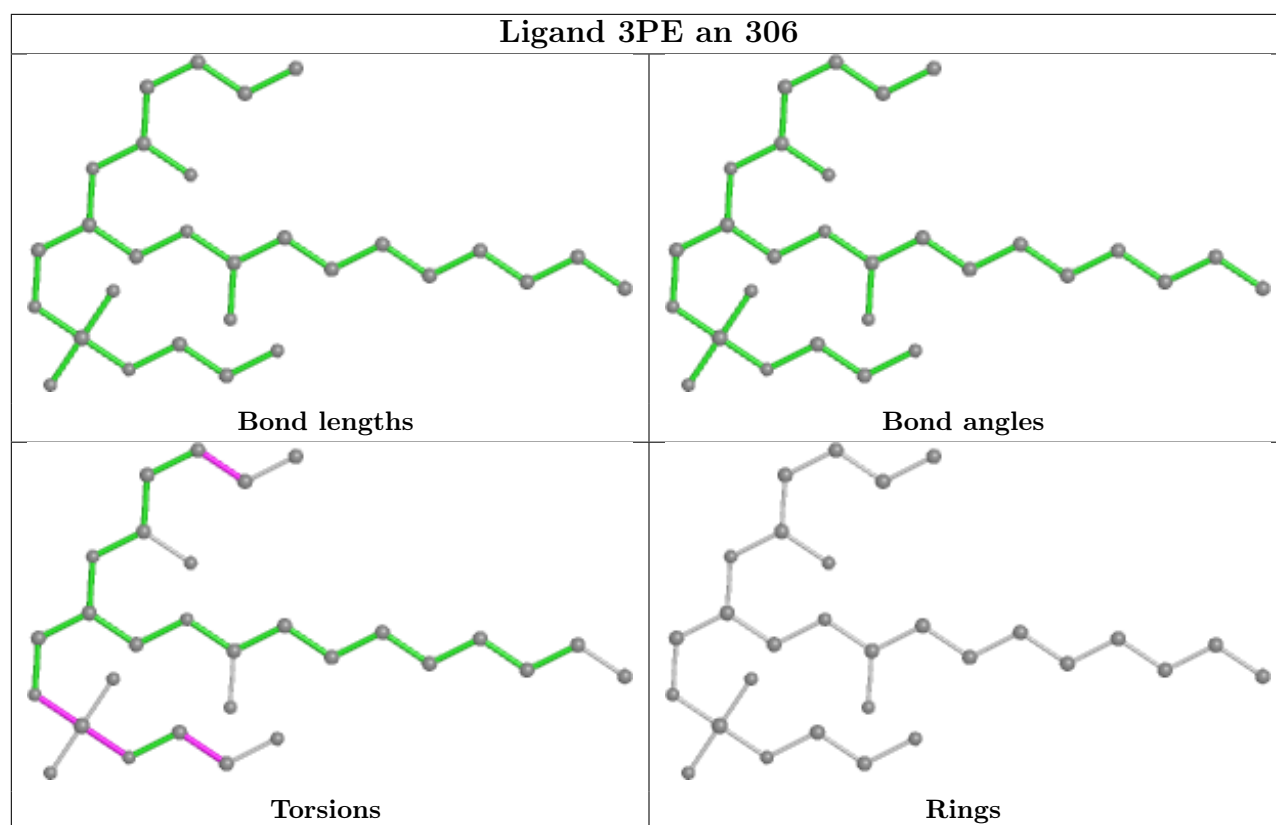


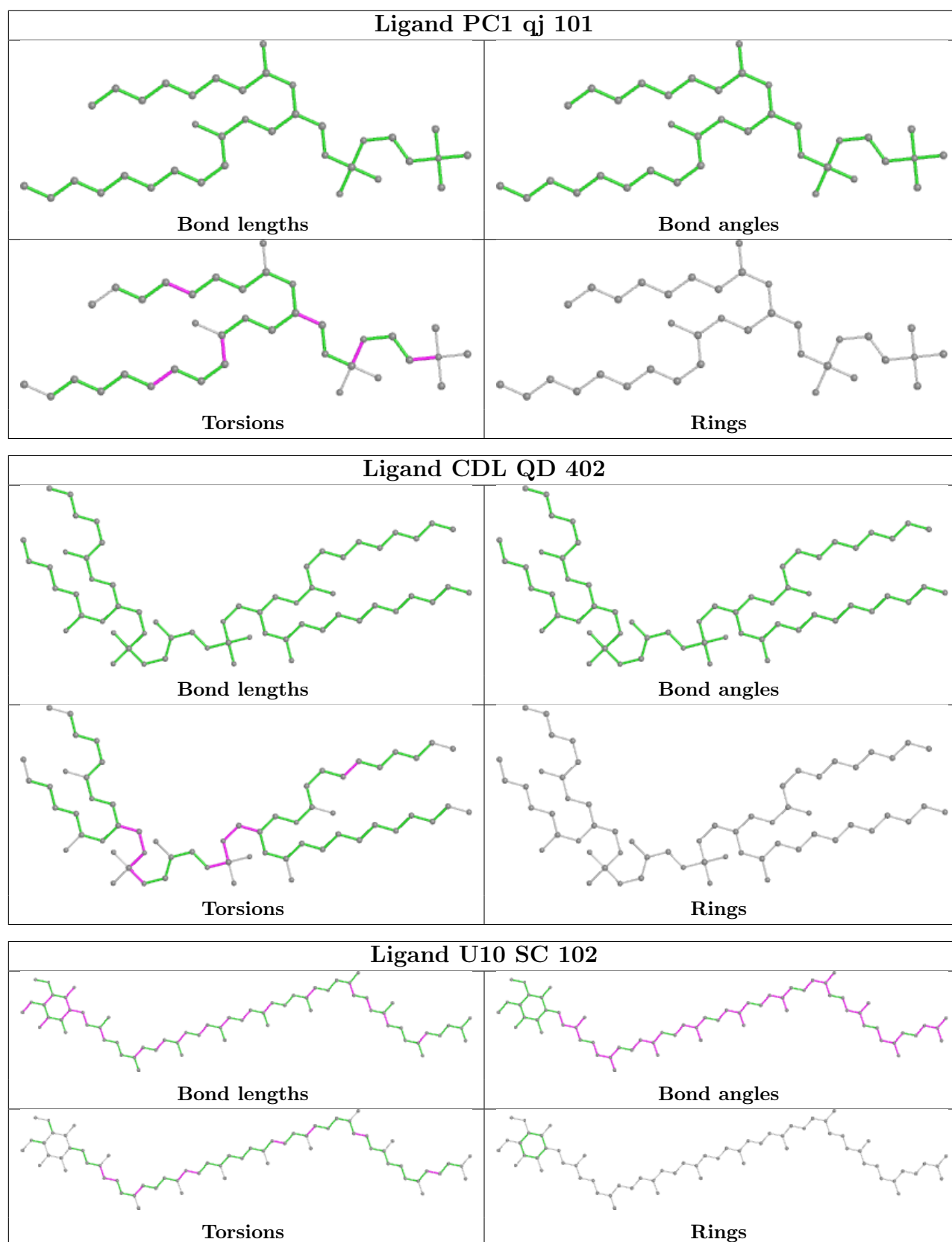


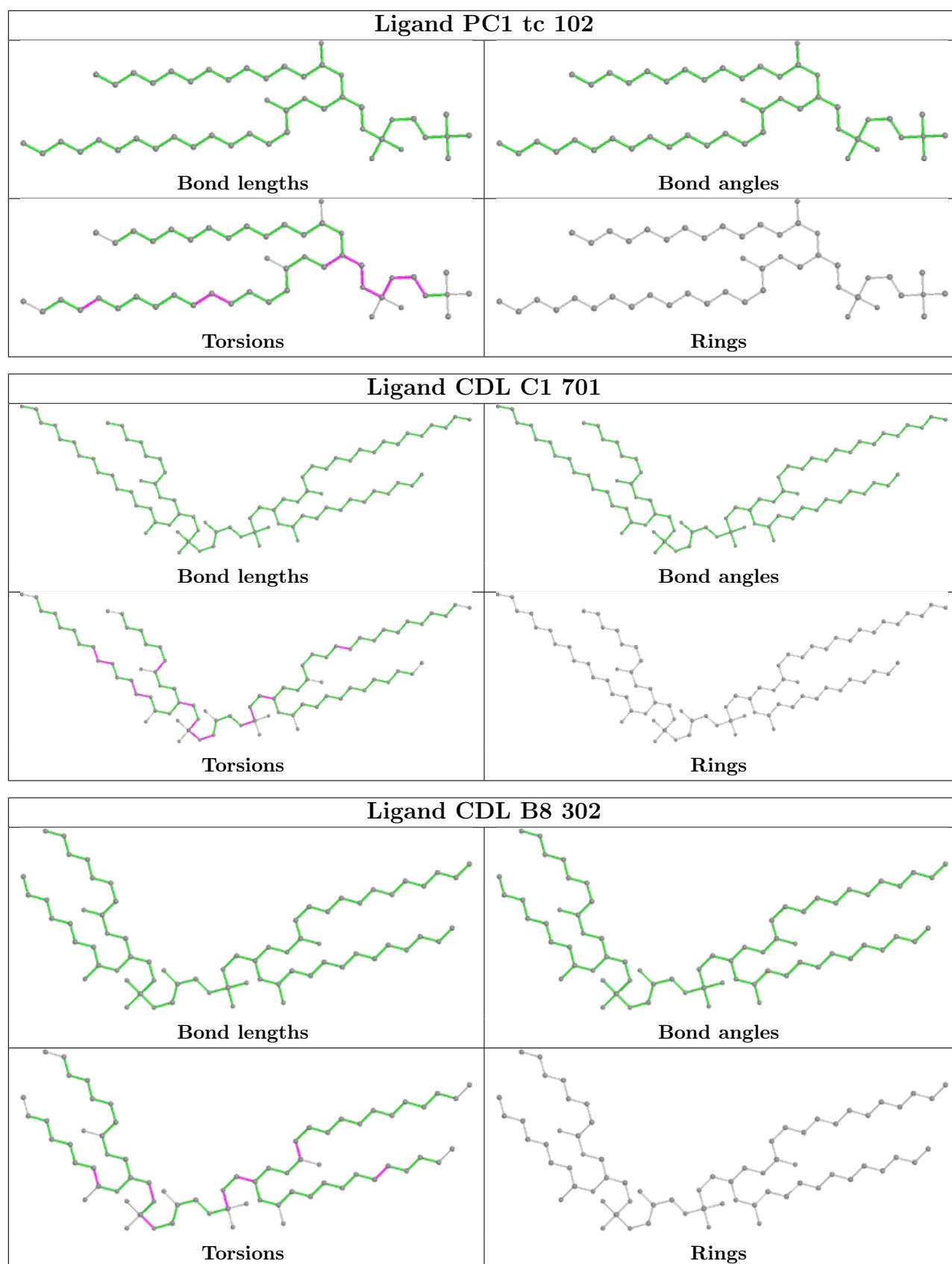
Ligand HEC Qd 401



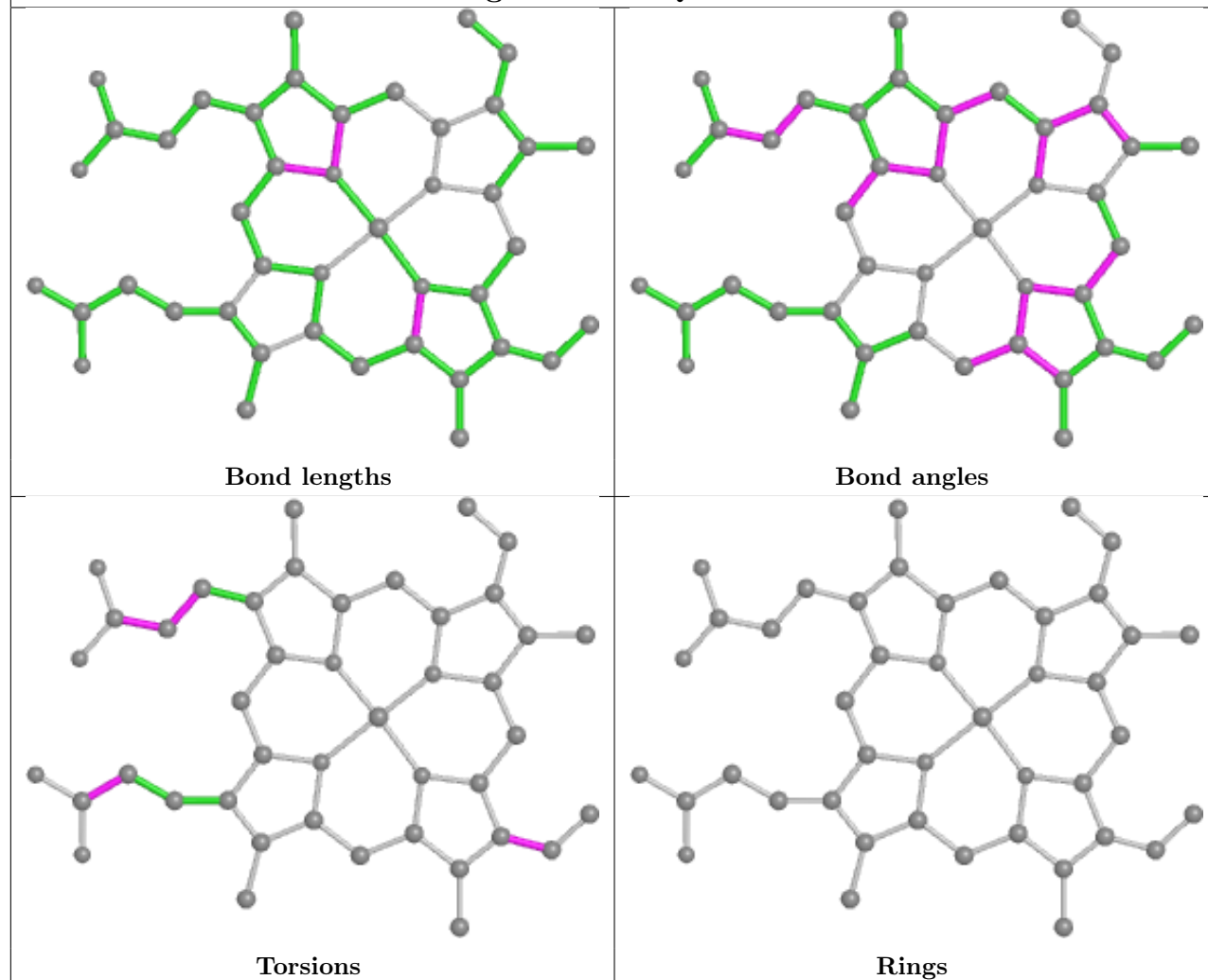




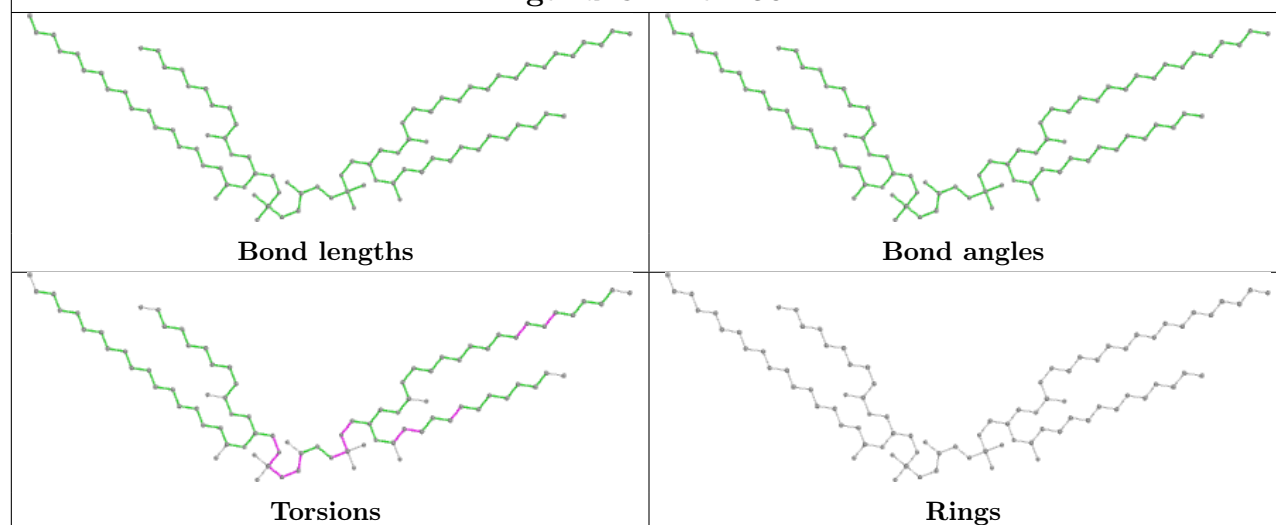


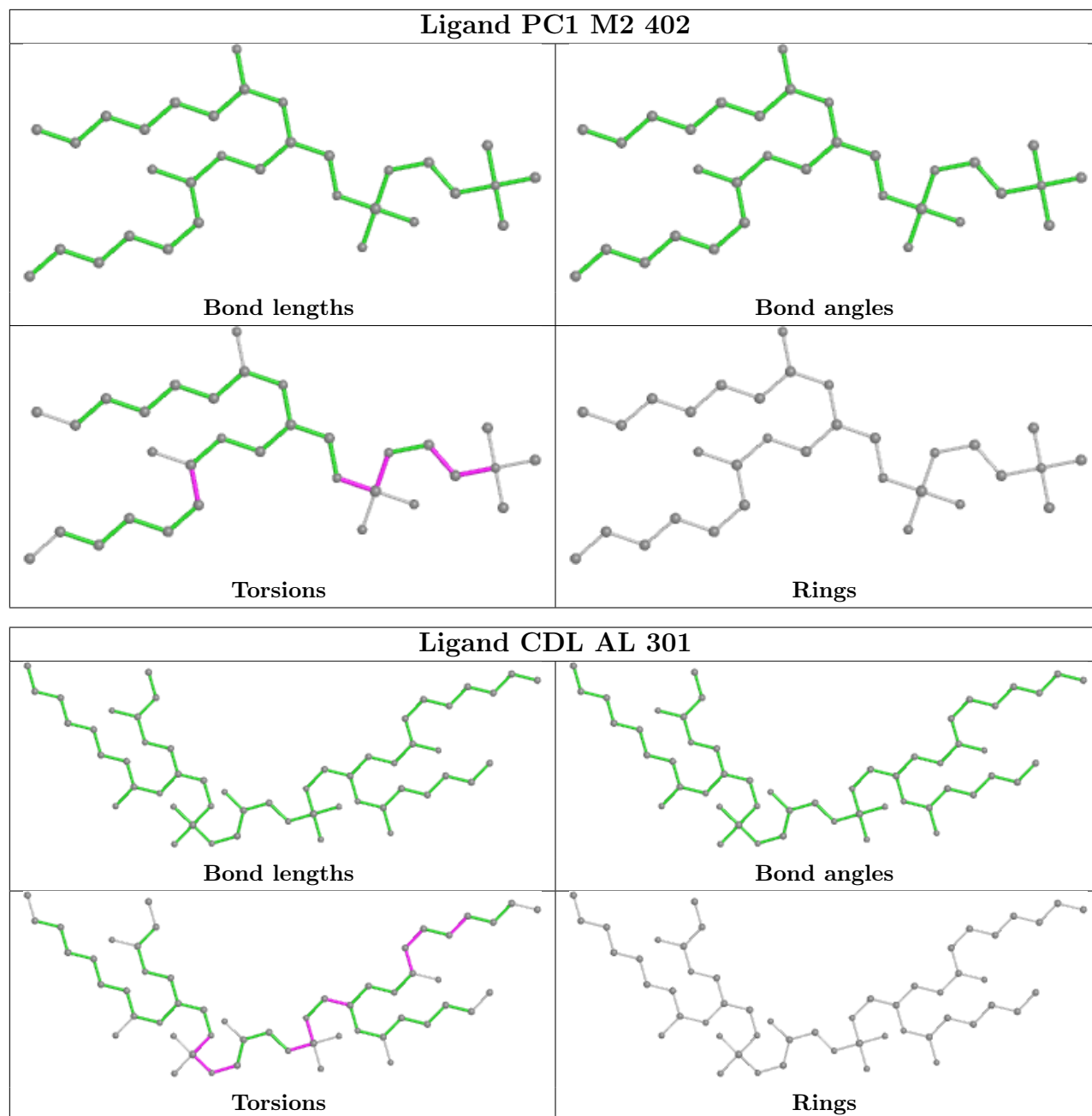


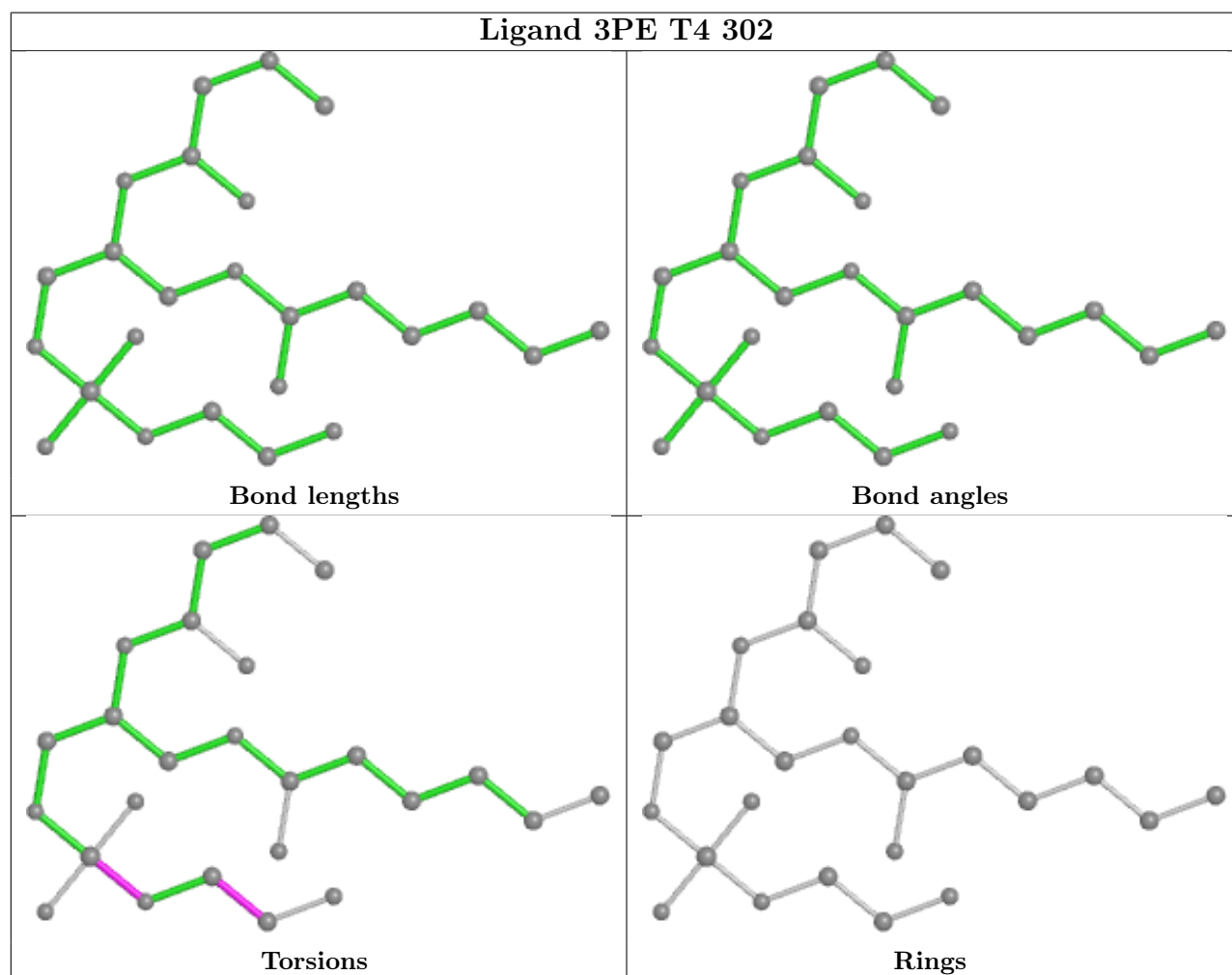
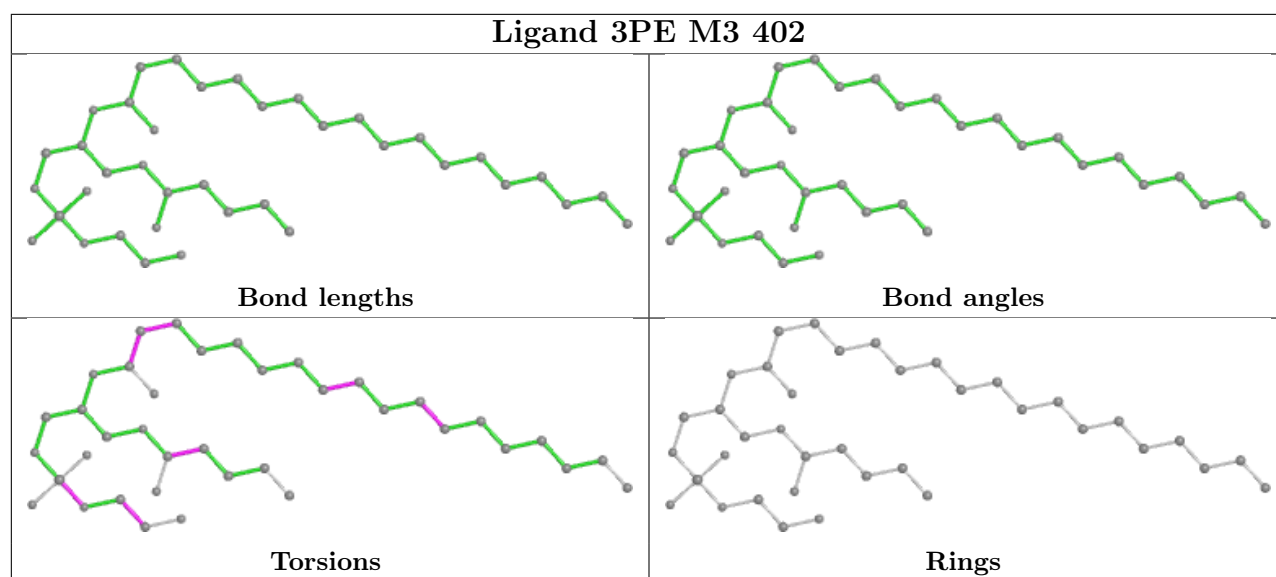
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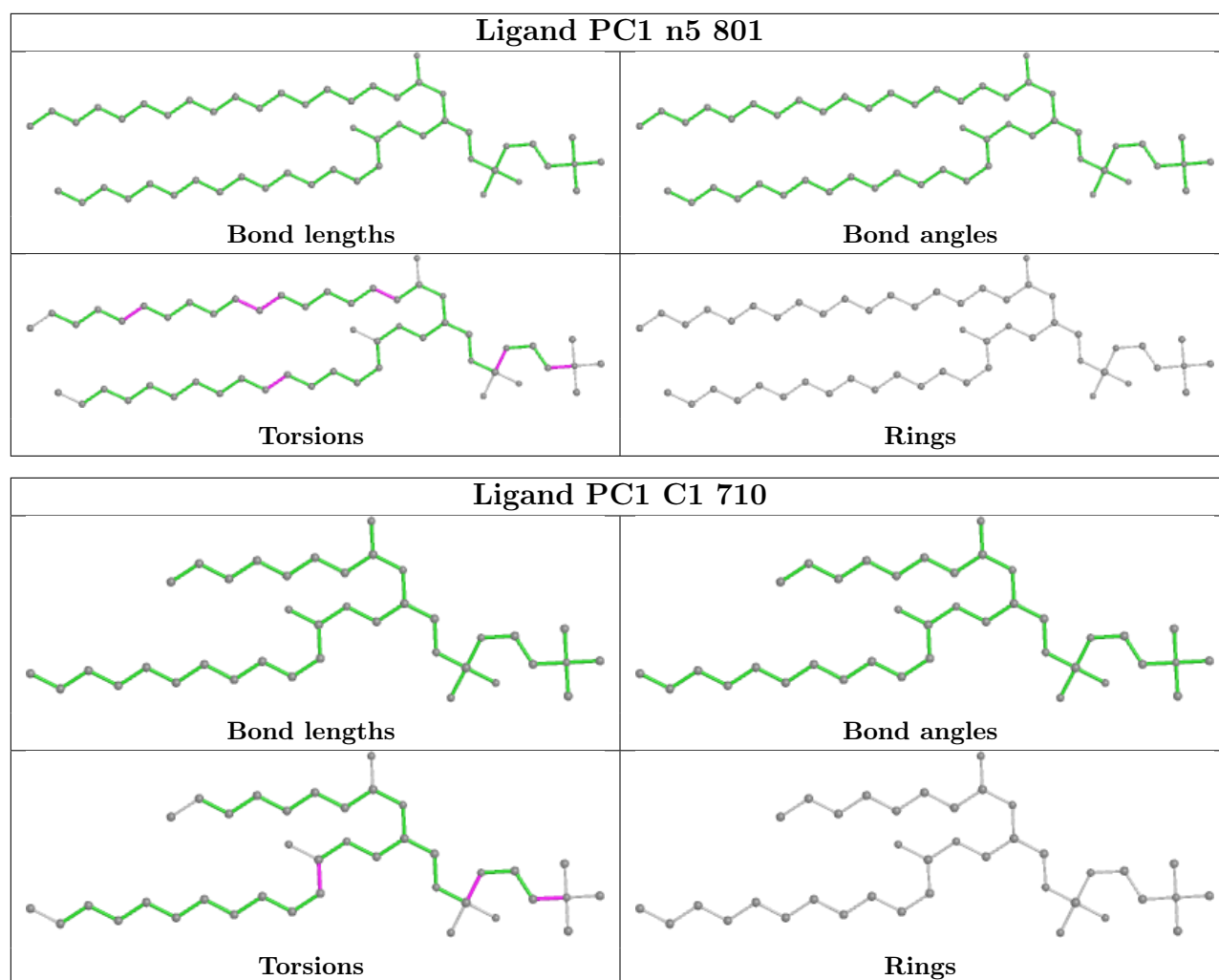


Ligand CDL an 302

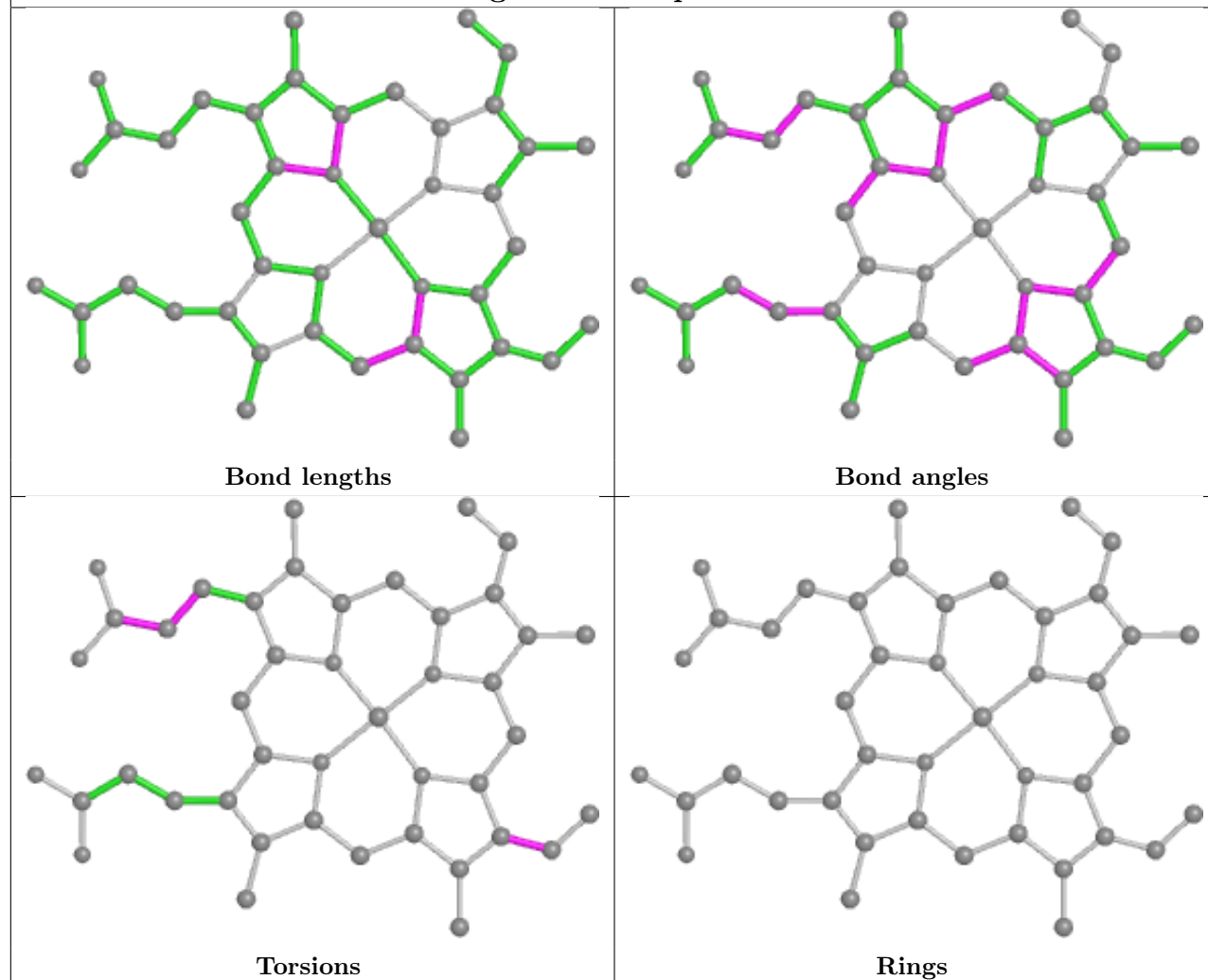




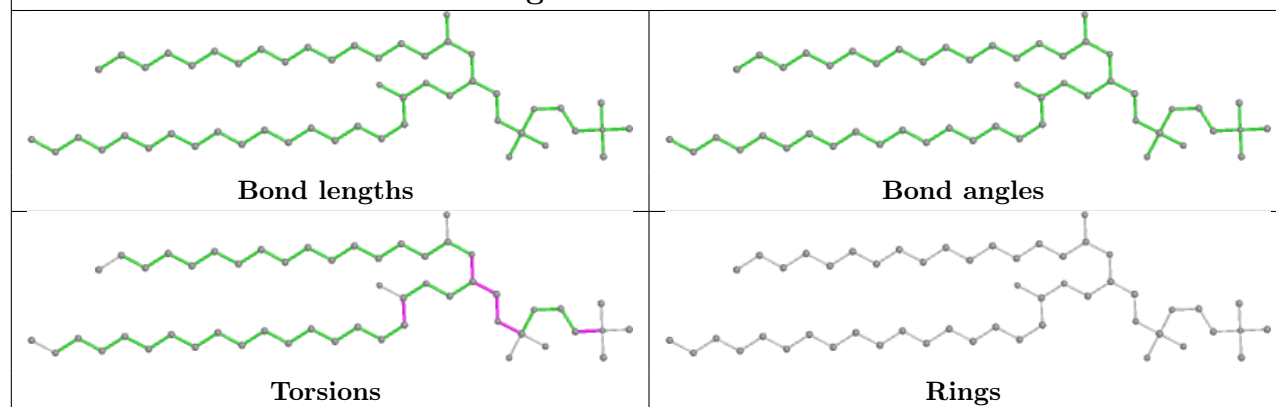


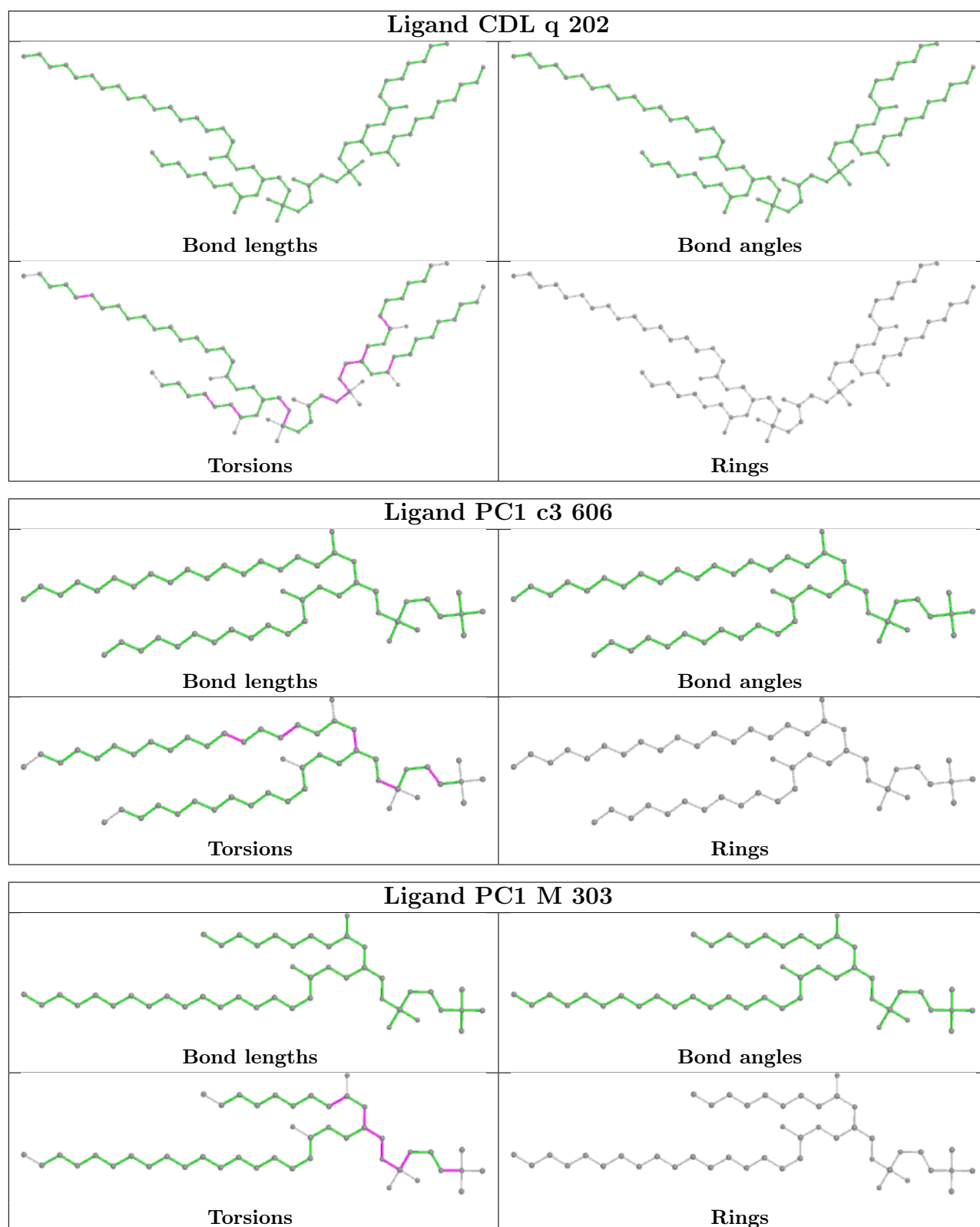


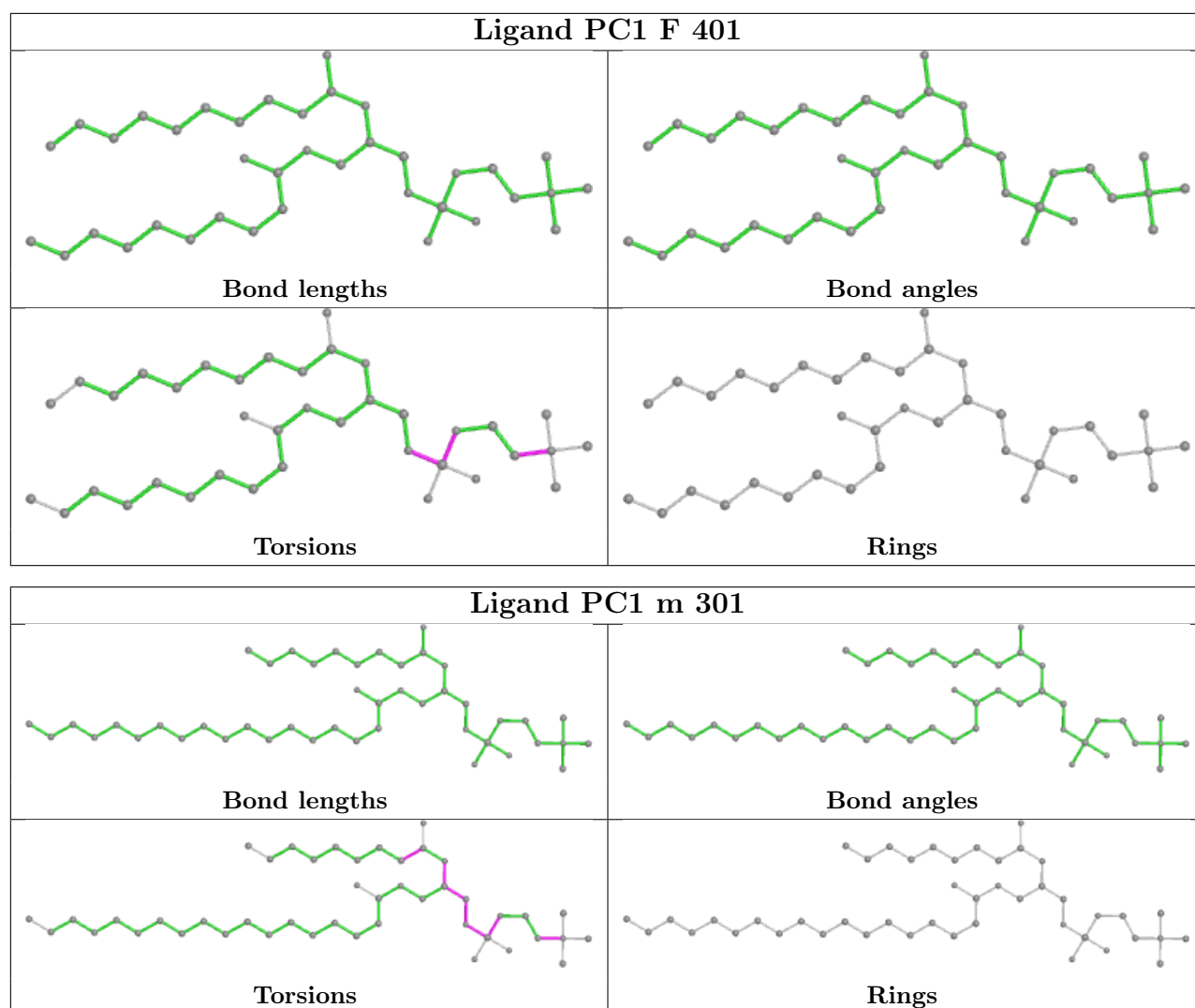
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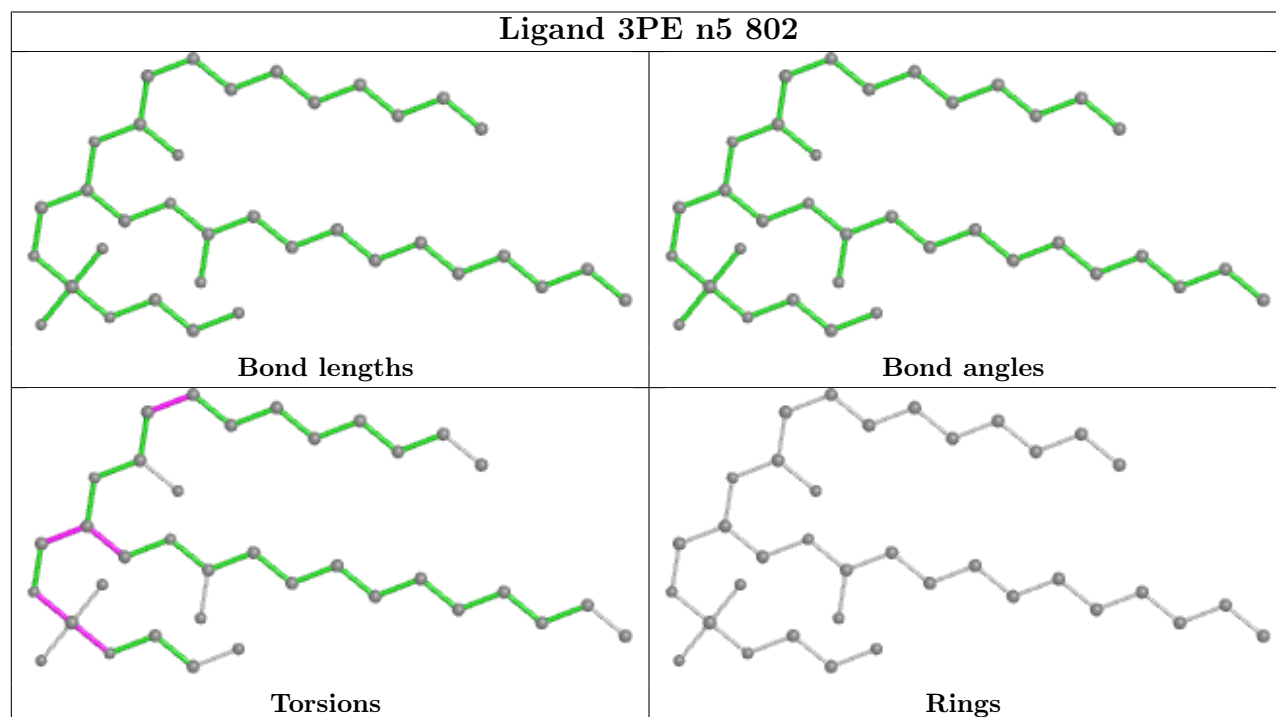
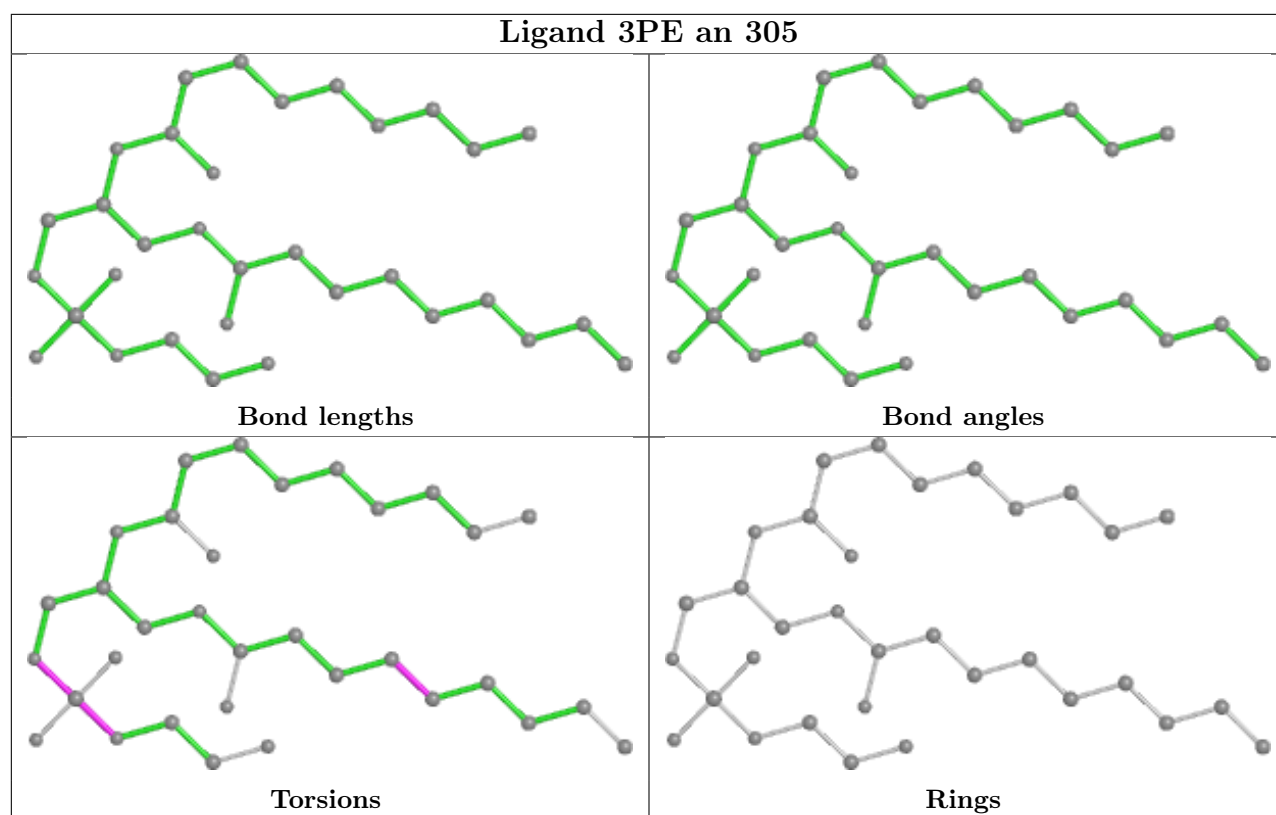


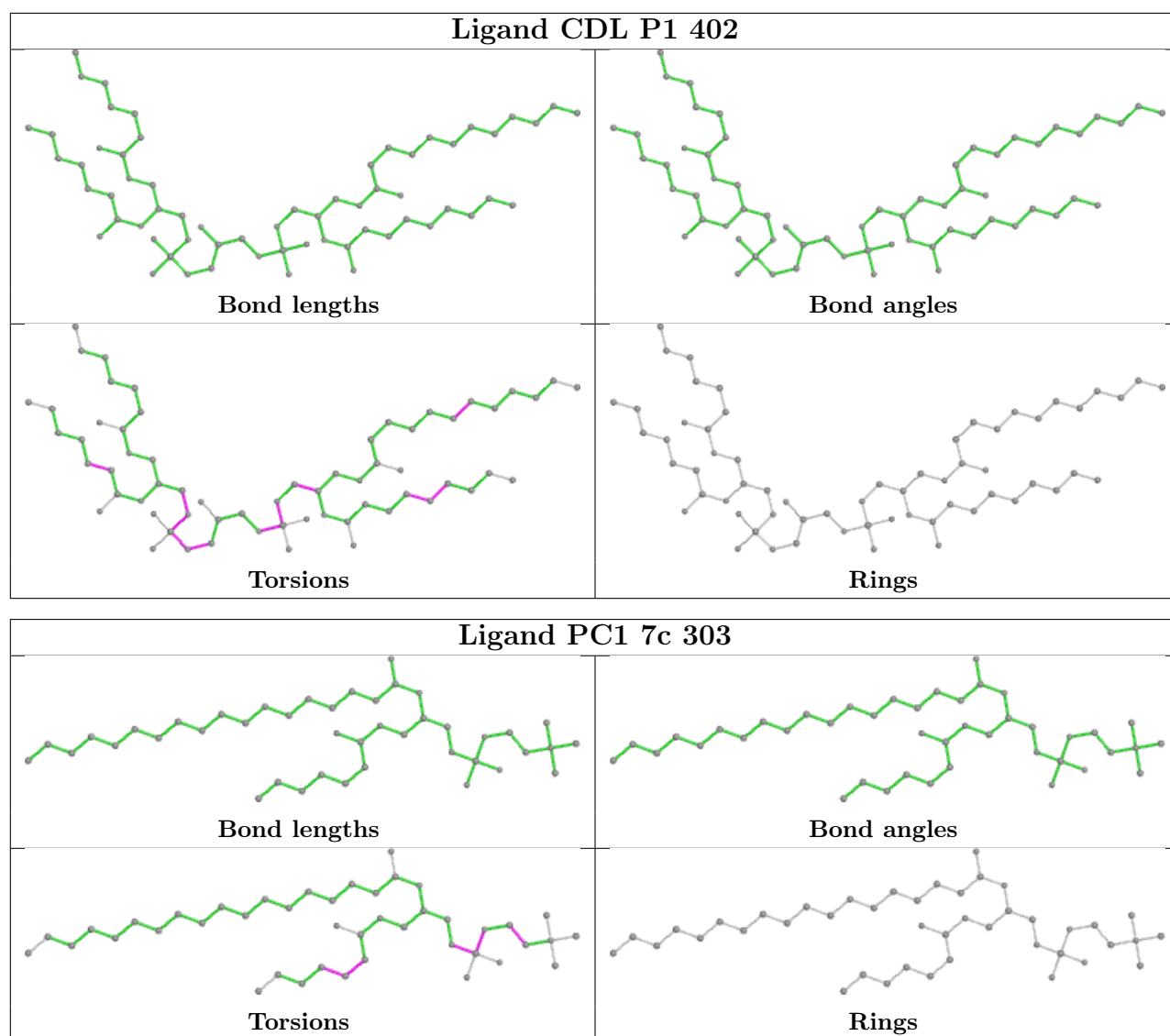
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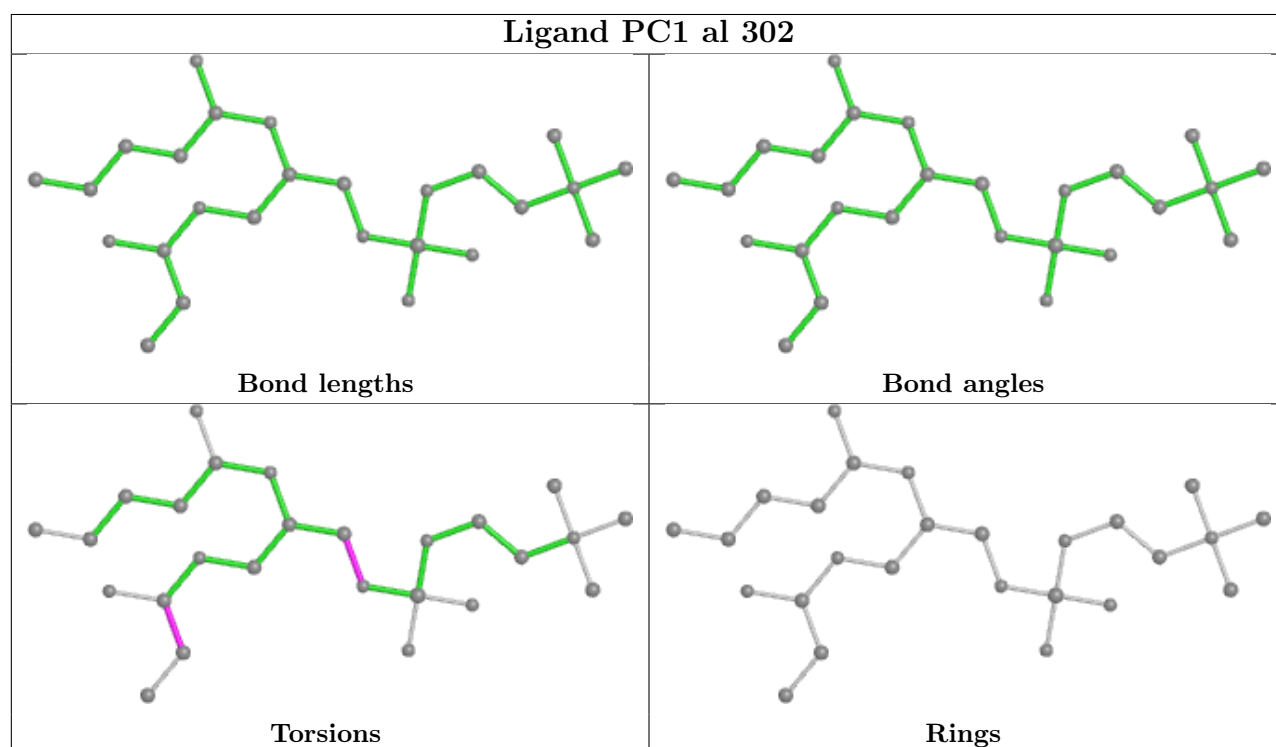
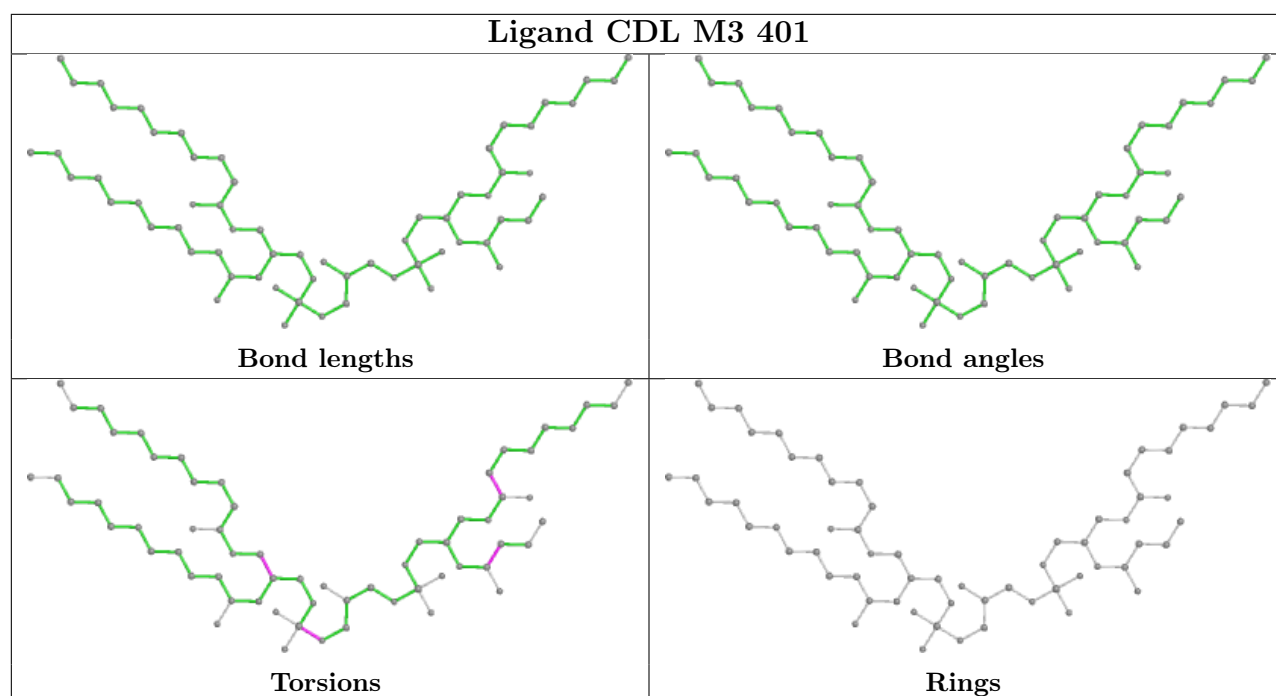


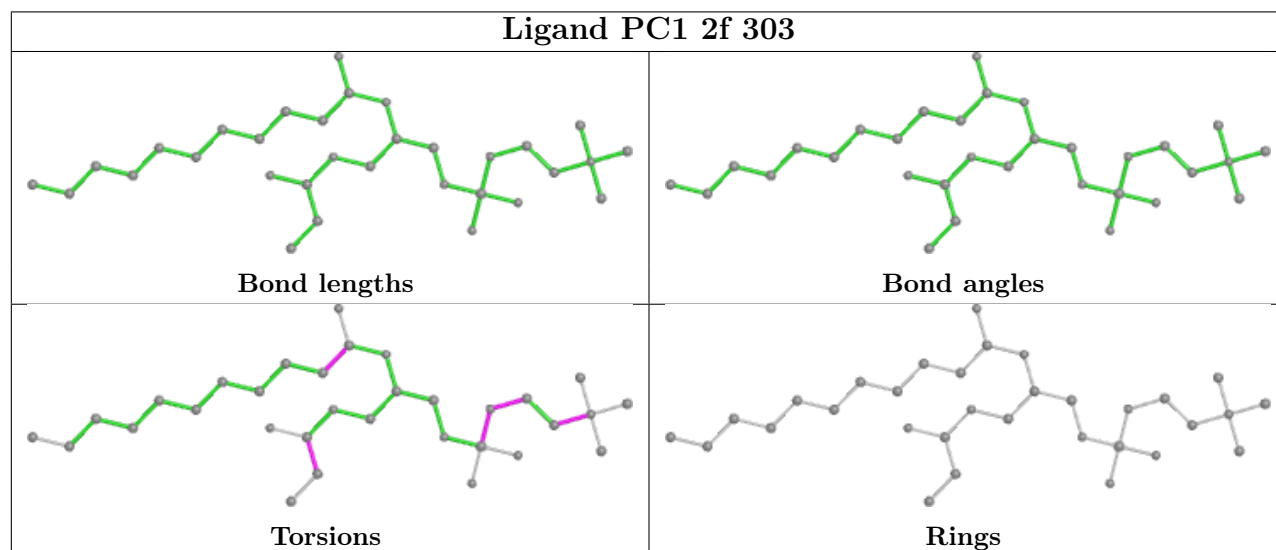
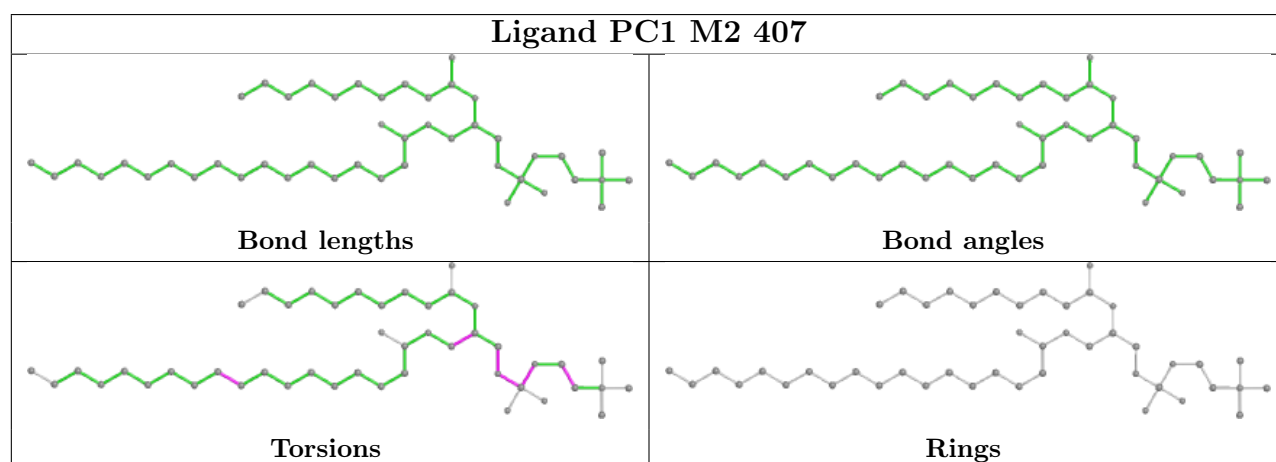
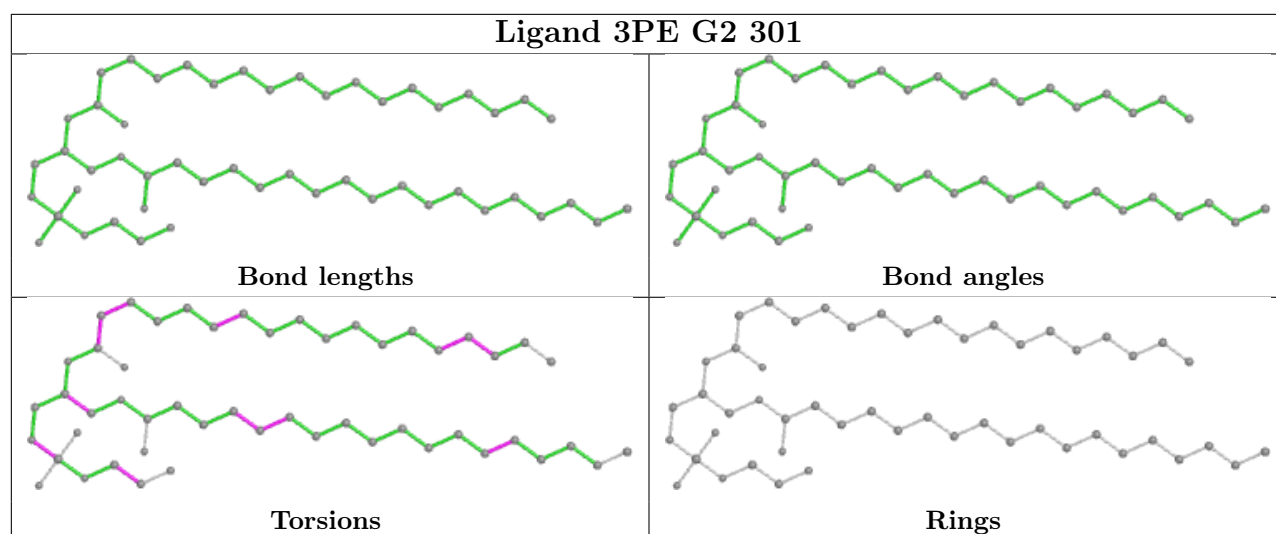


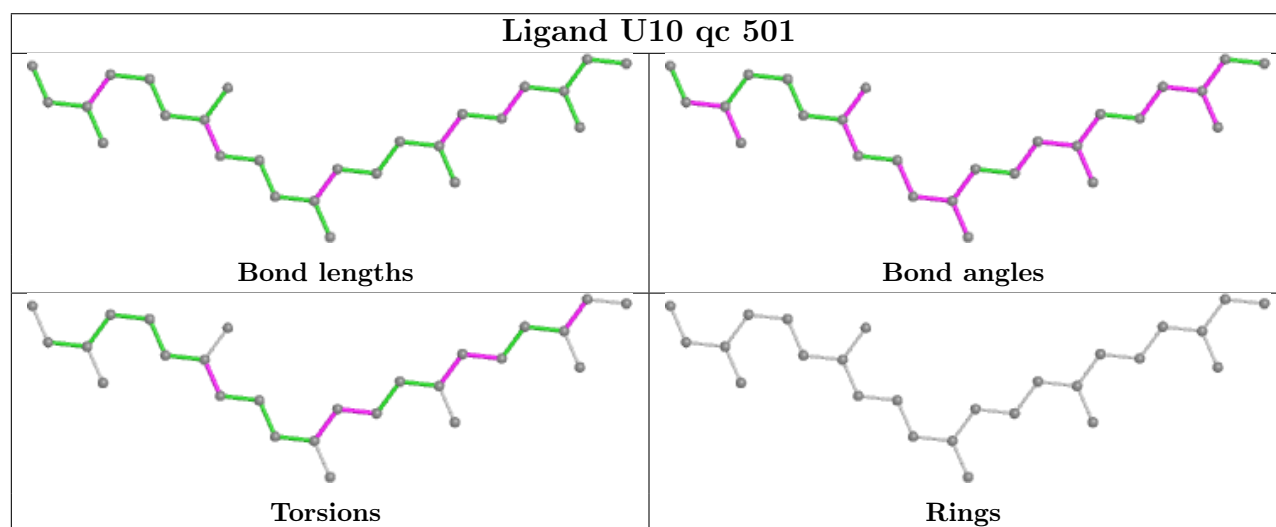
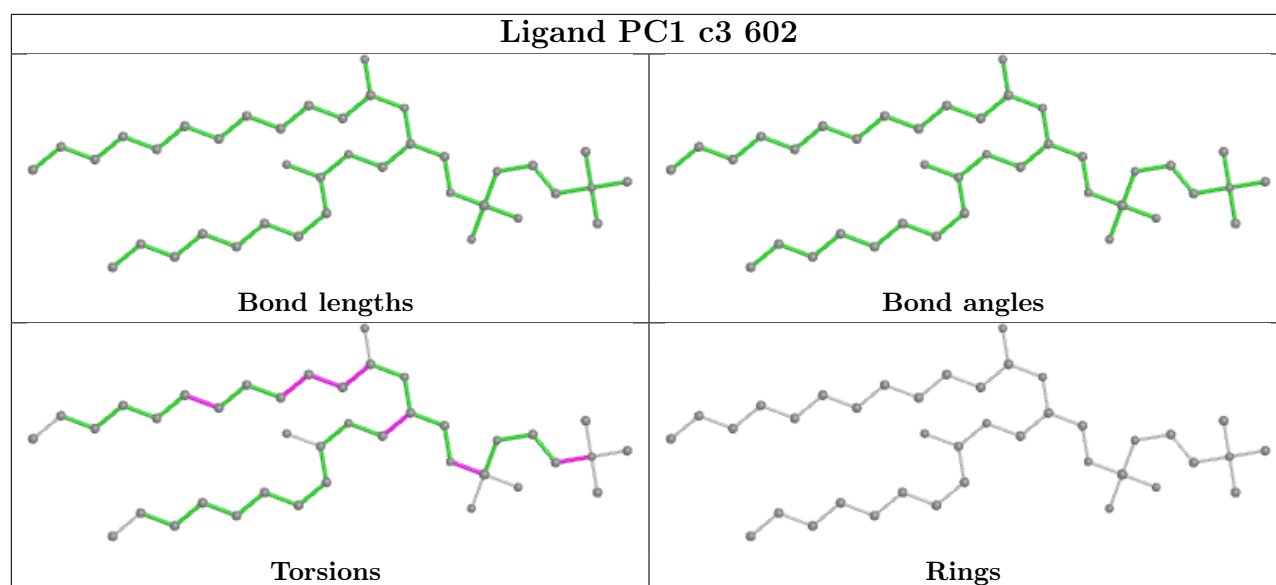


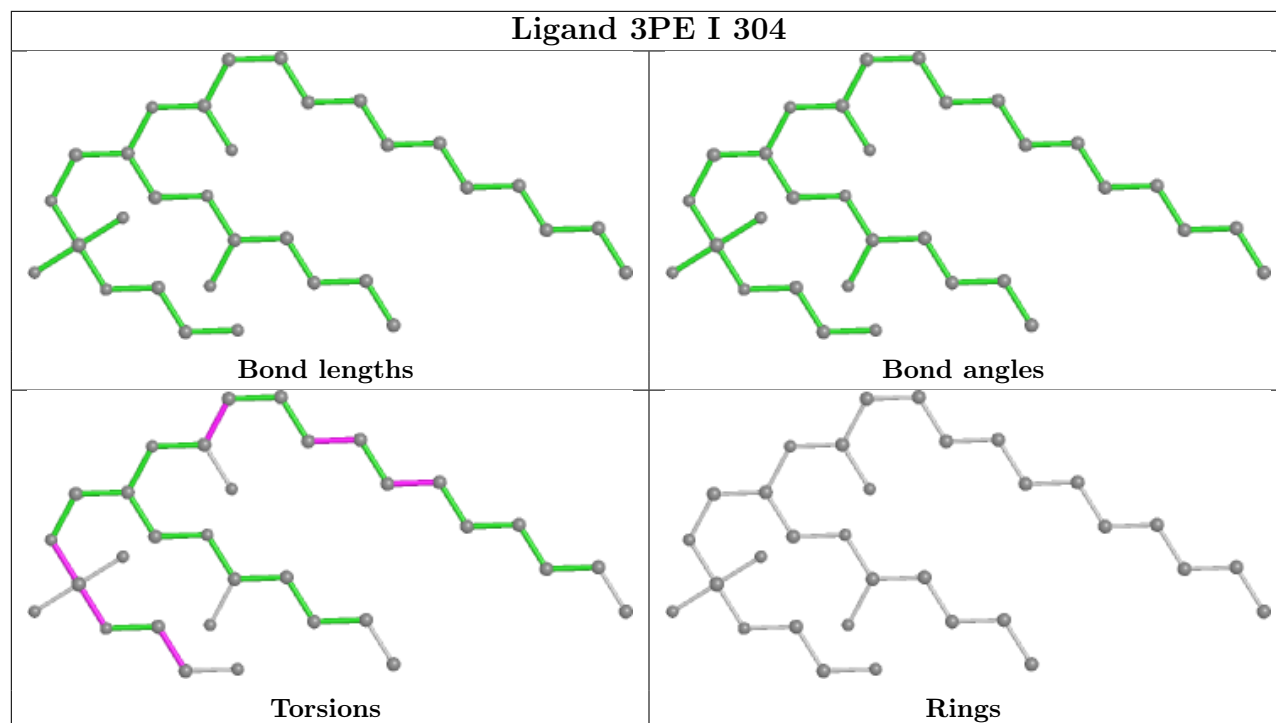
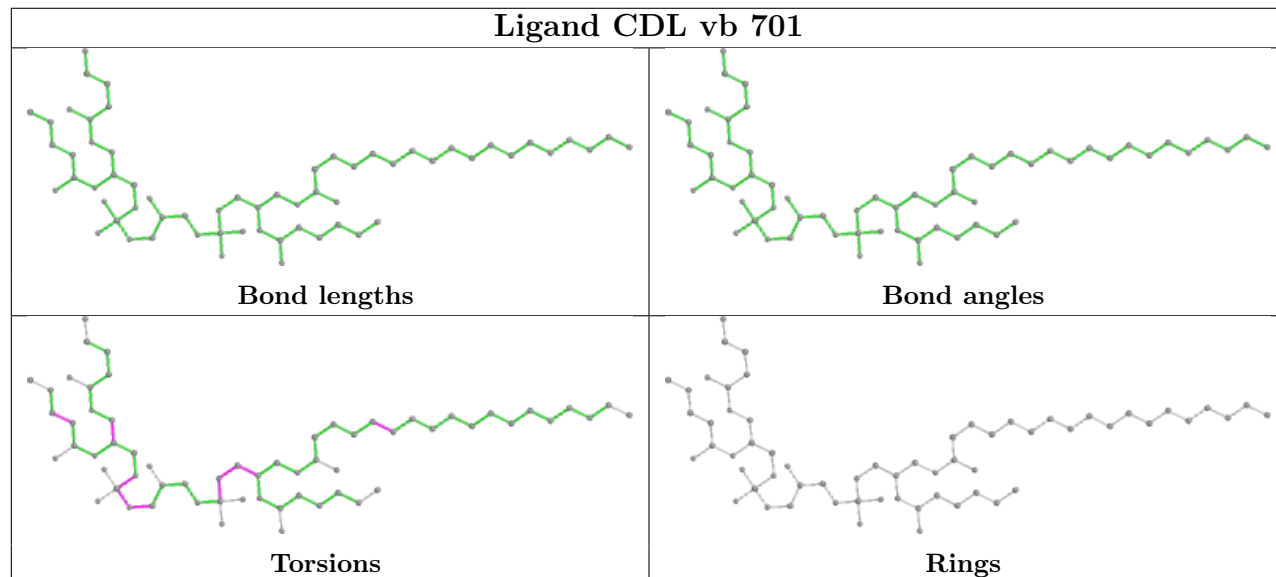


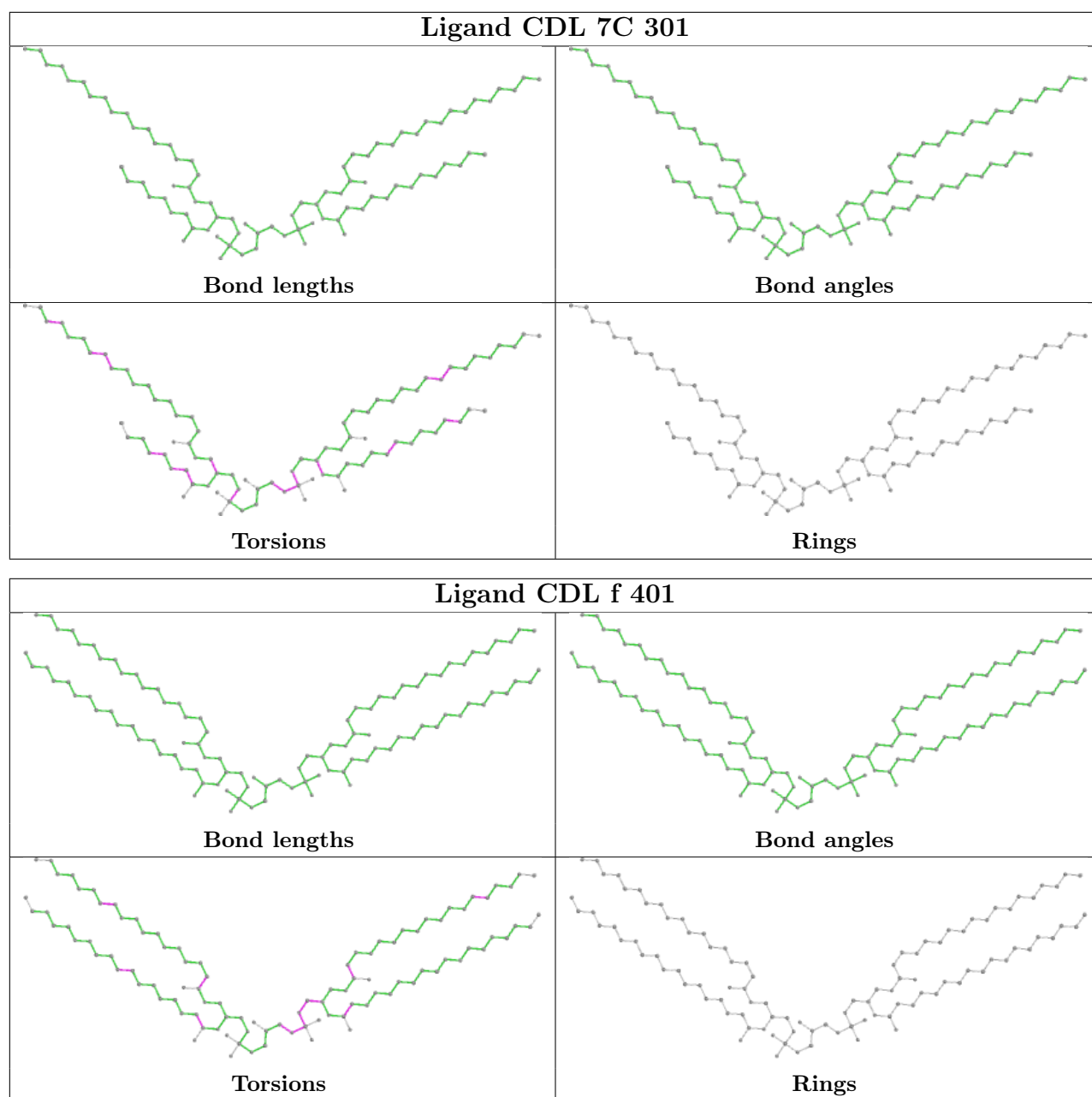


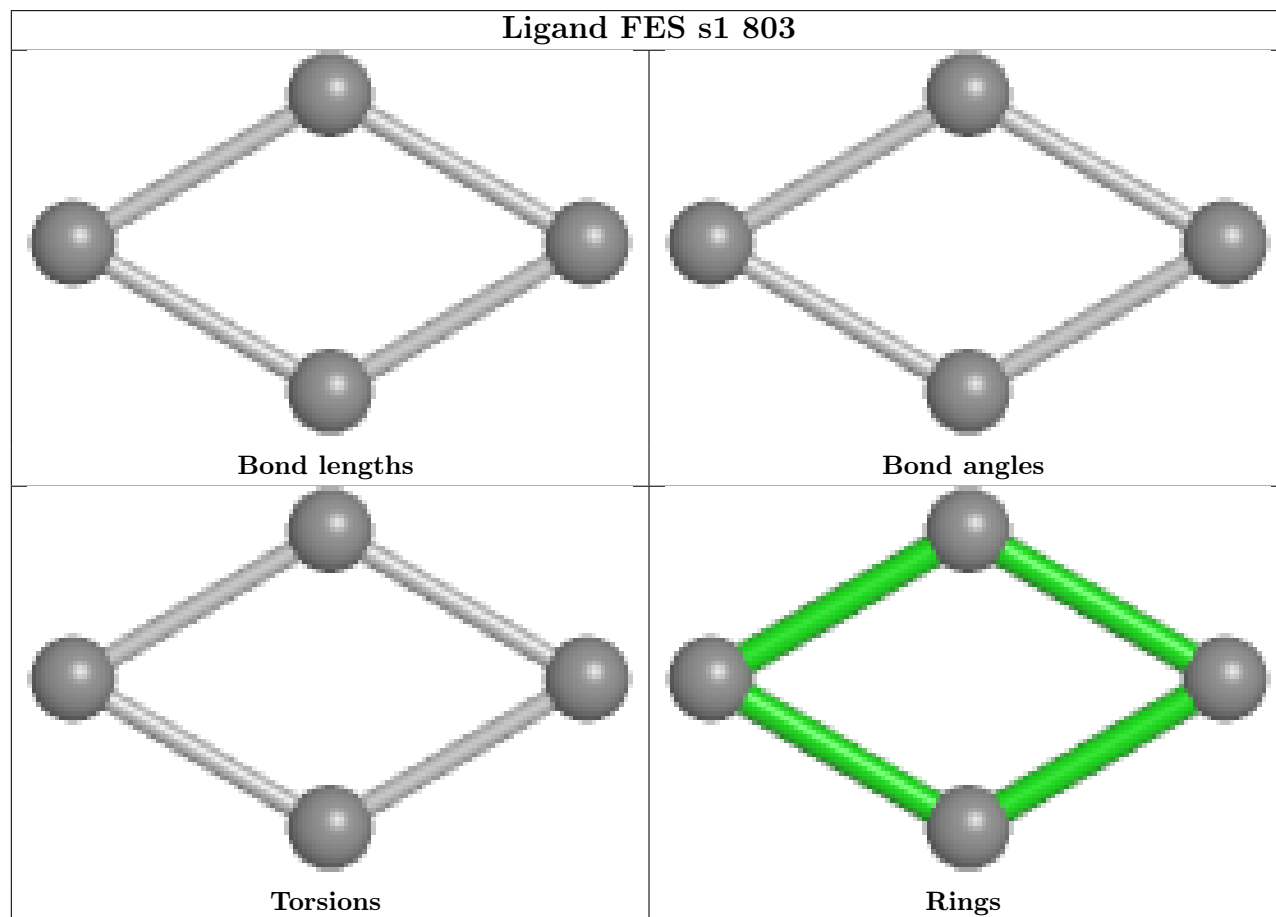
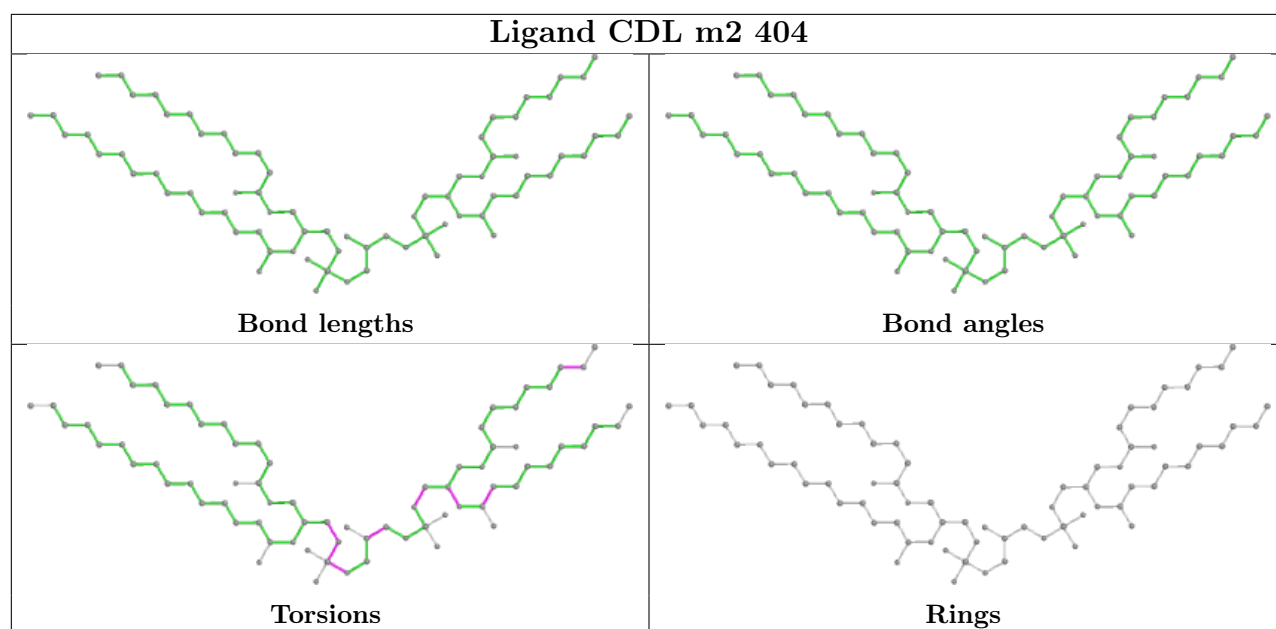


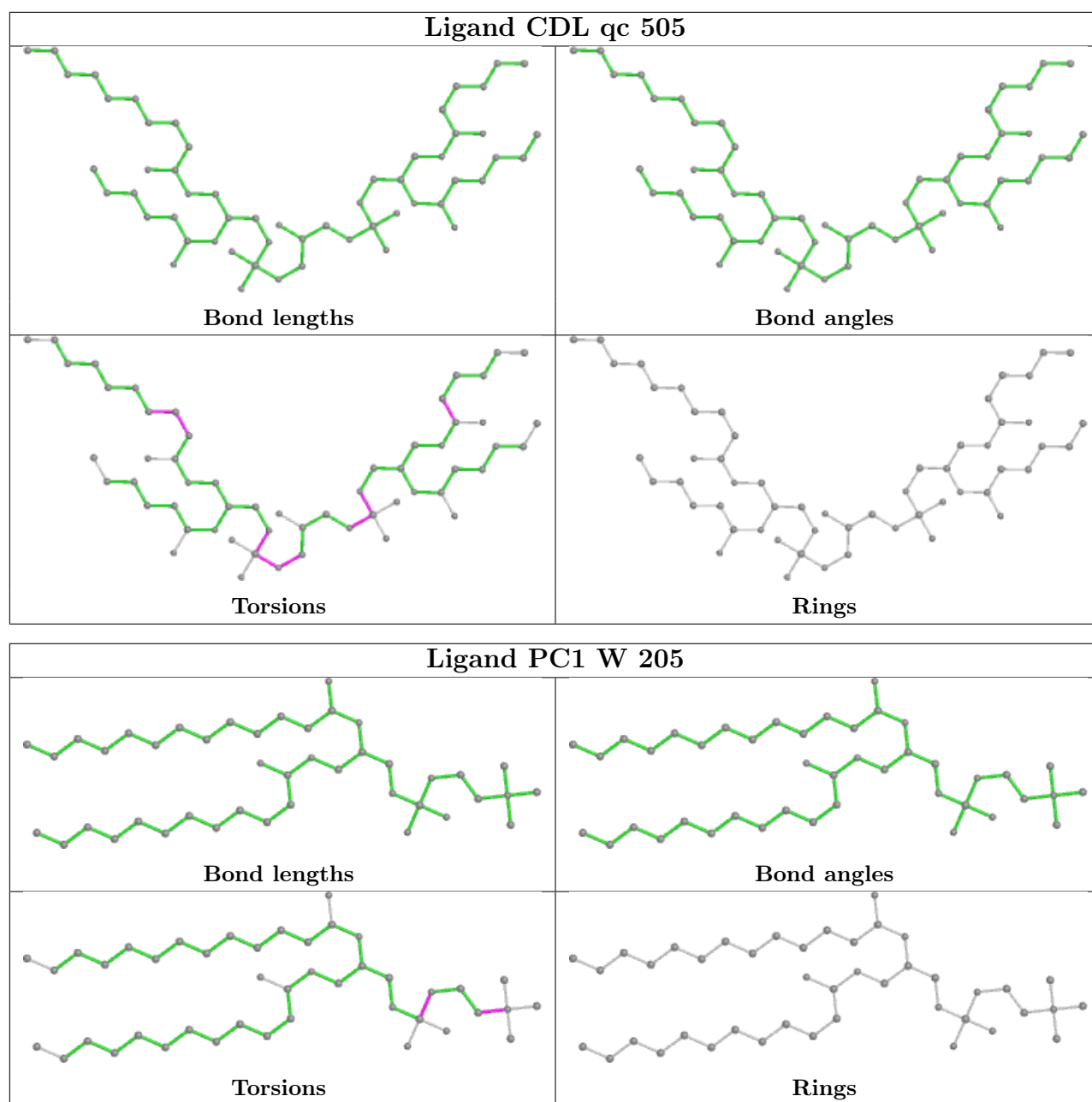


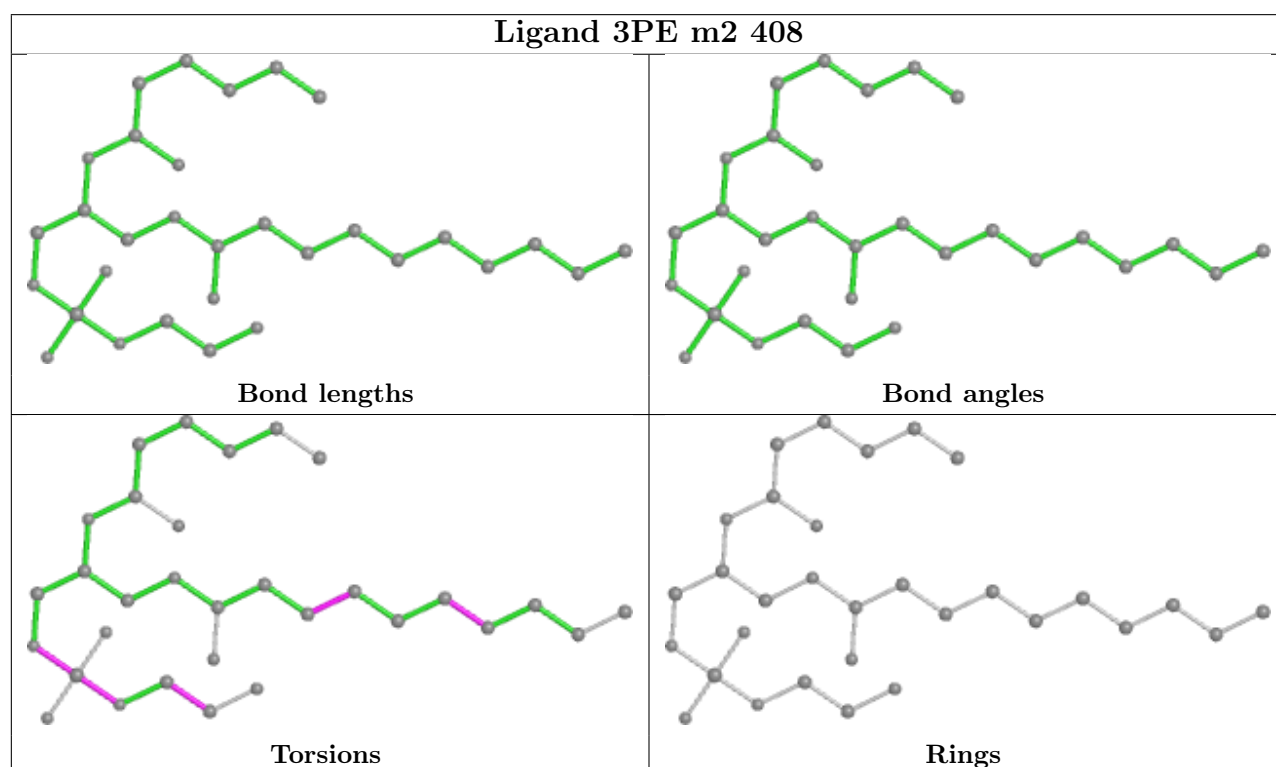
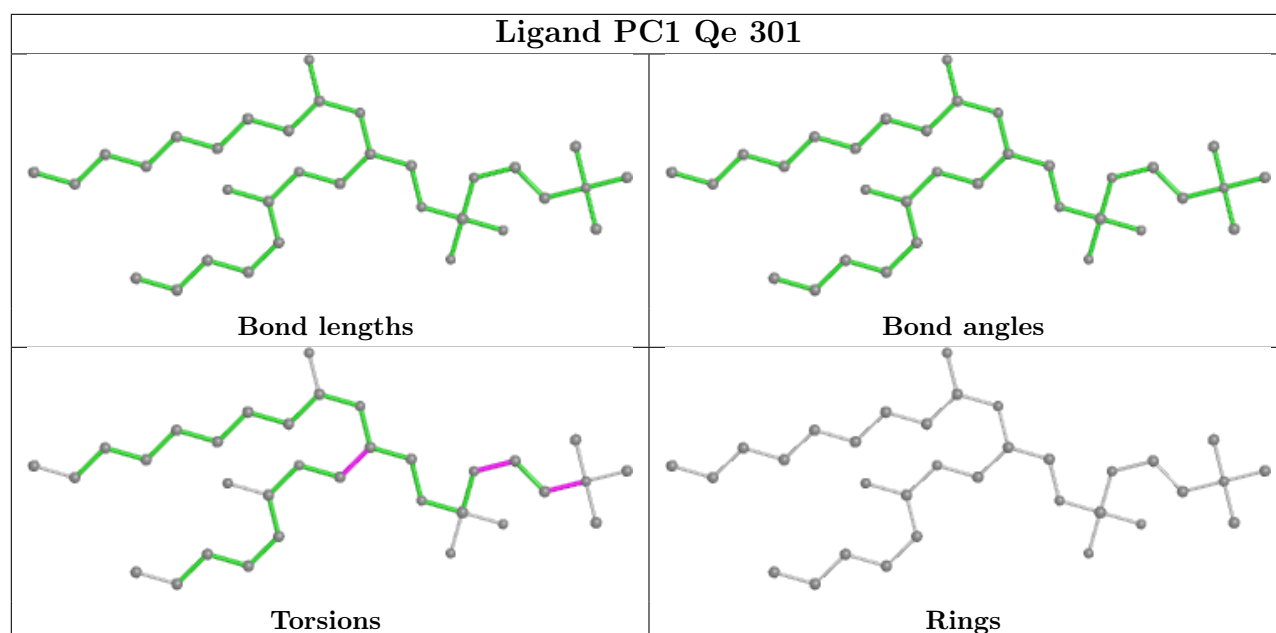


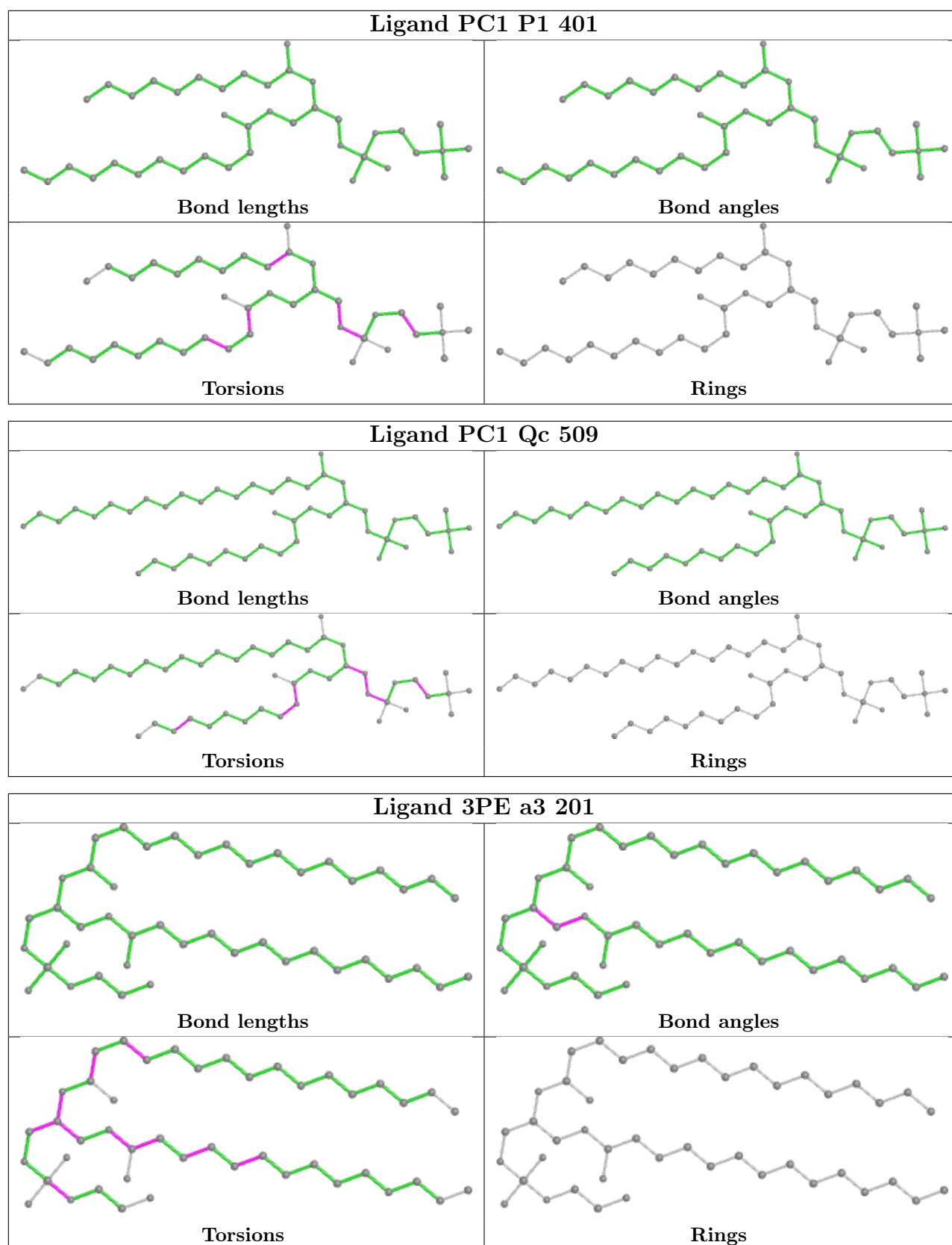
Ligand 3PE I 304**Ligand CDL vb 701**

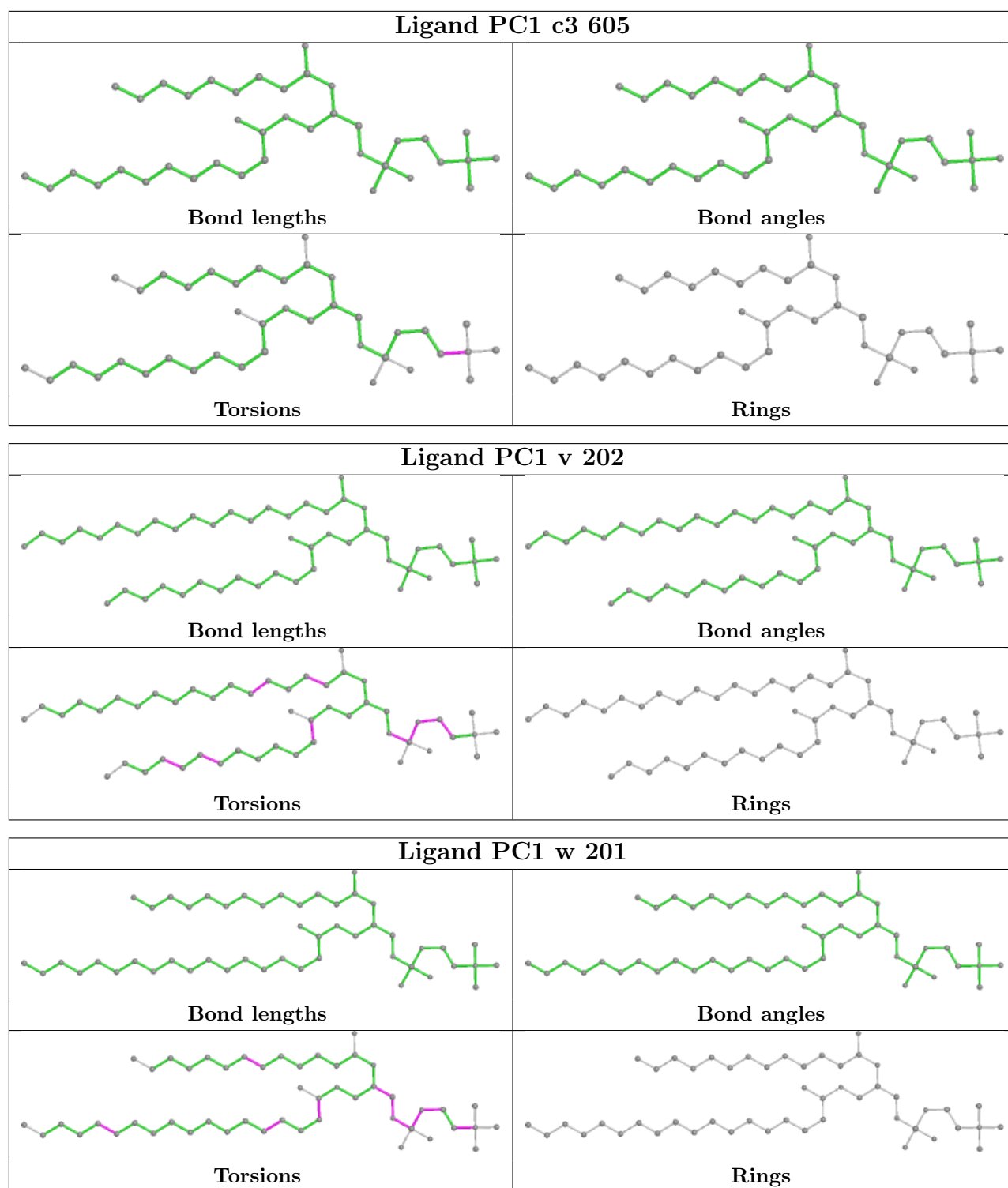


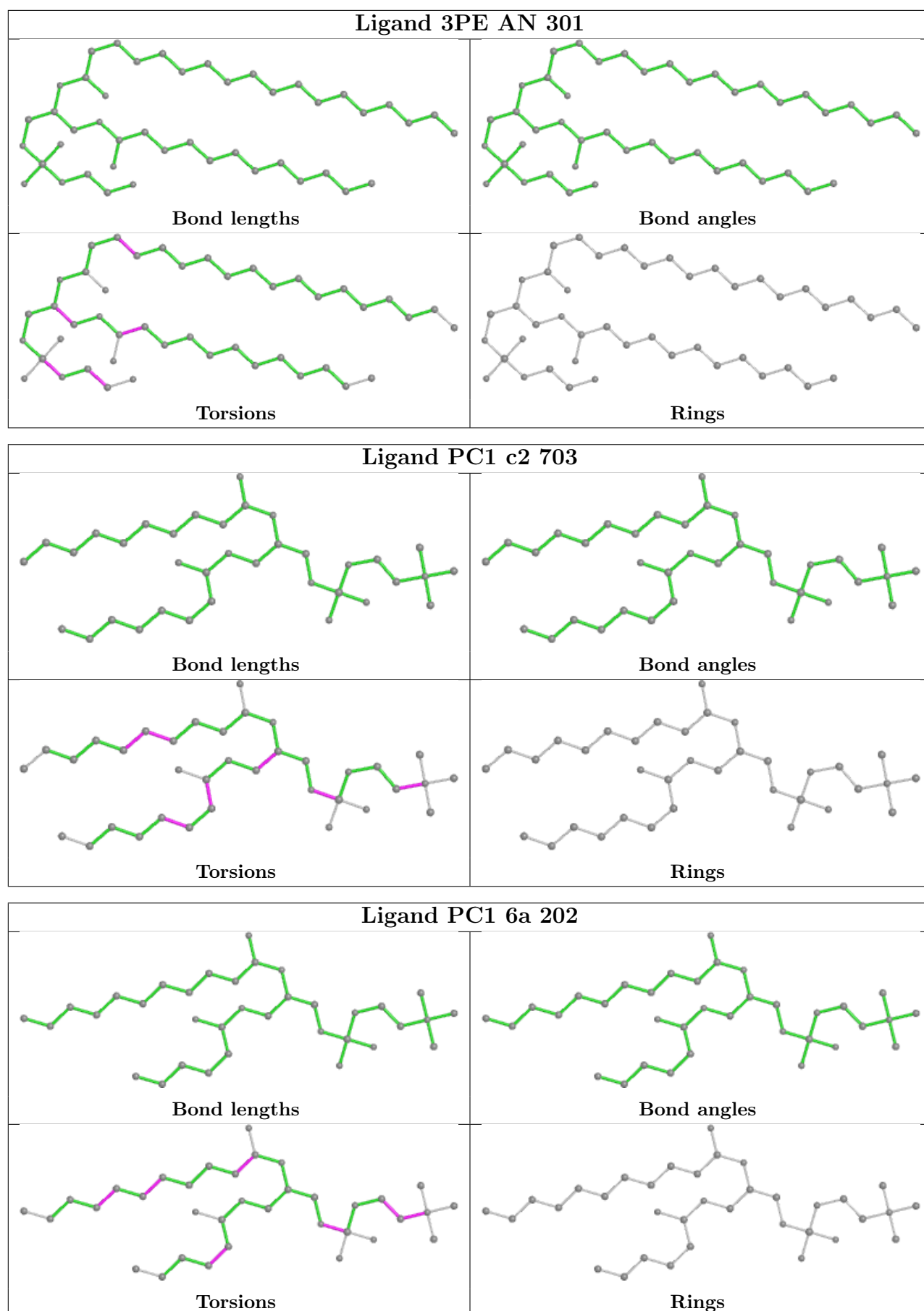


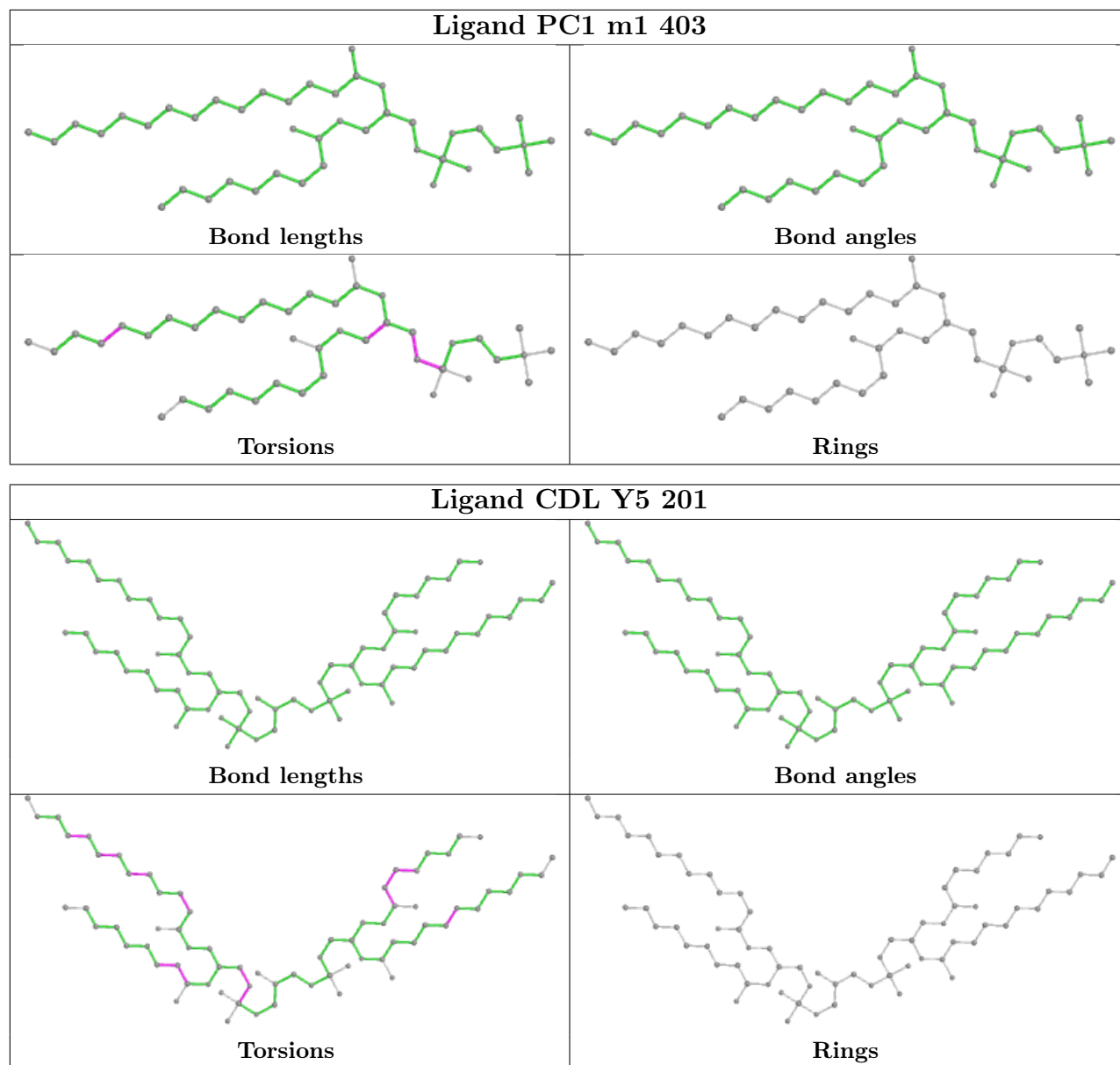


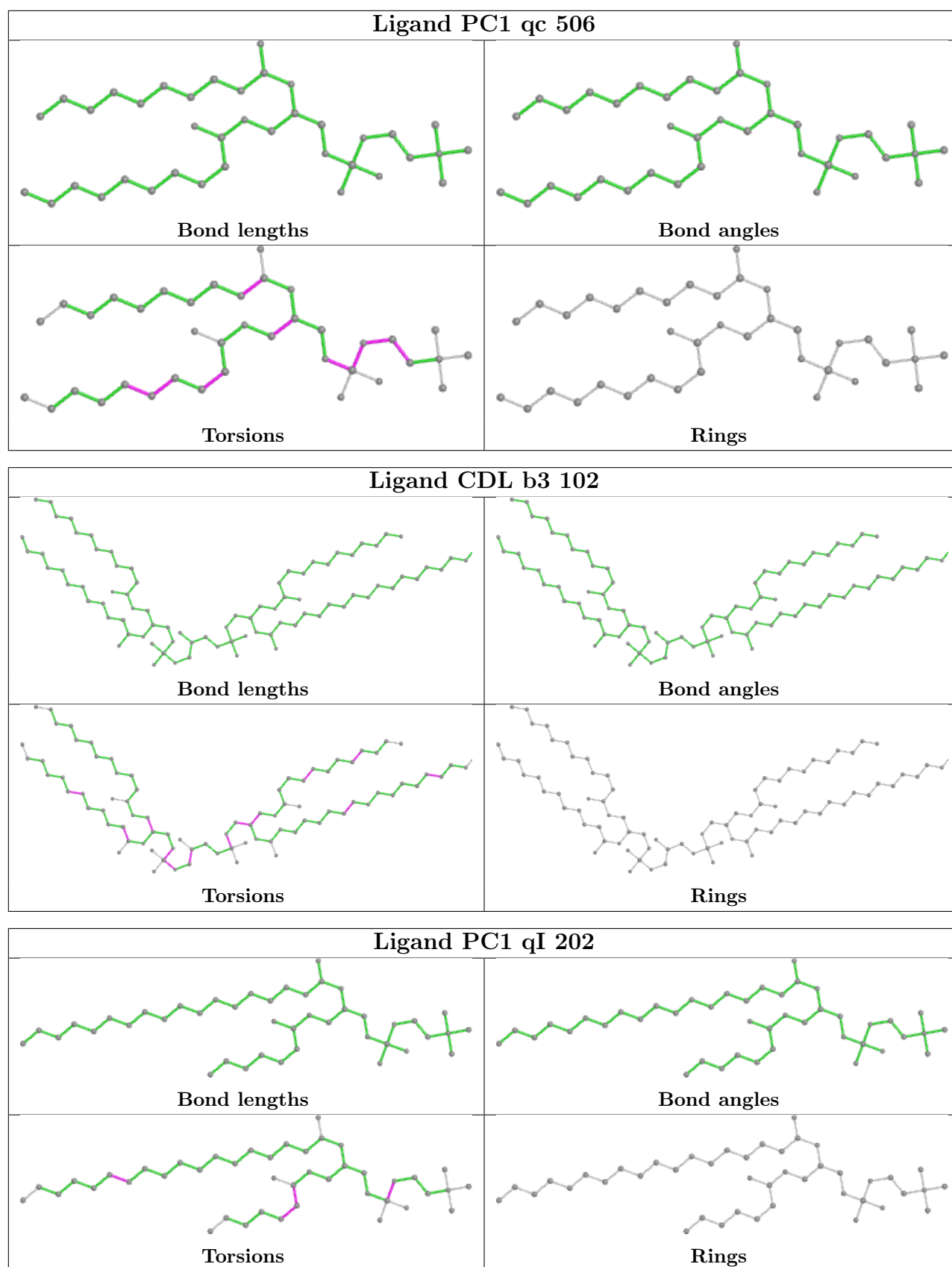


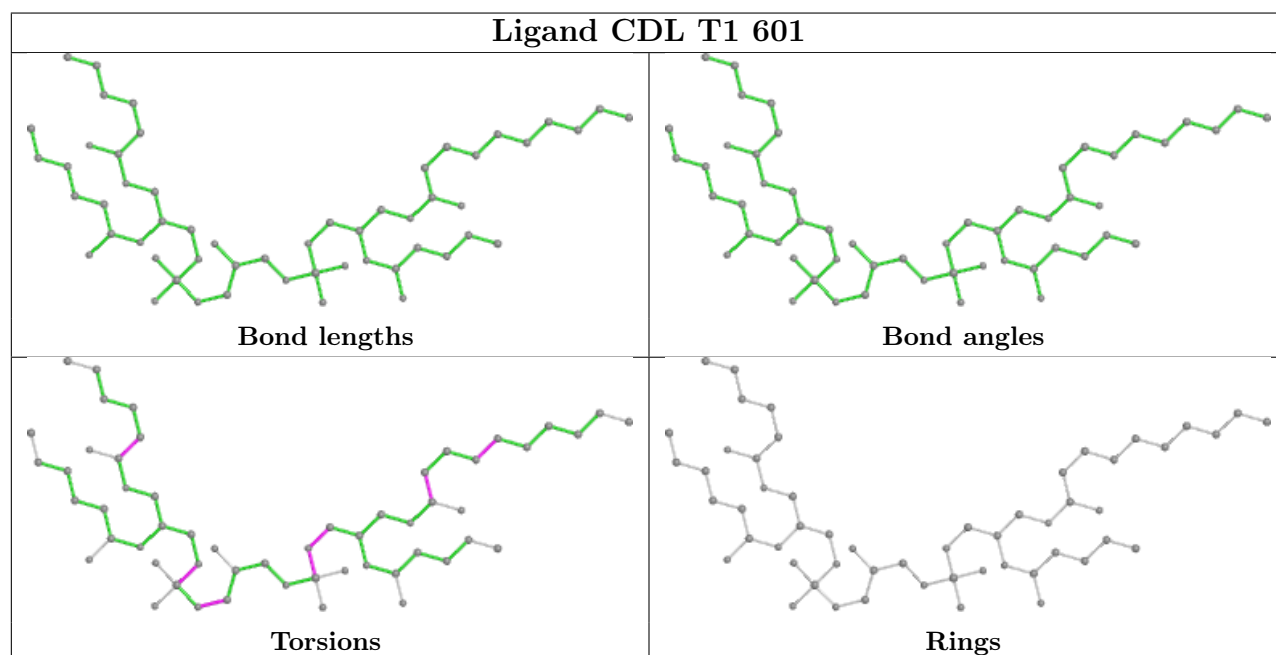
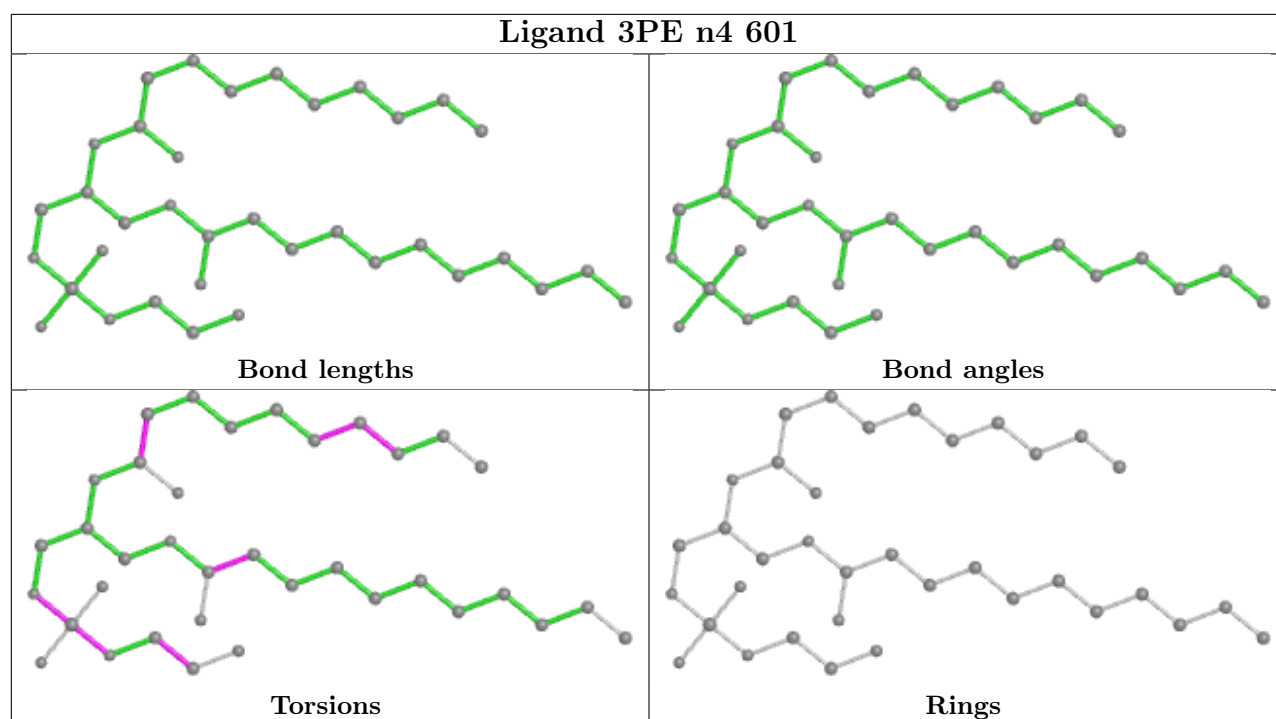


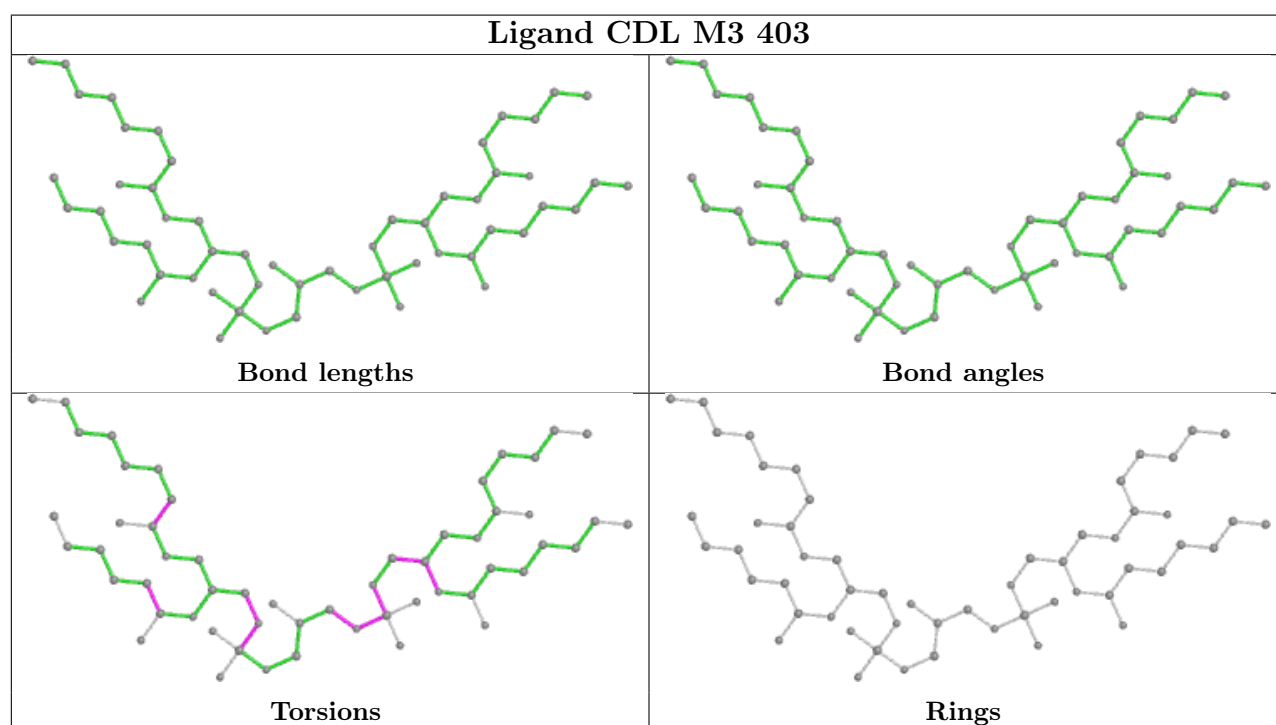
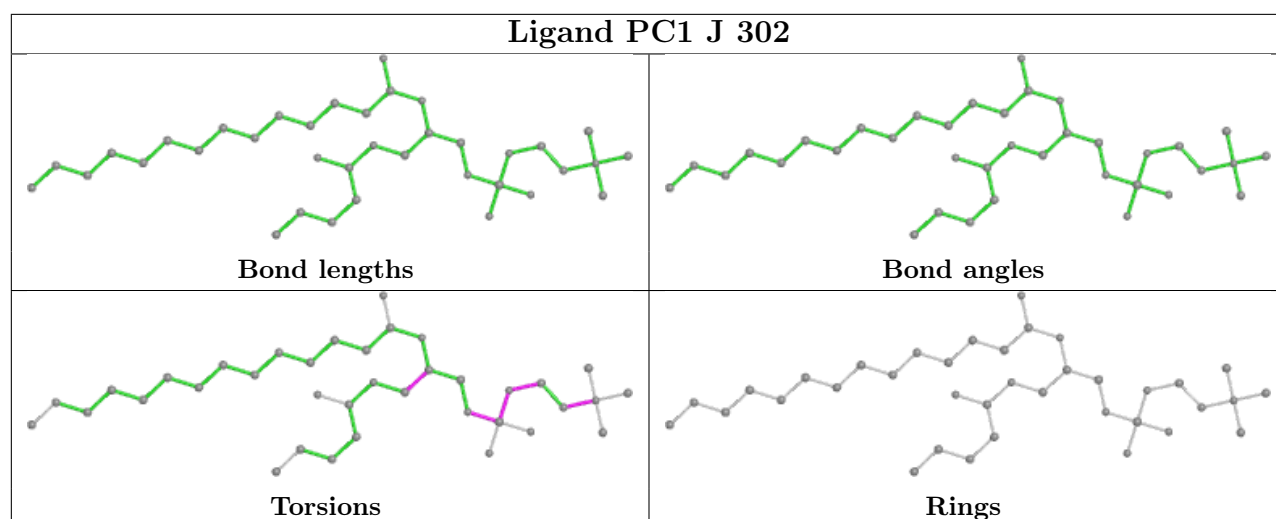


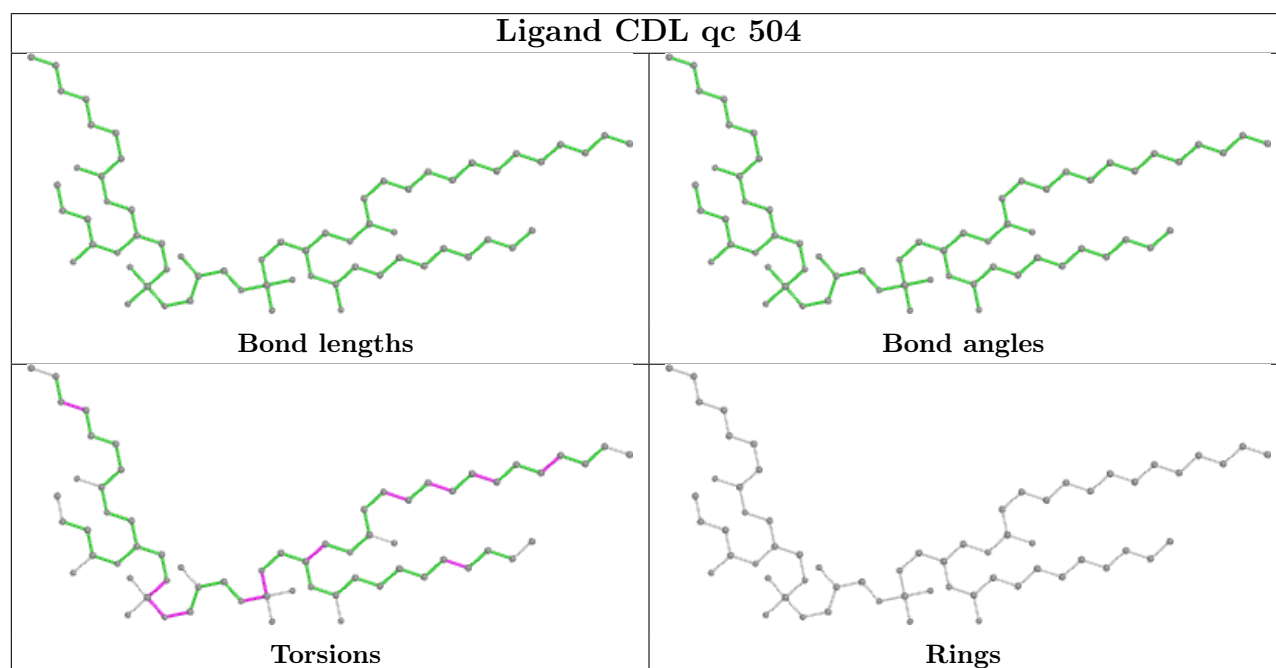
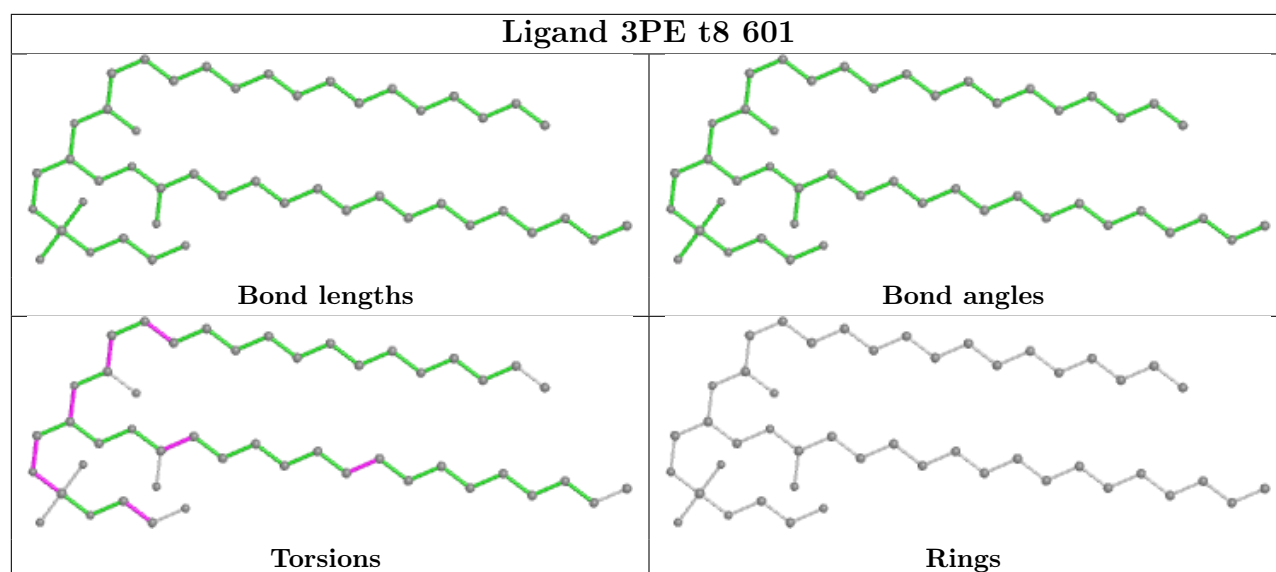


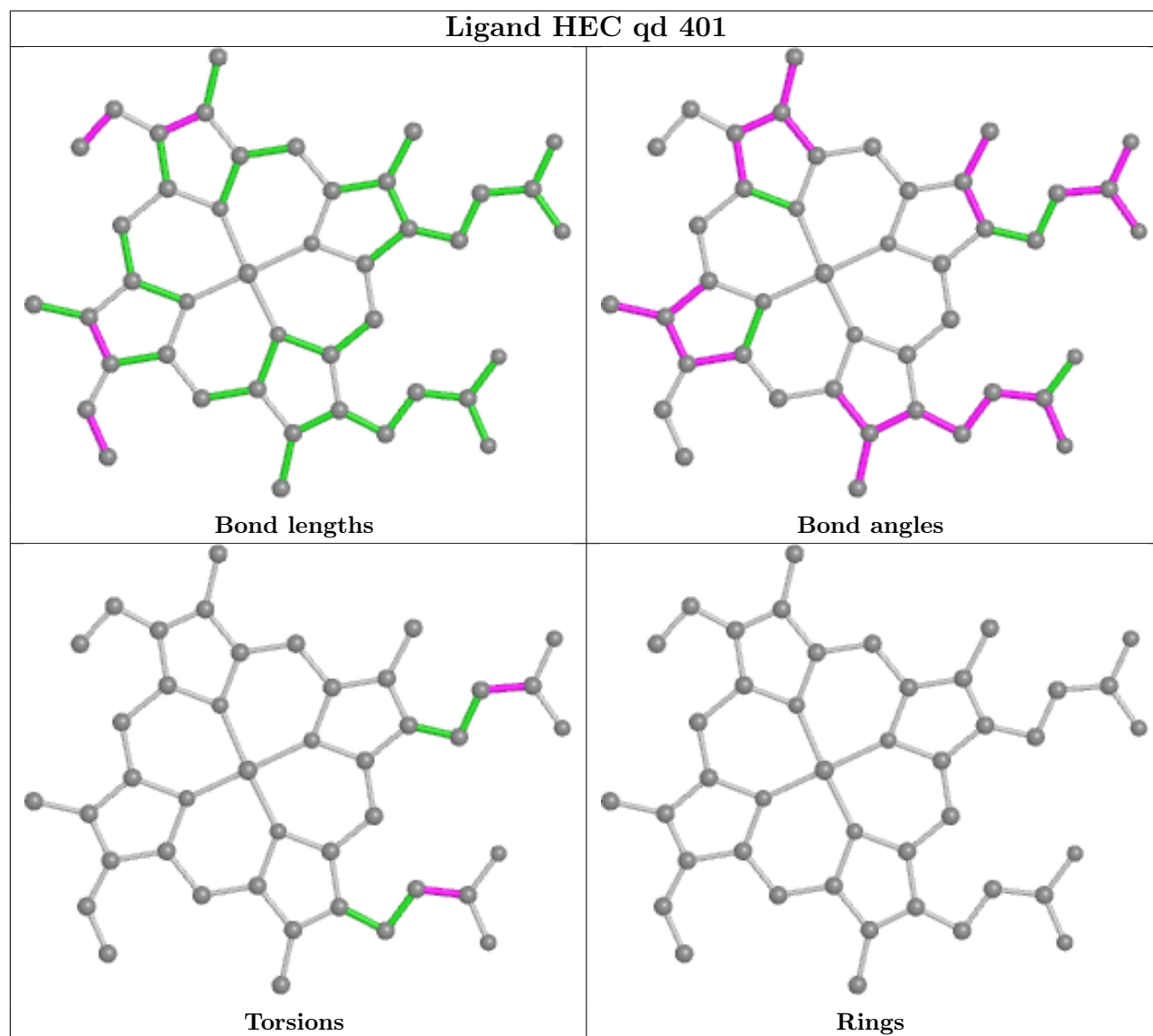
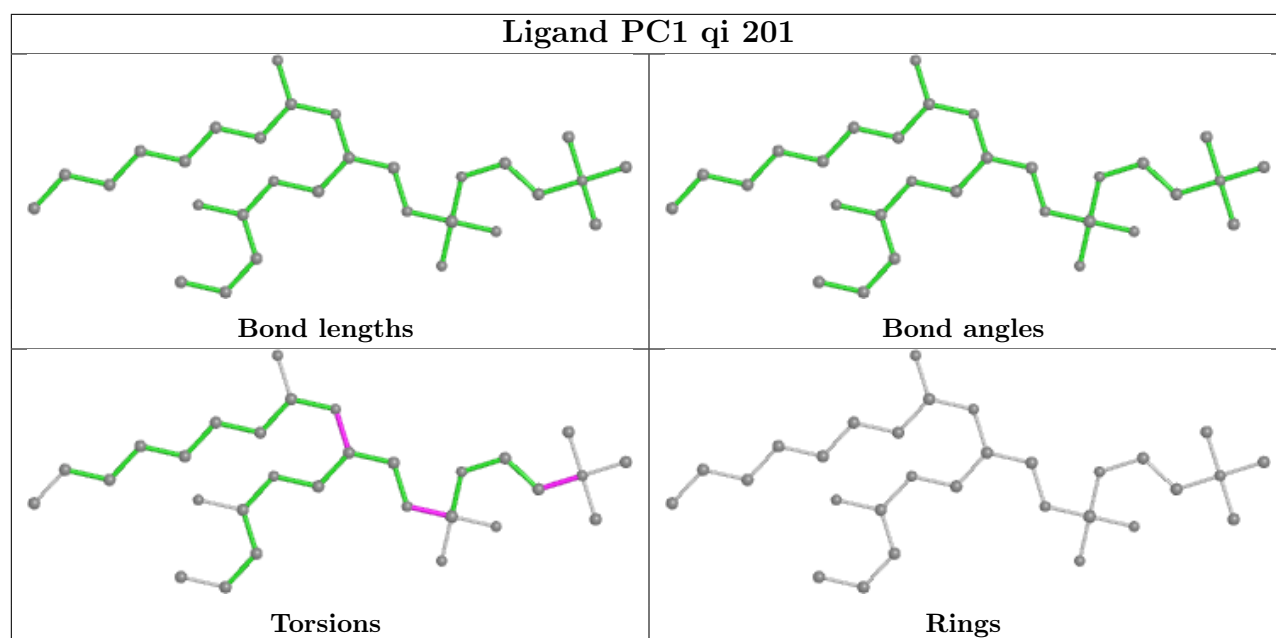


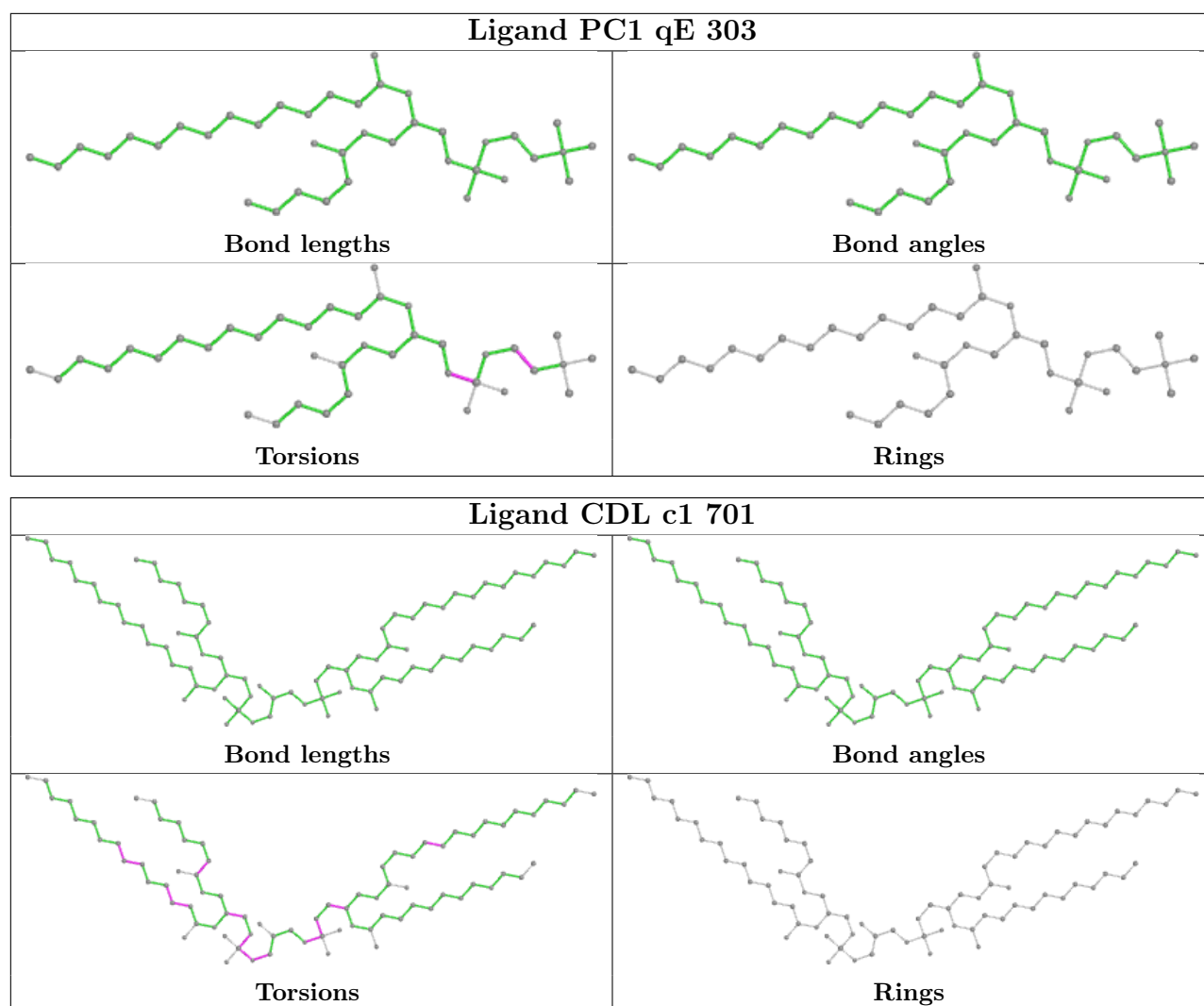




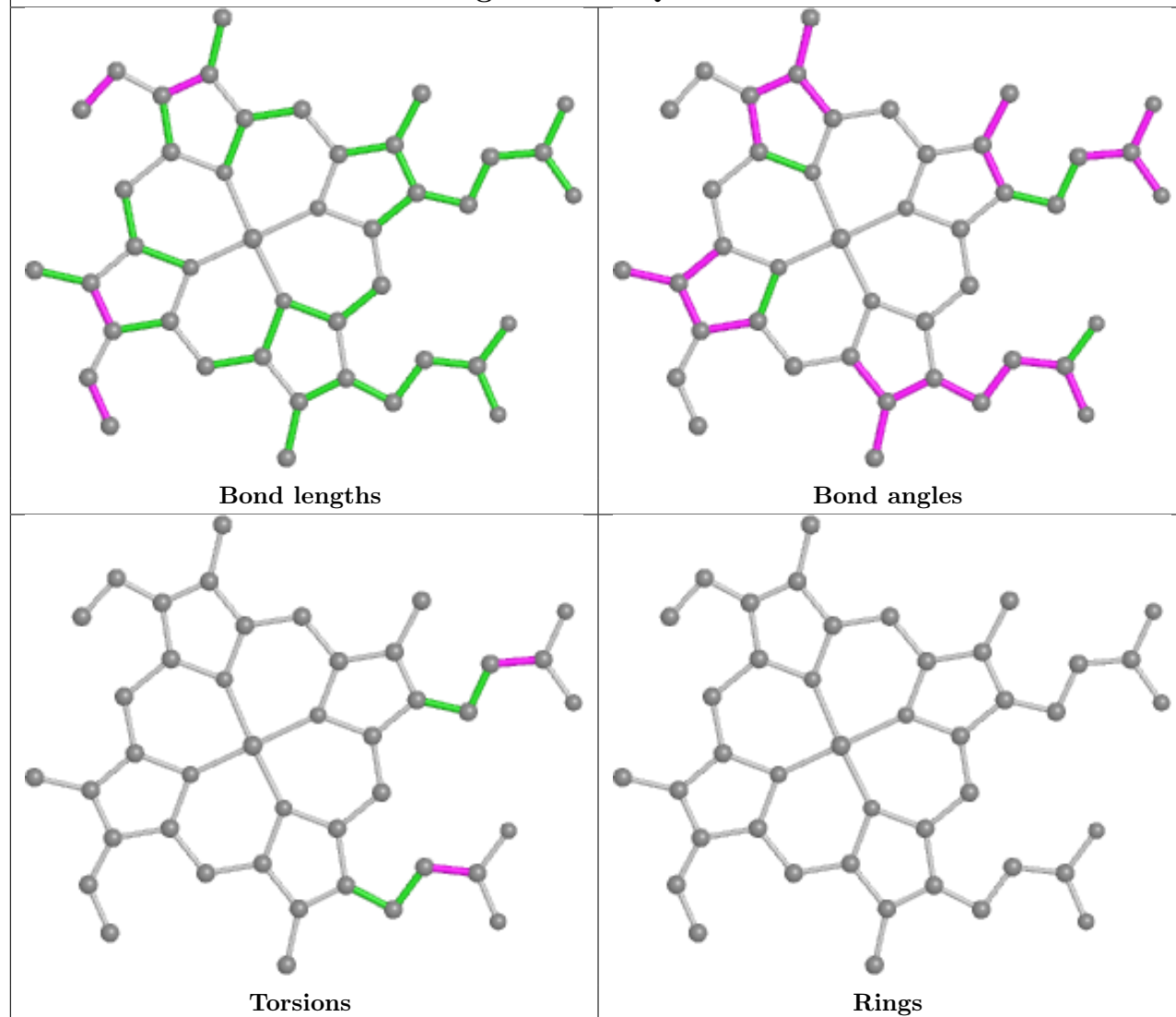




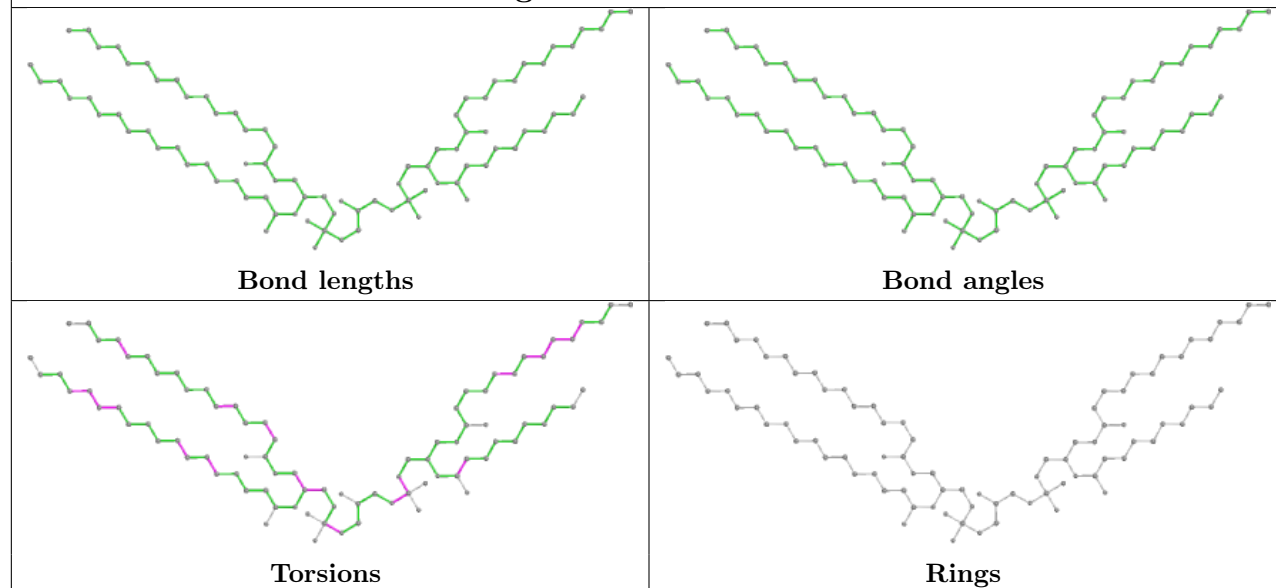


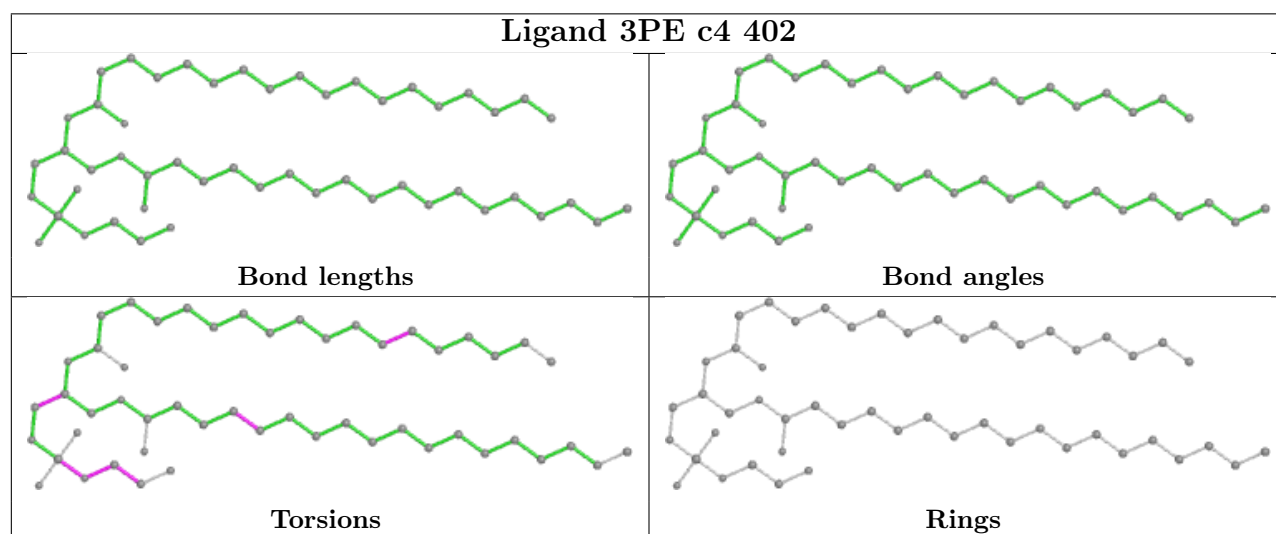
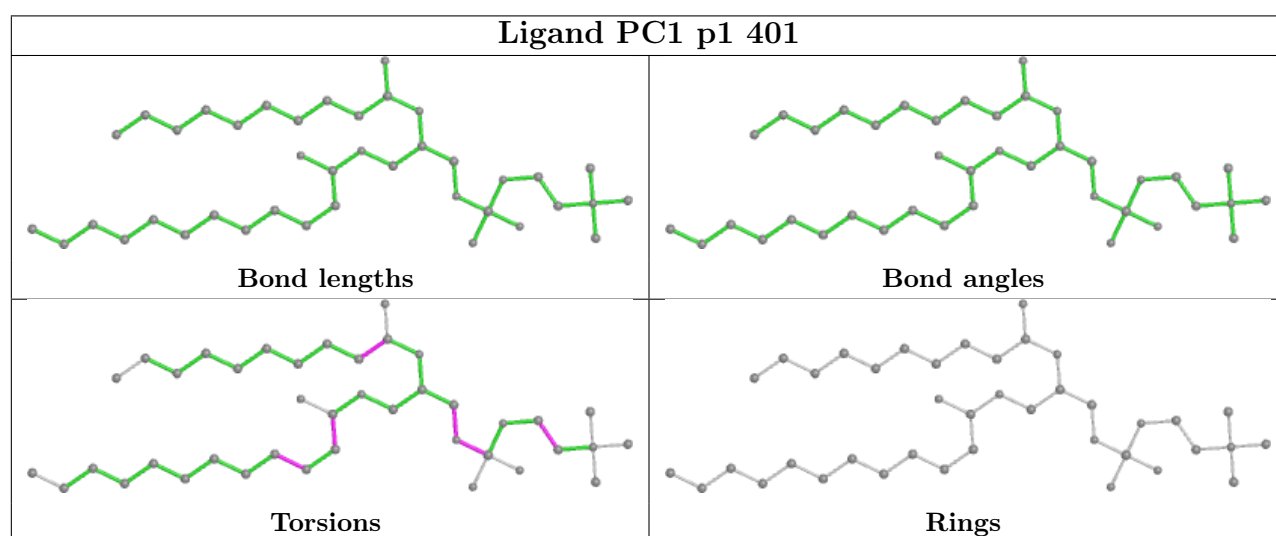
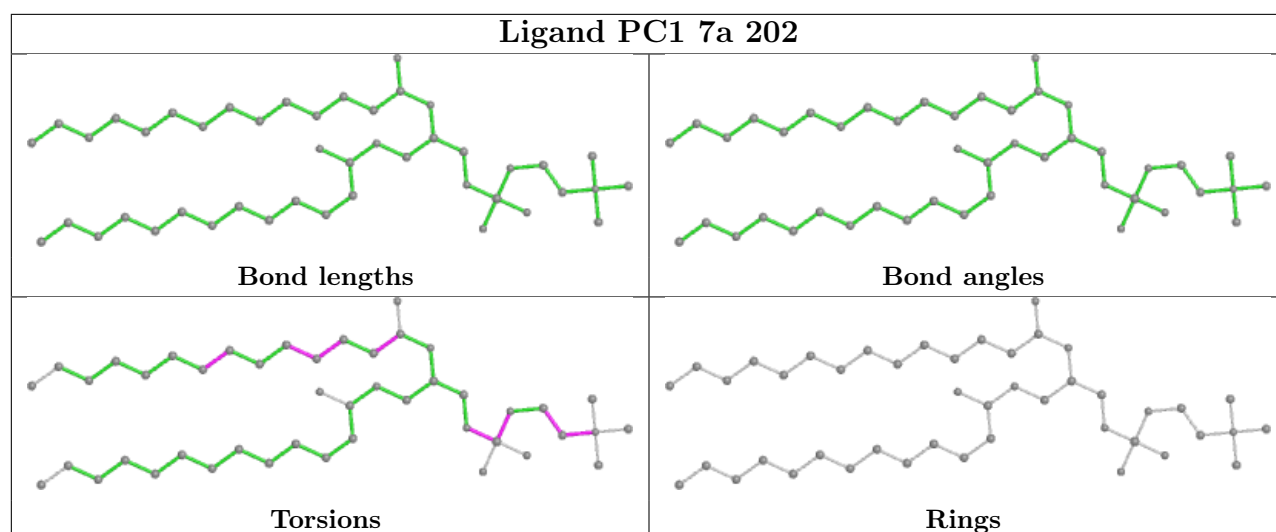


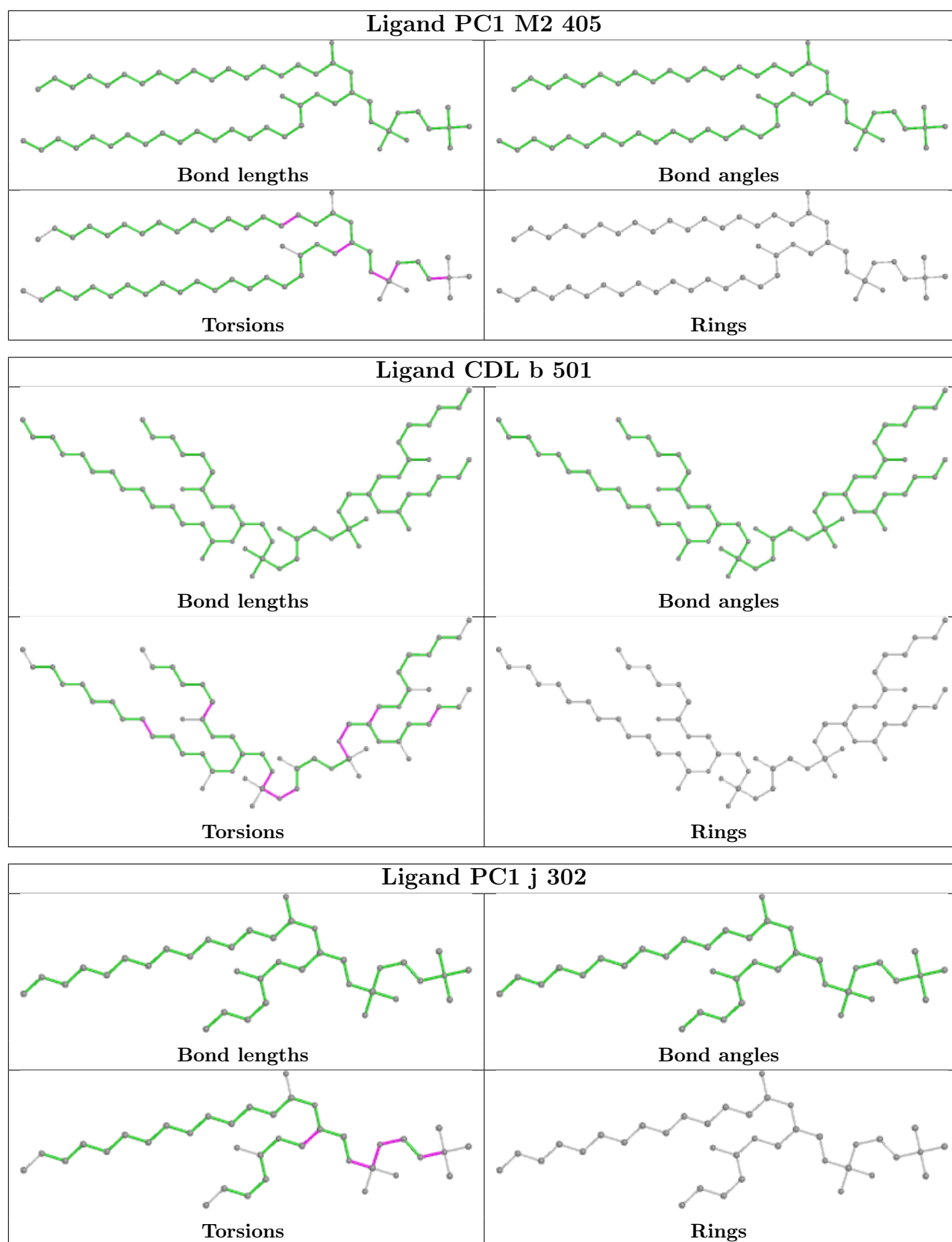
Ligand HEC QD 401

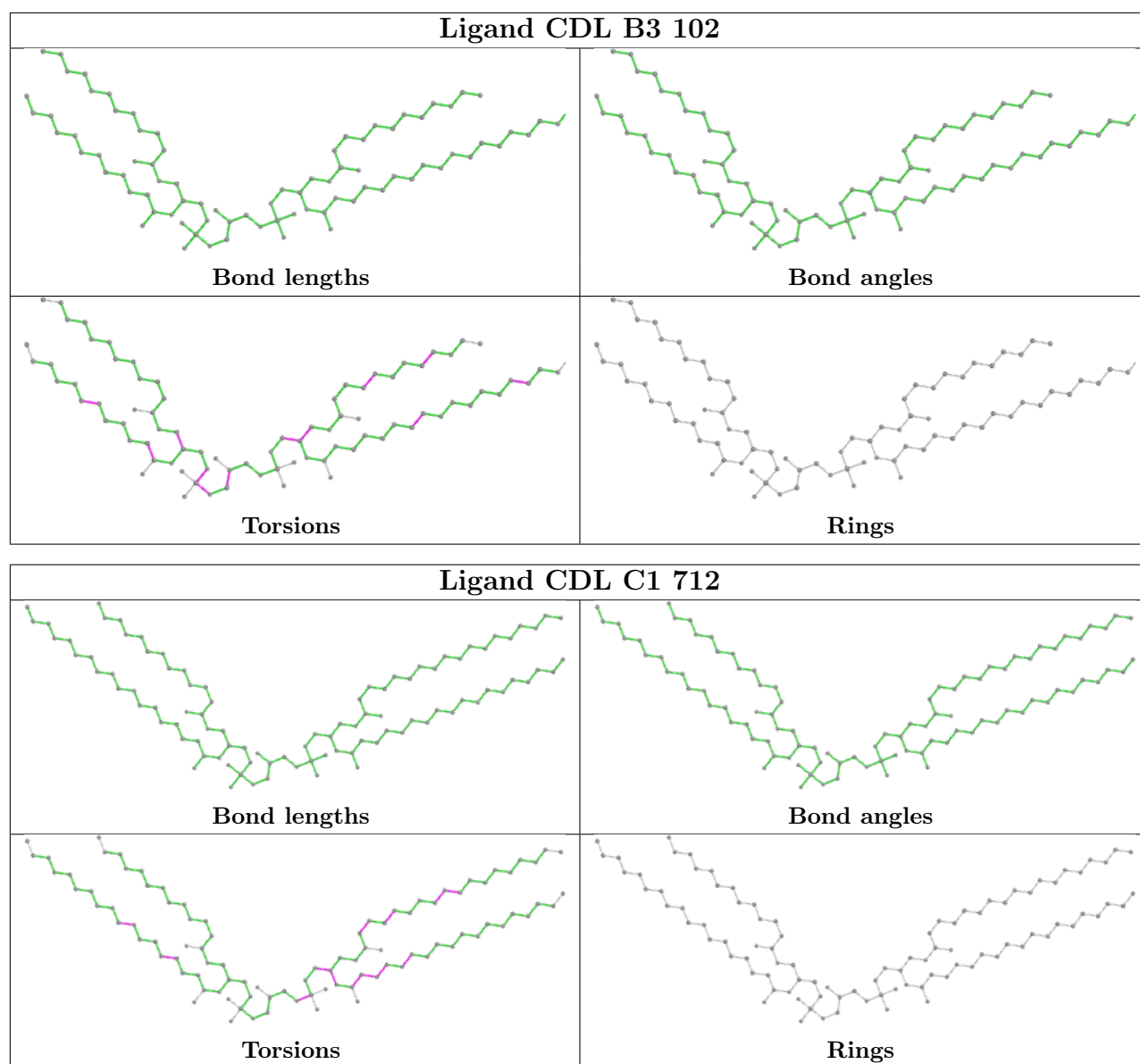


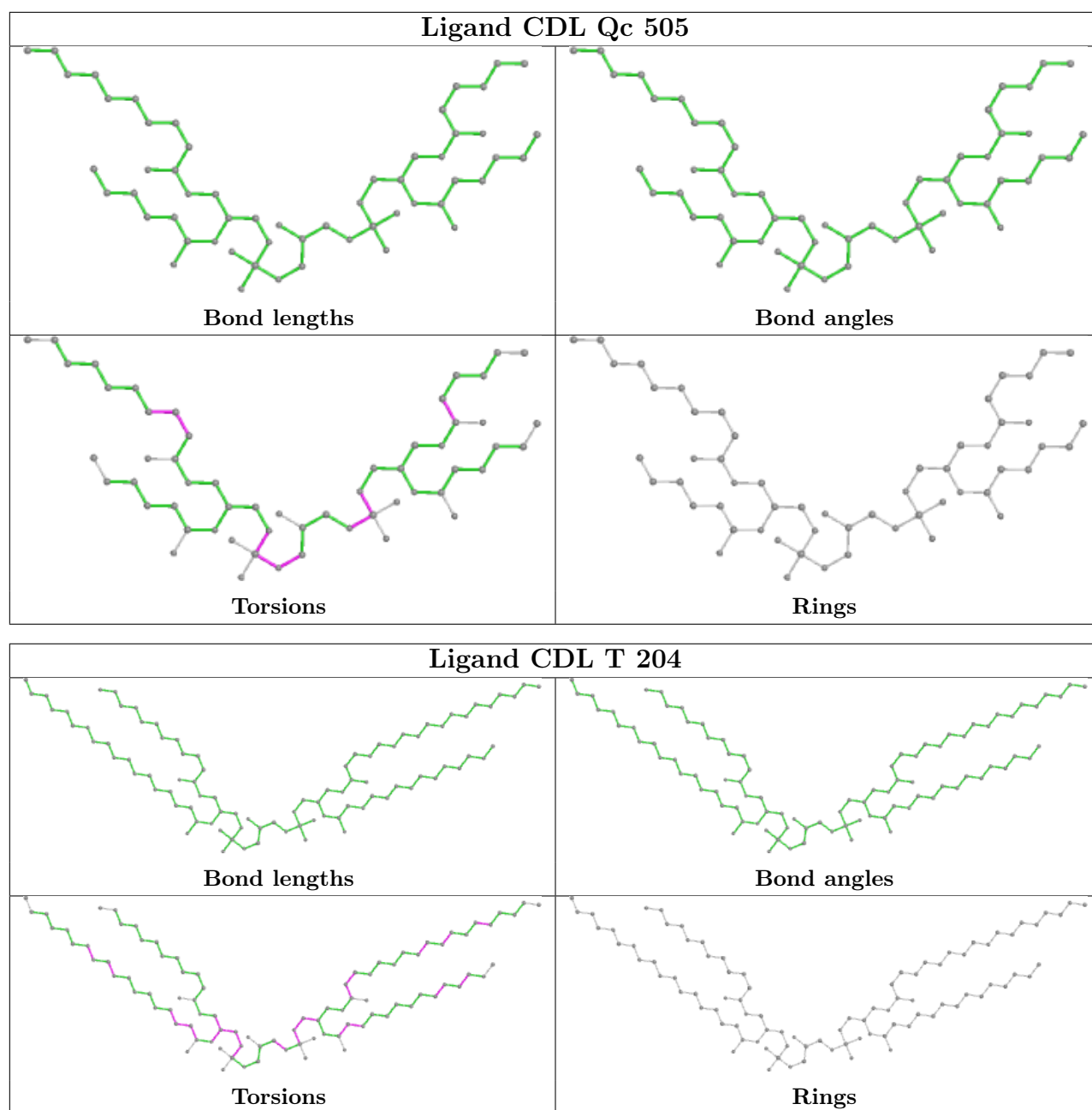
Ligand CDL BM 301

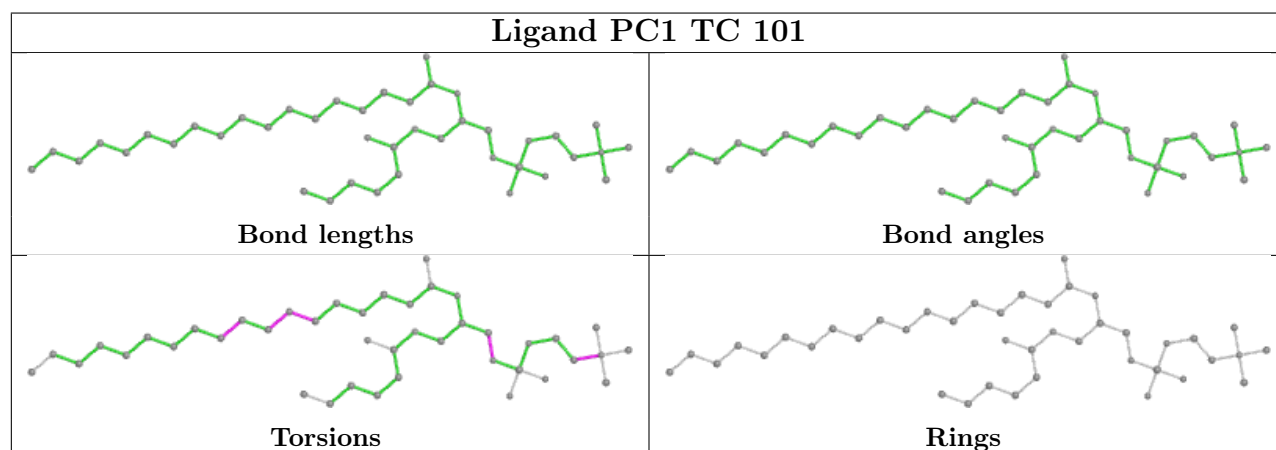
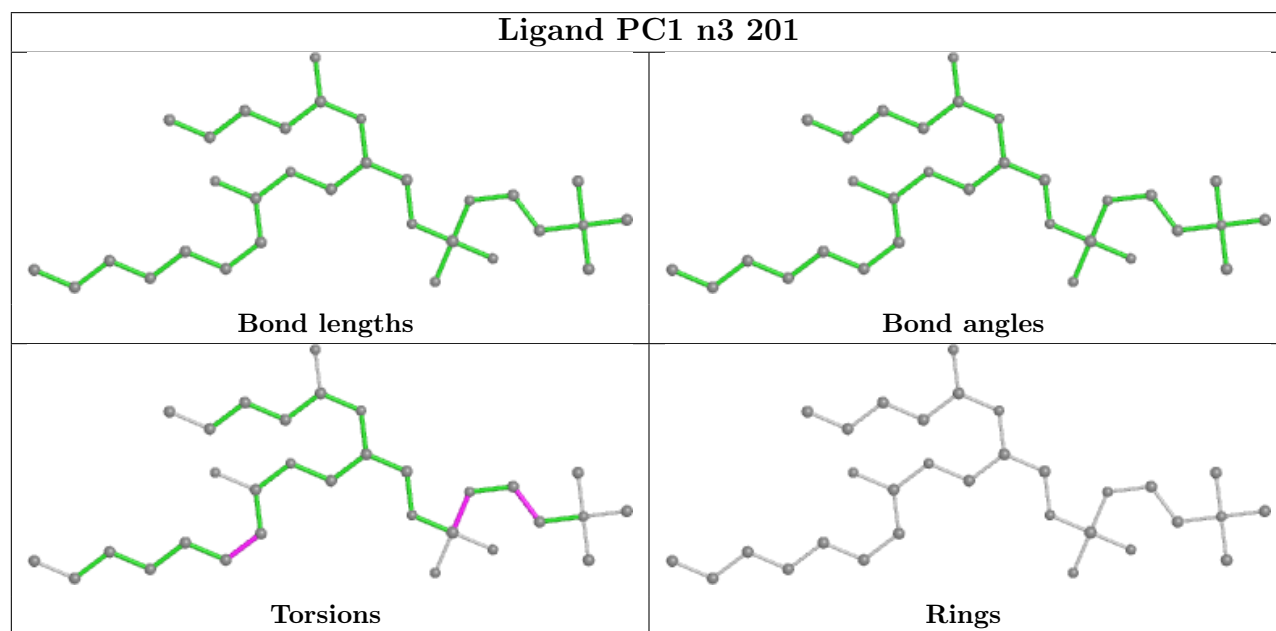
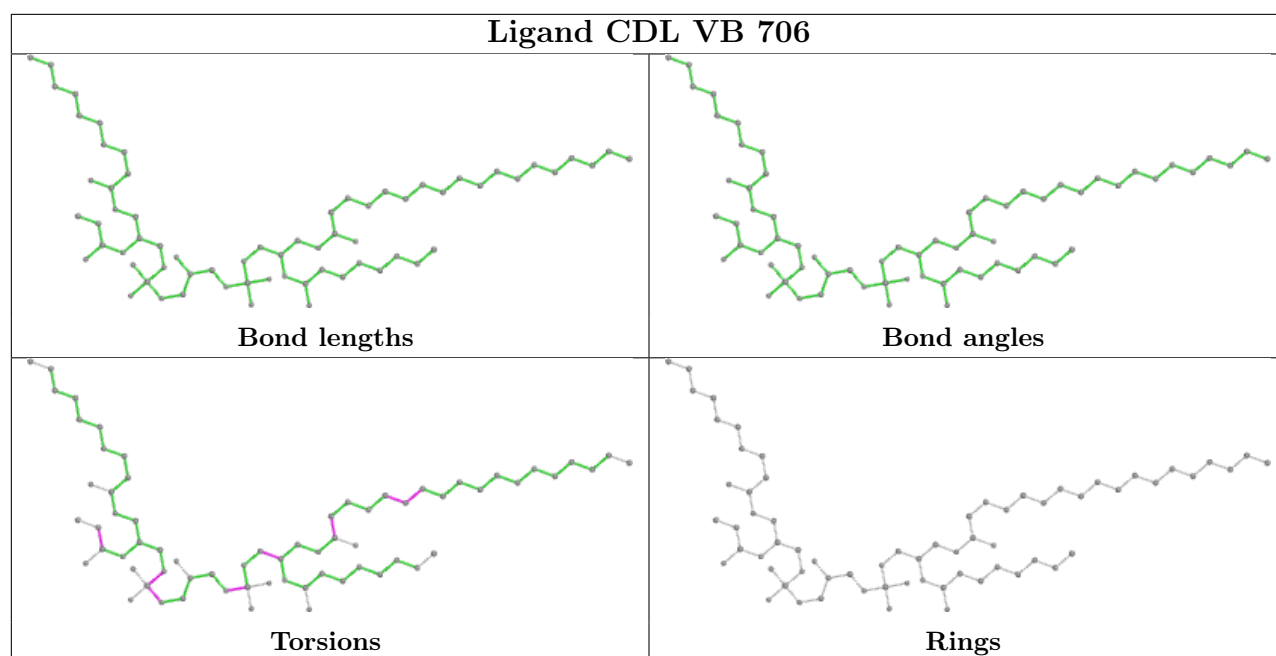


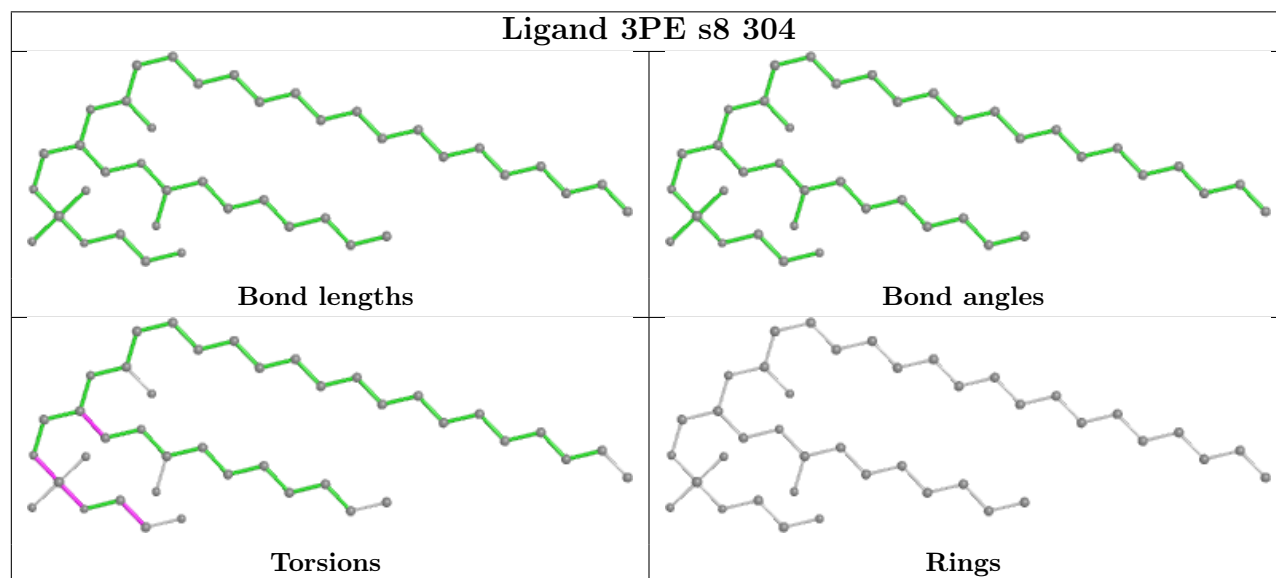
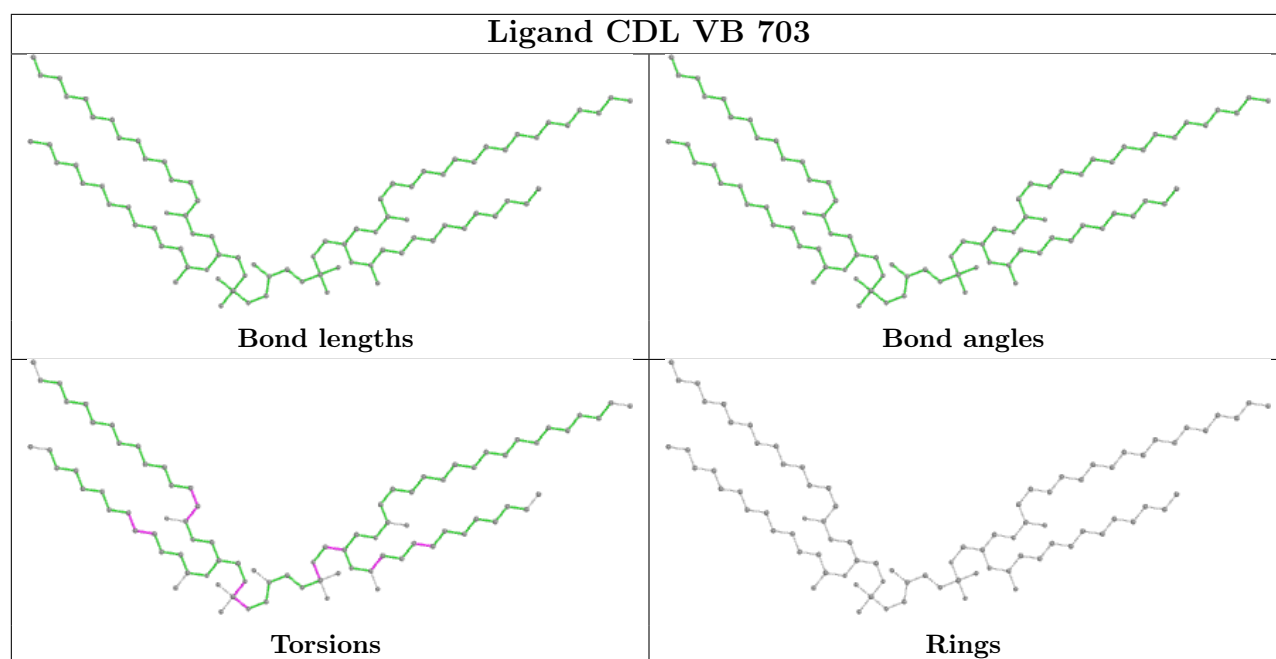


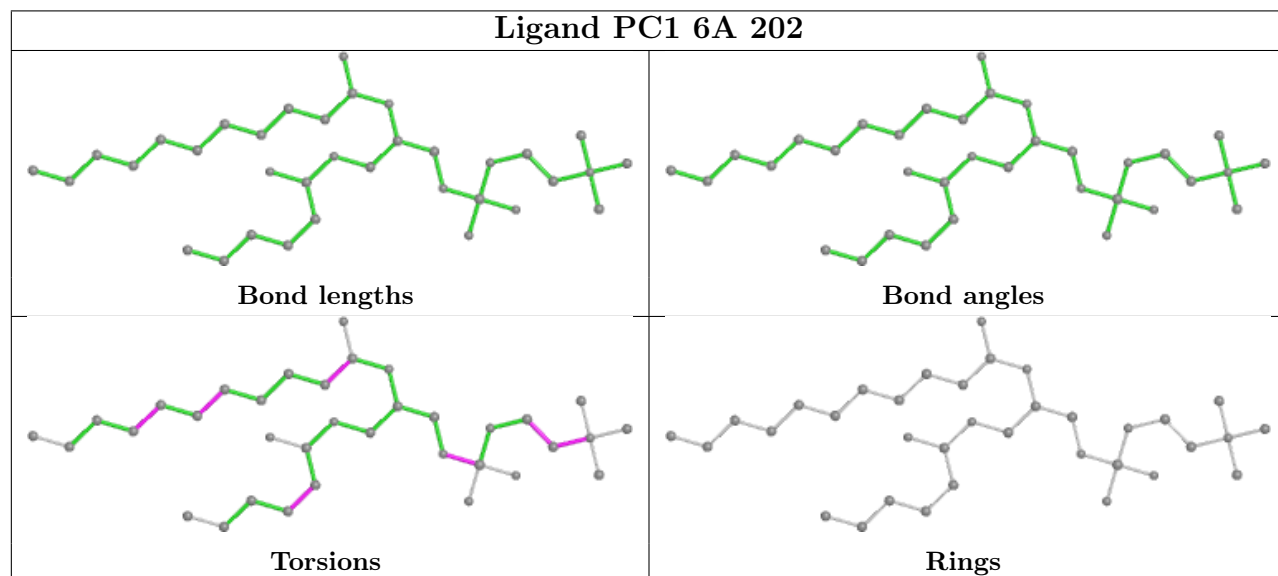
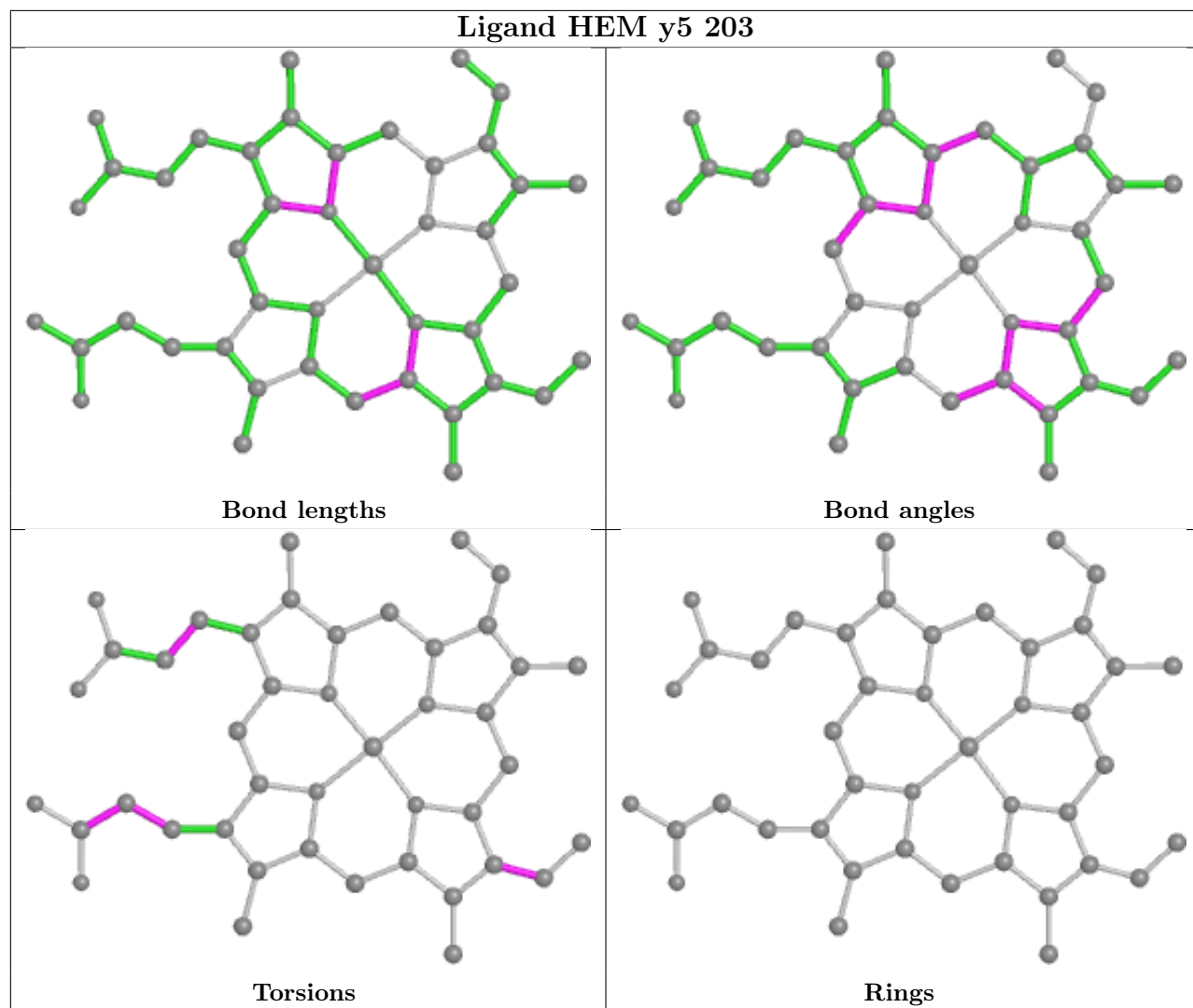


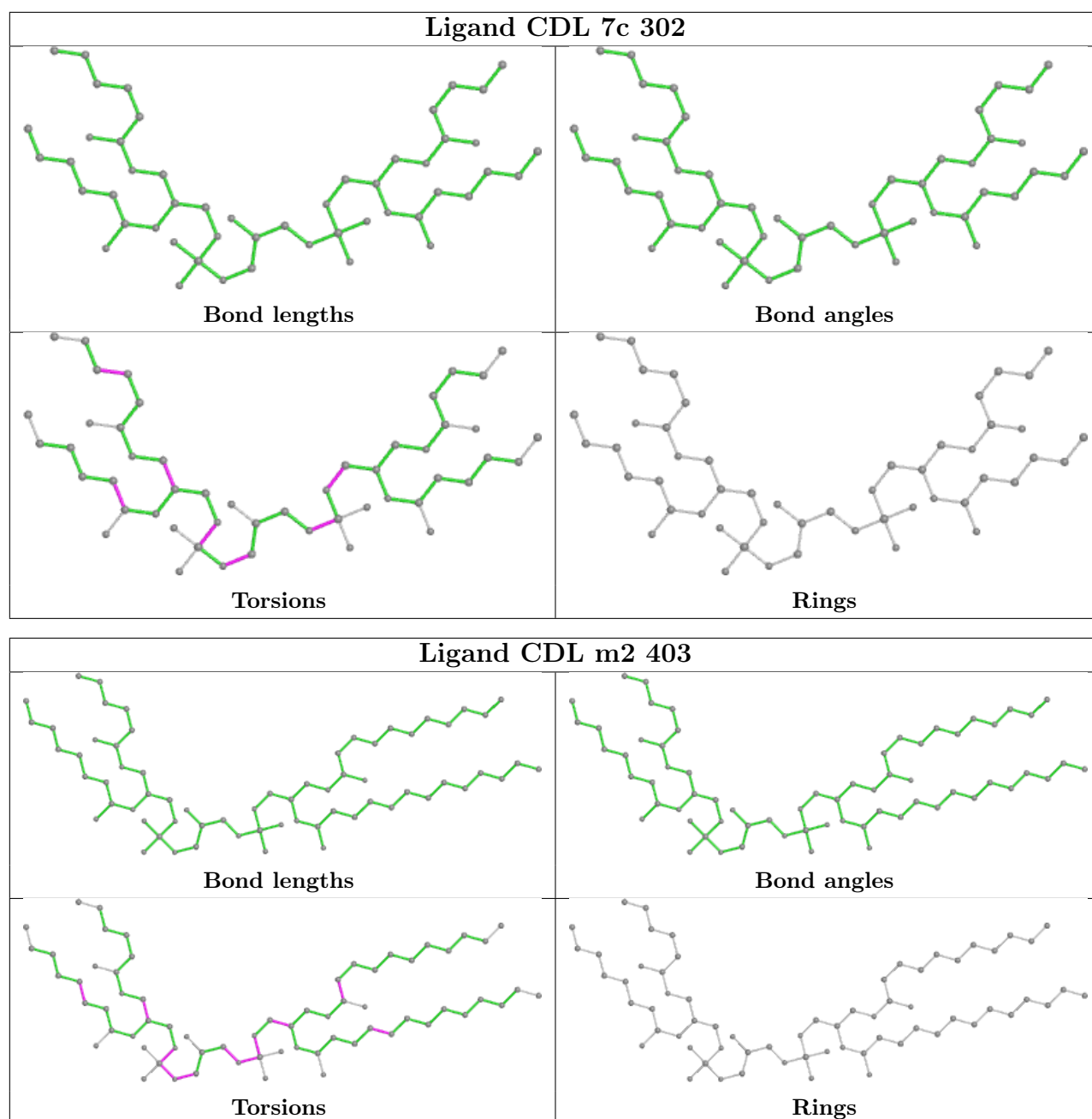


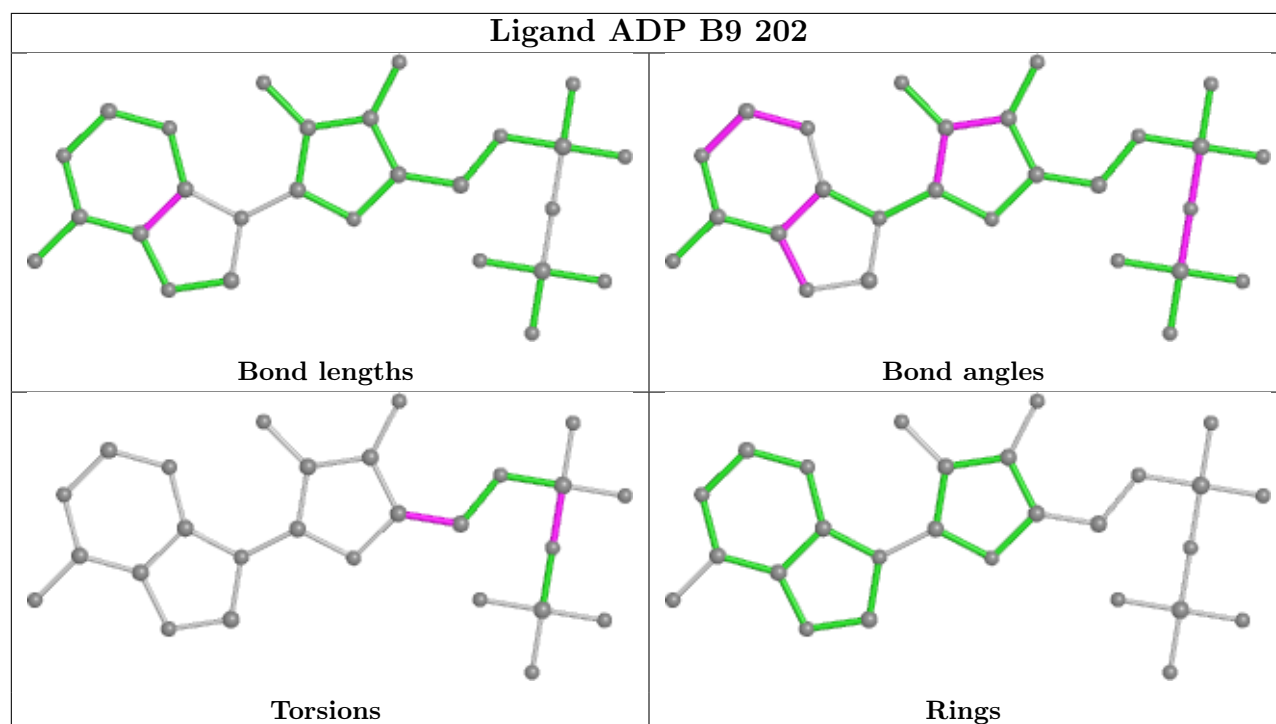
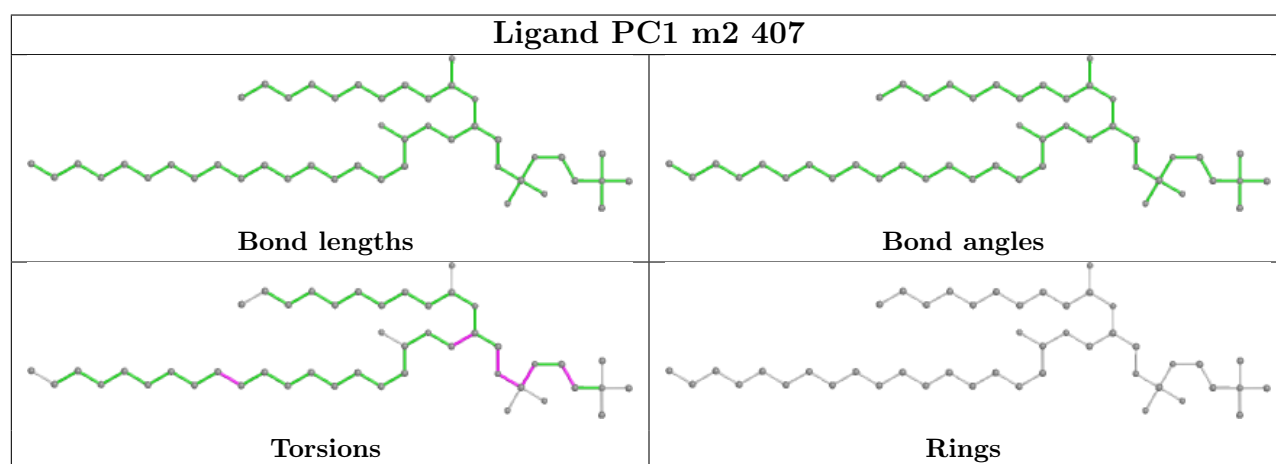
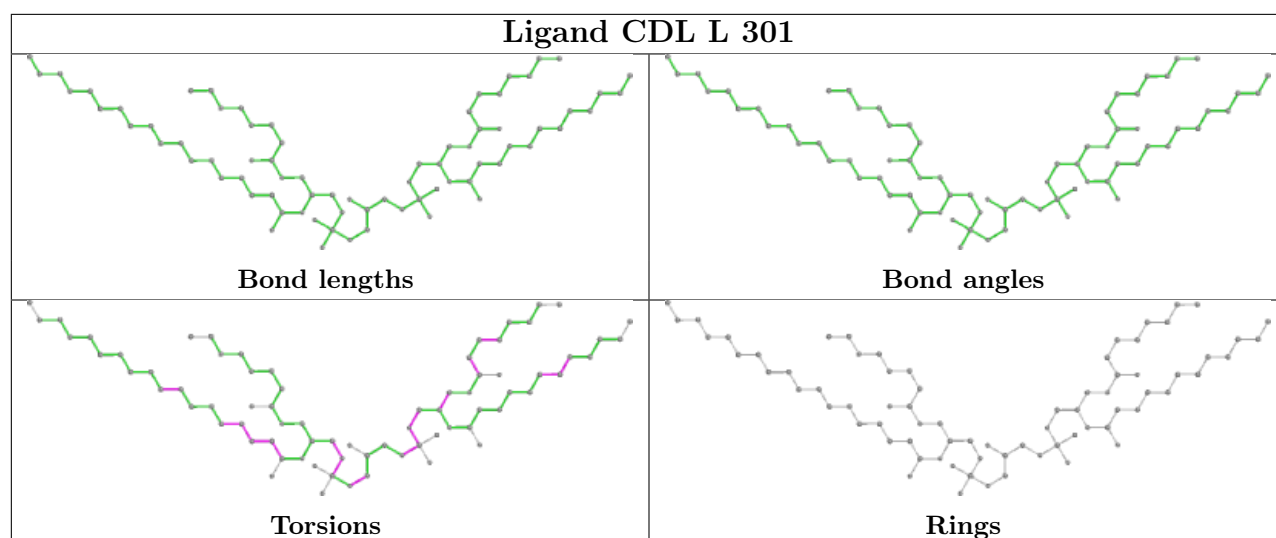


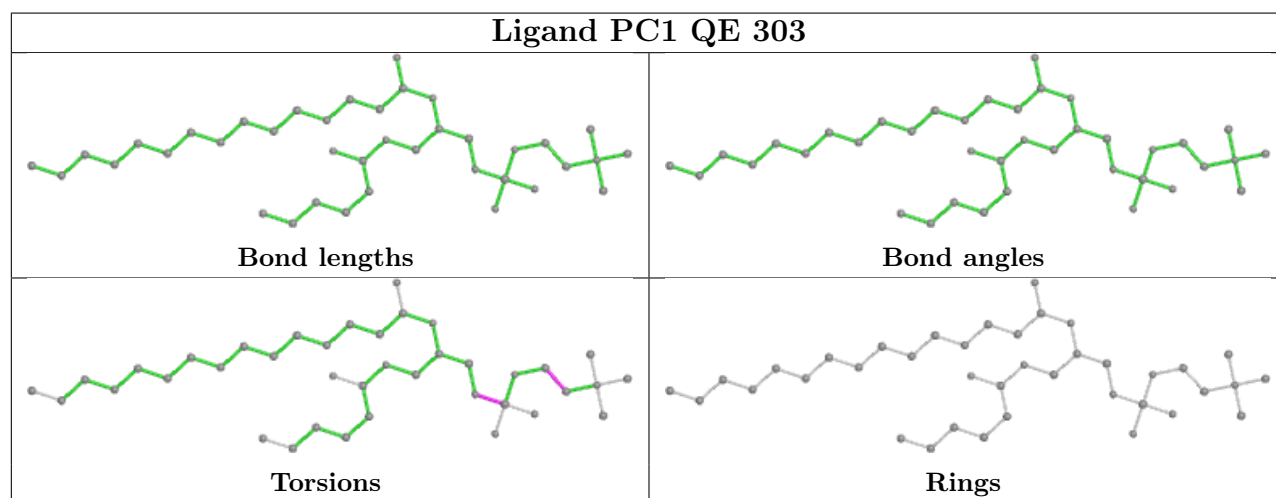
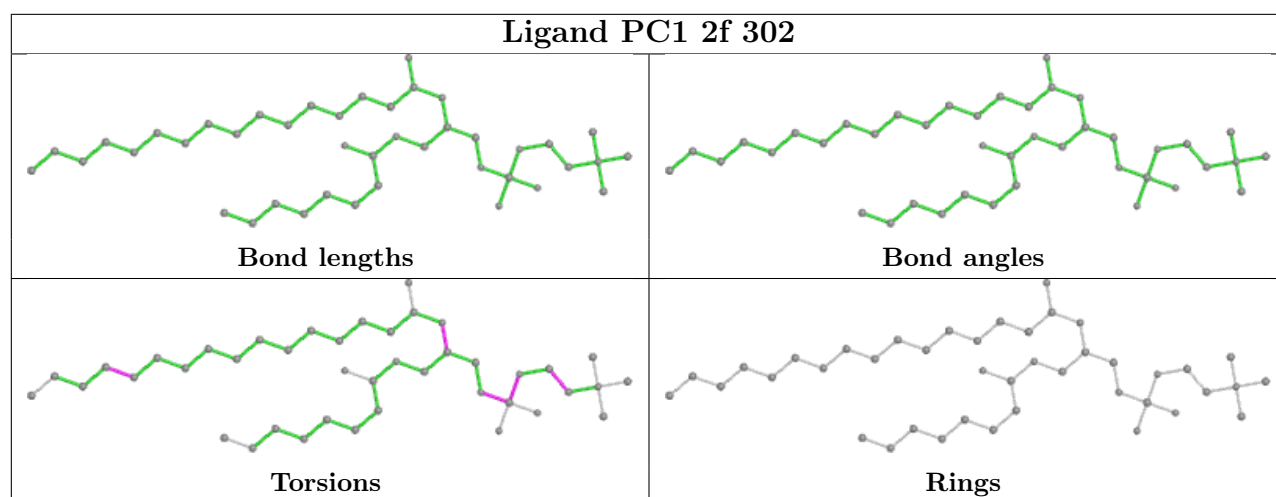
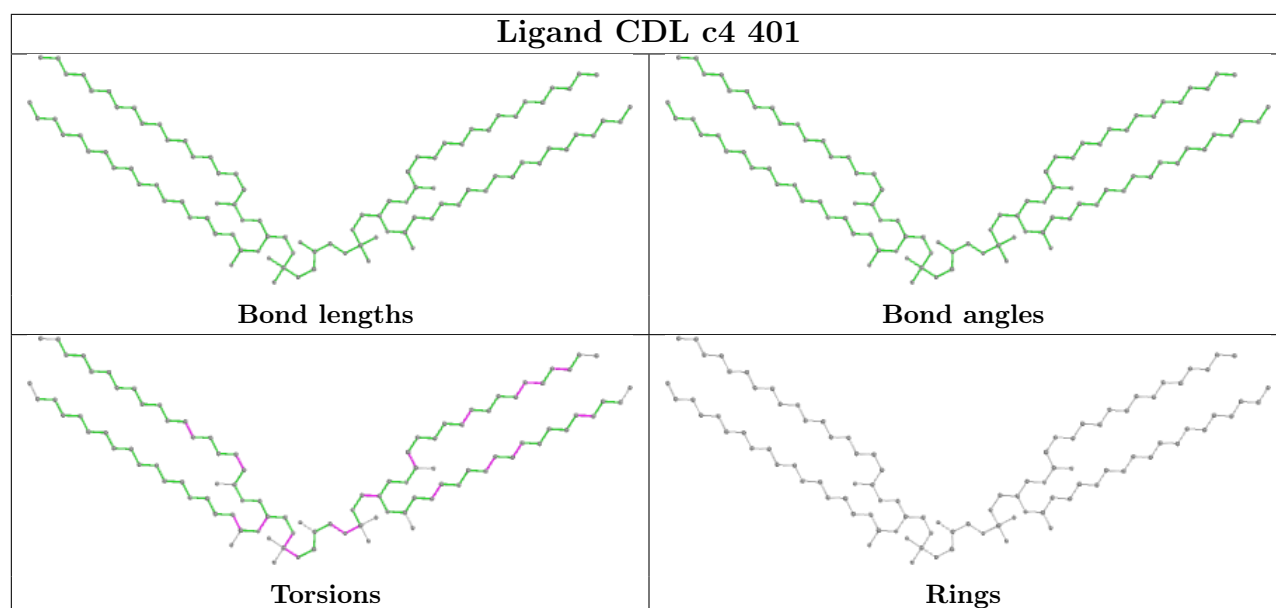


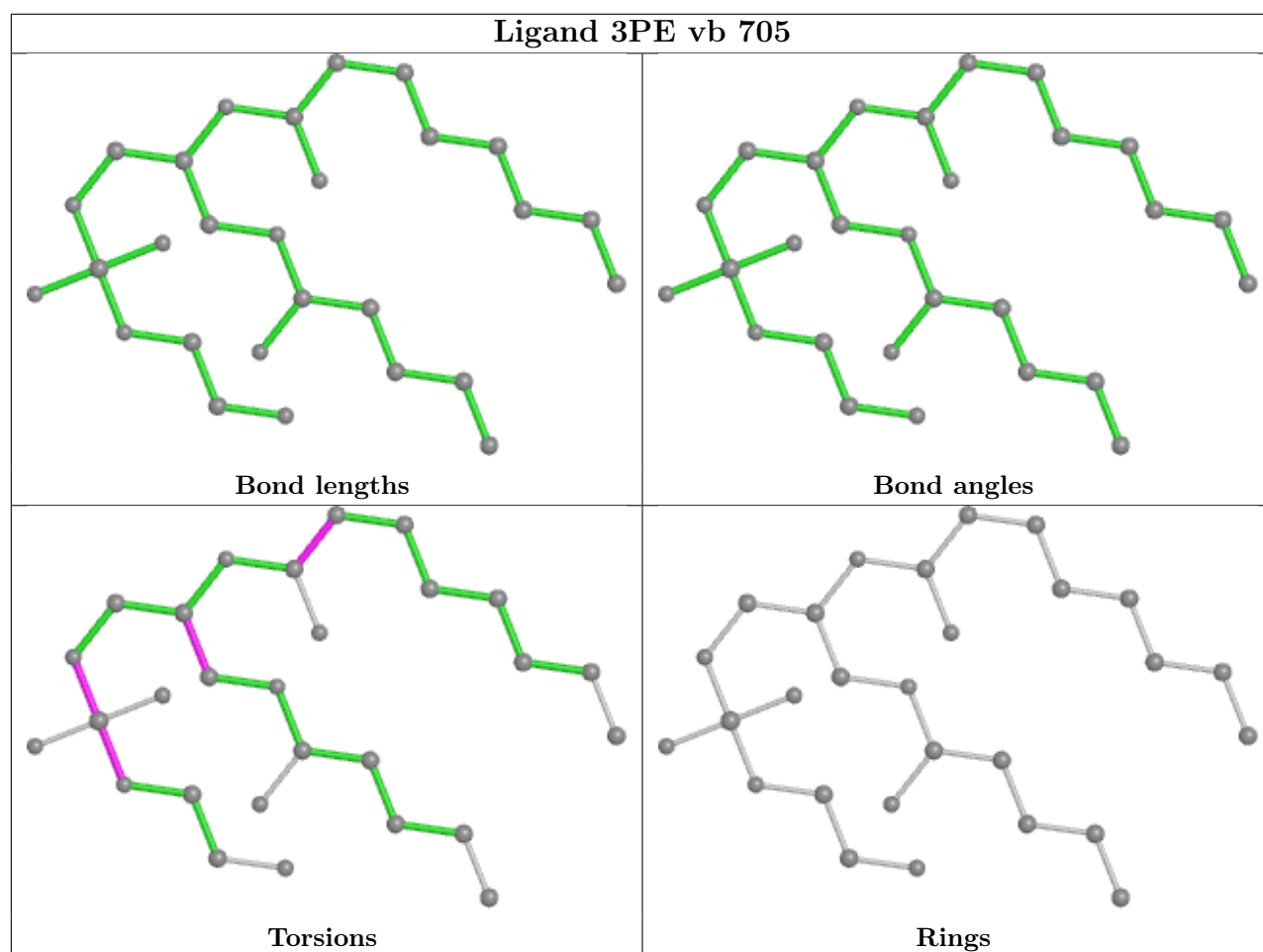
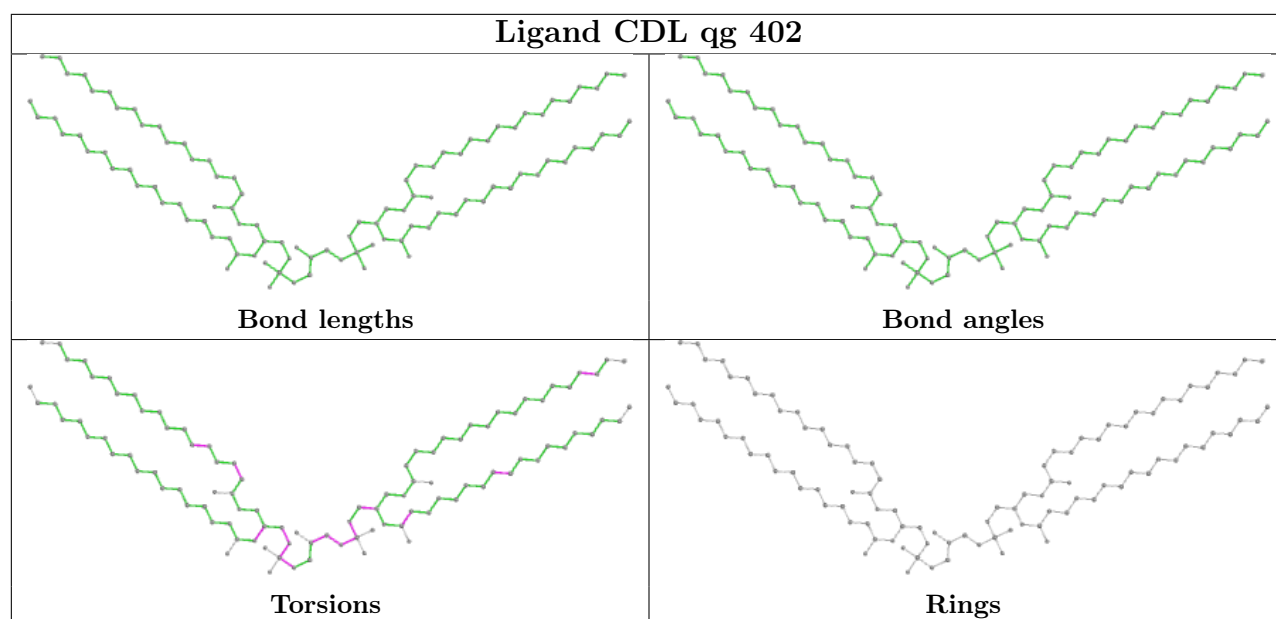


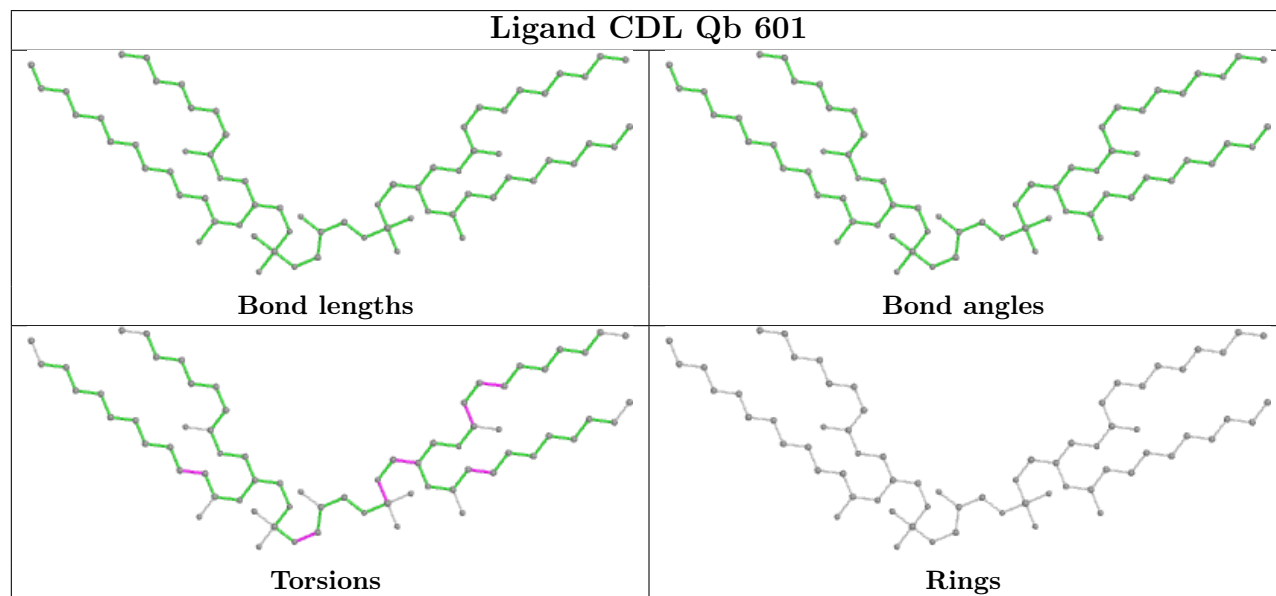
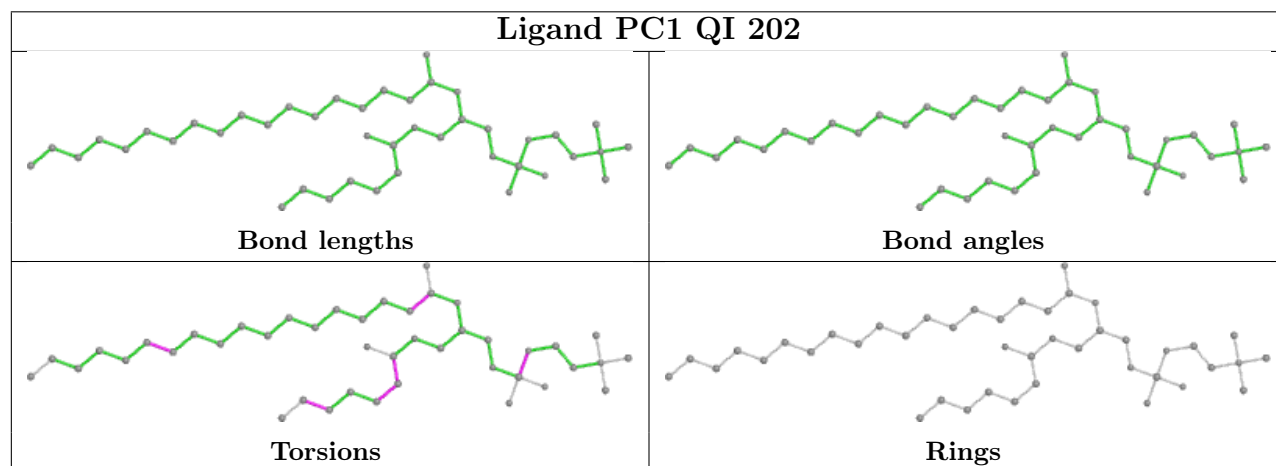
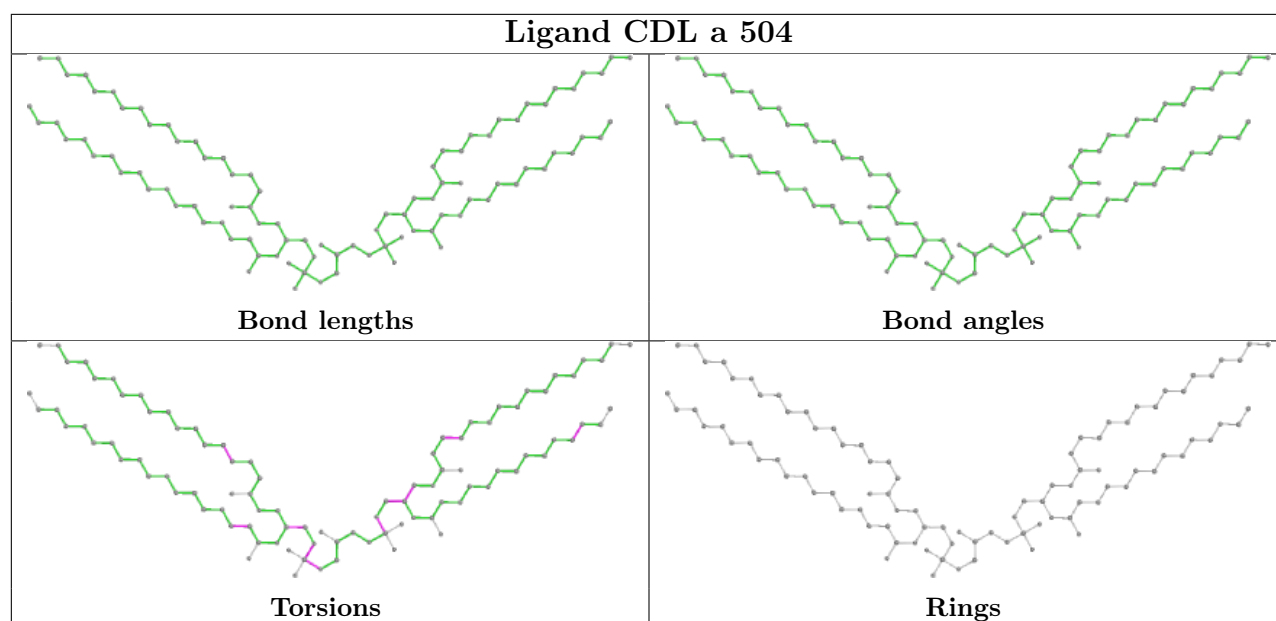


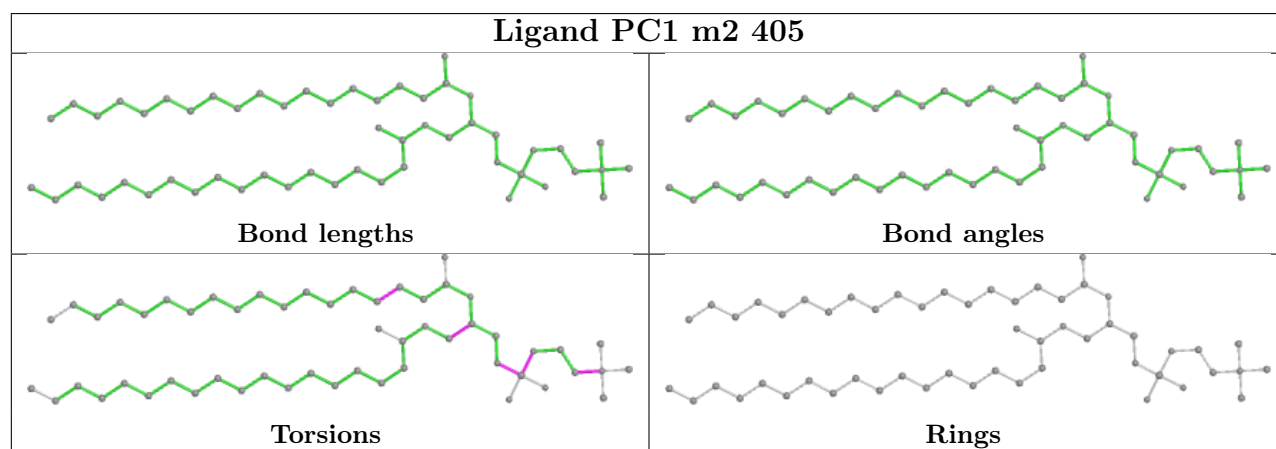
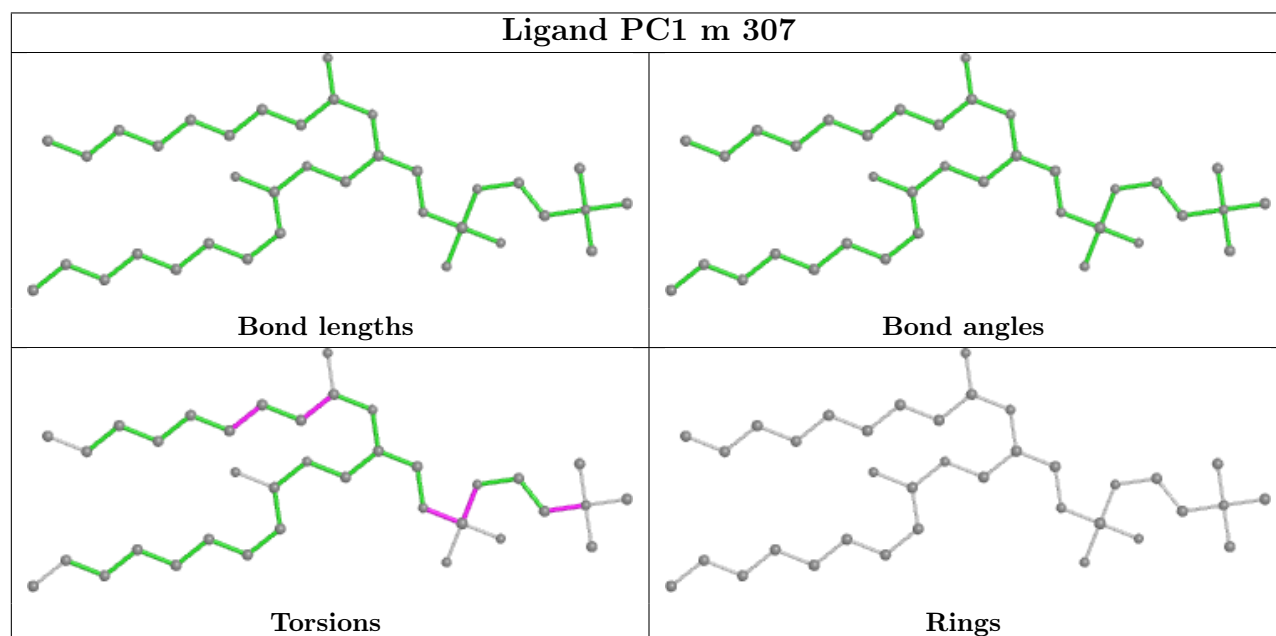
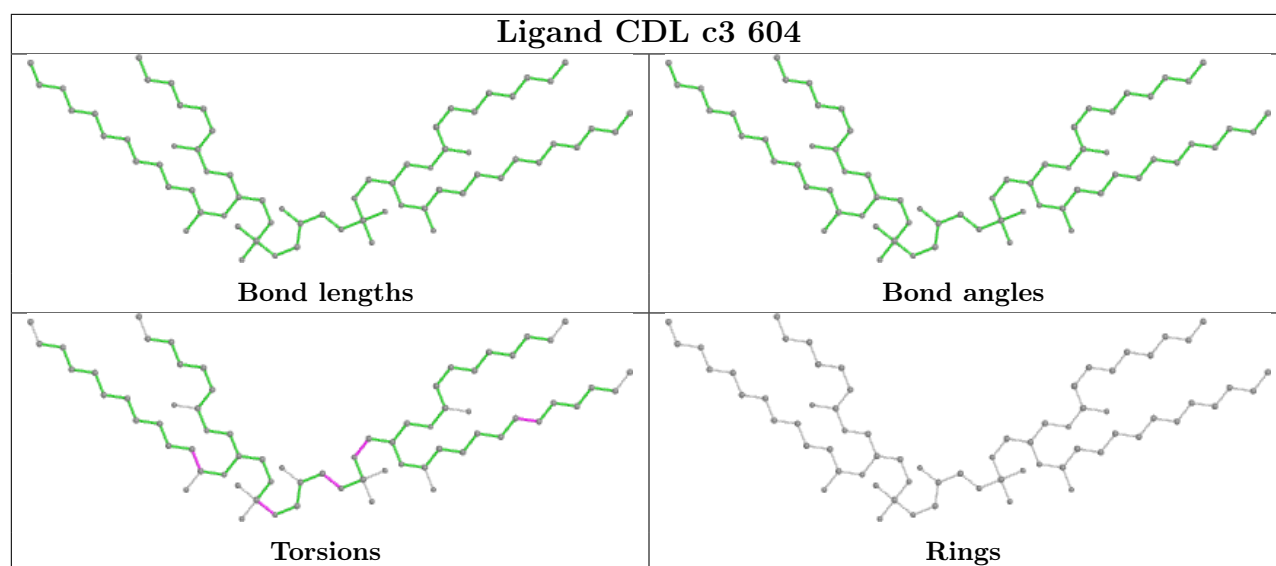


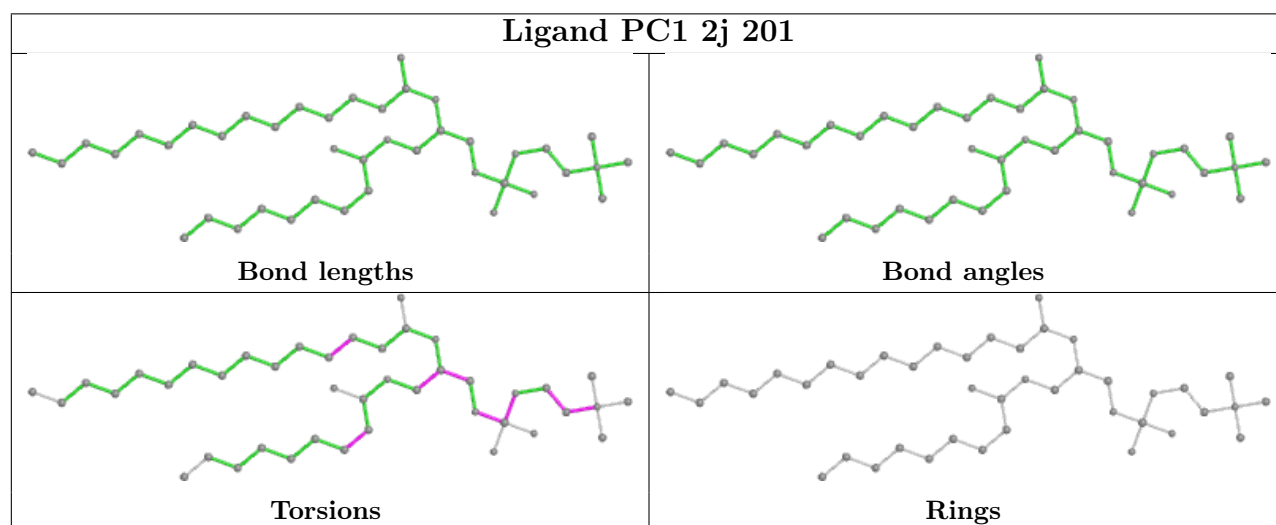
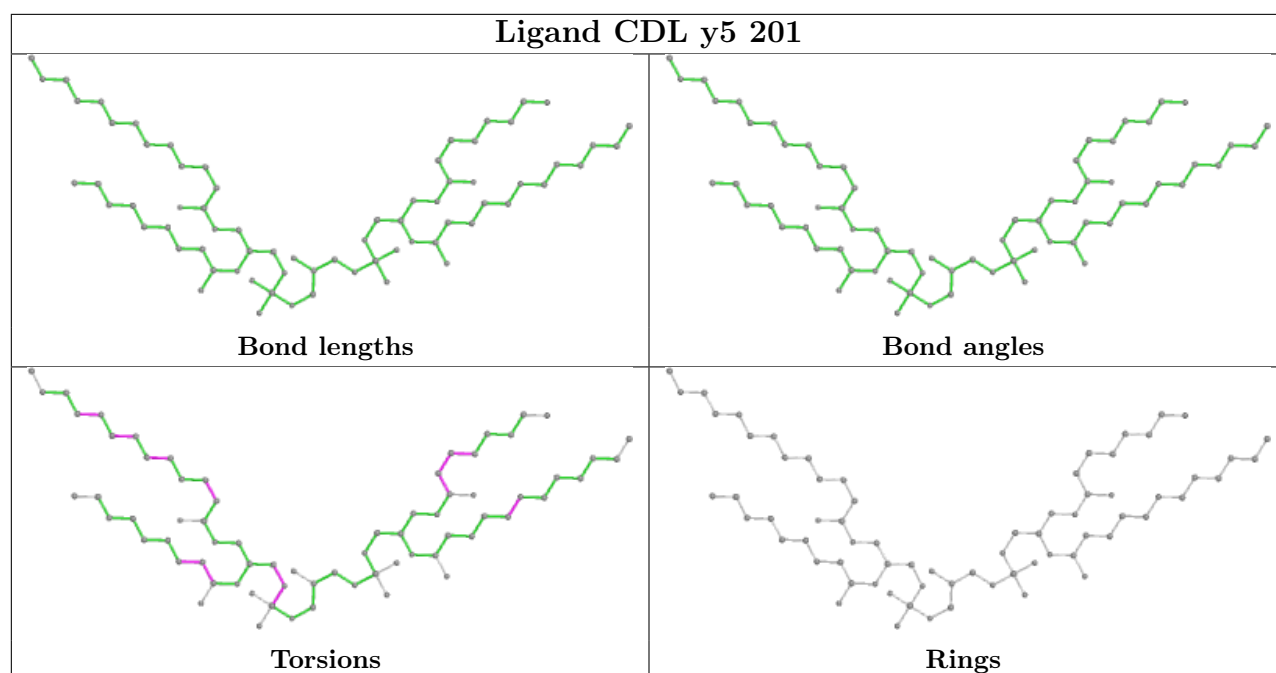


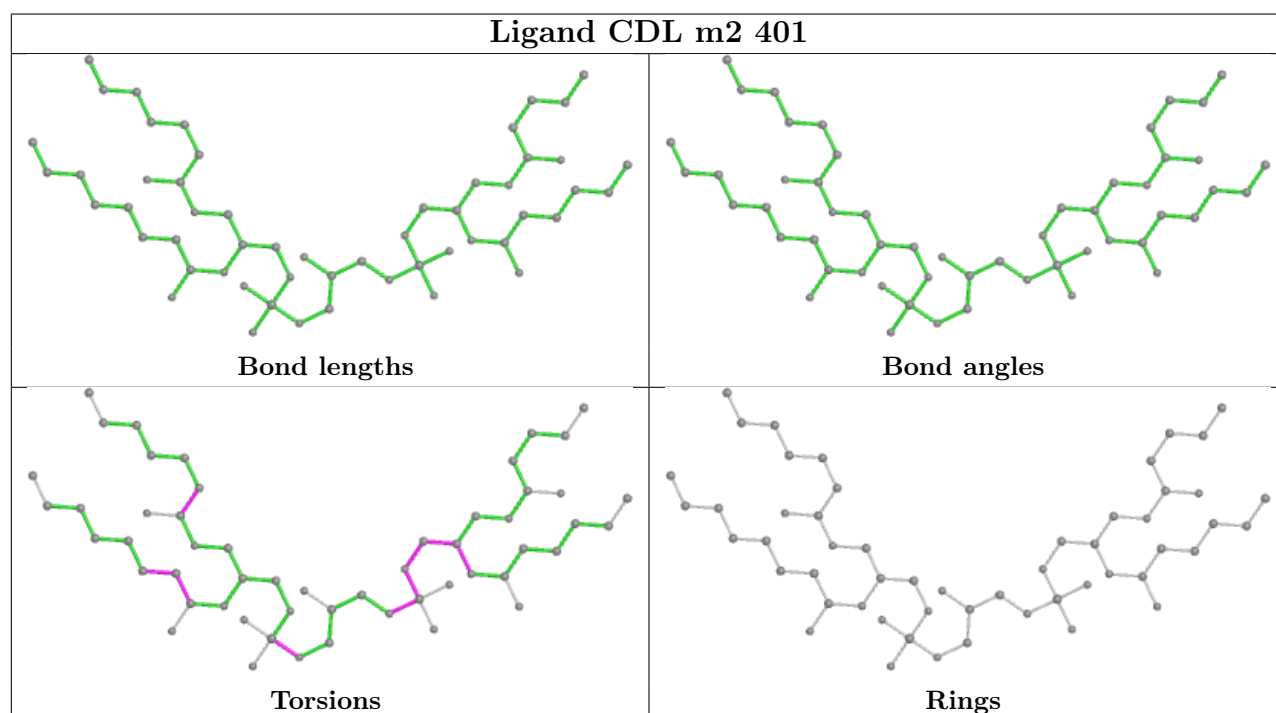
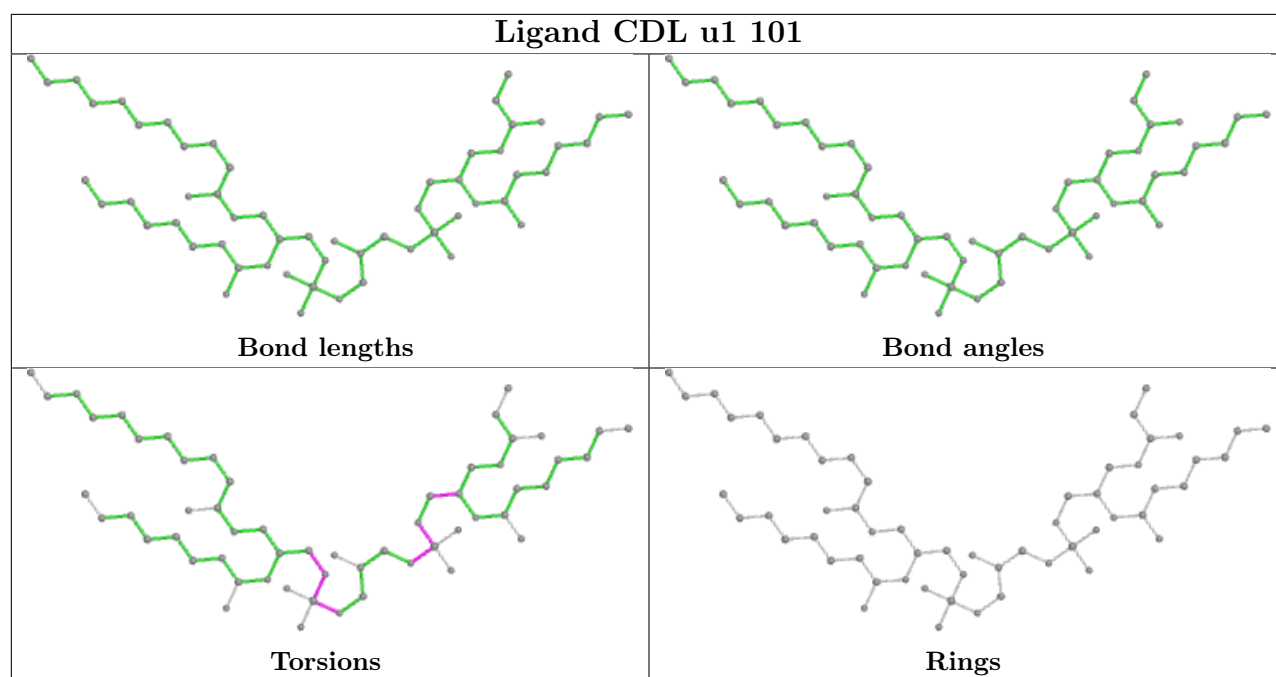


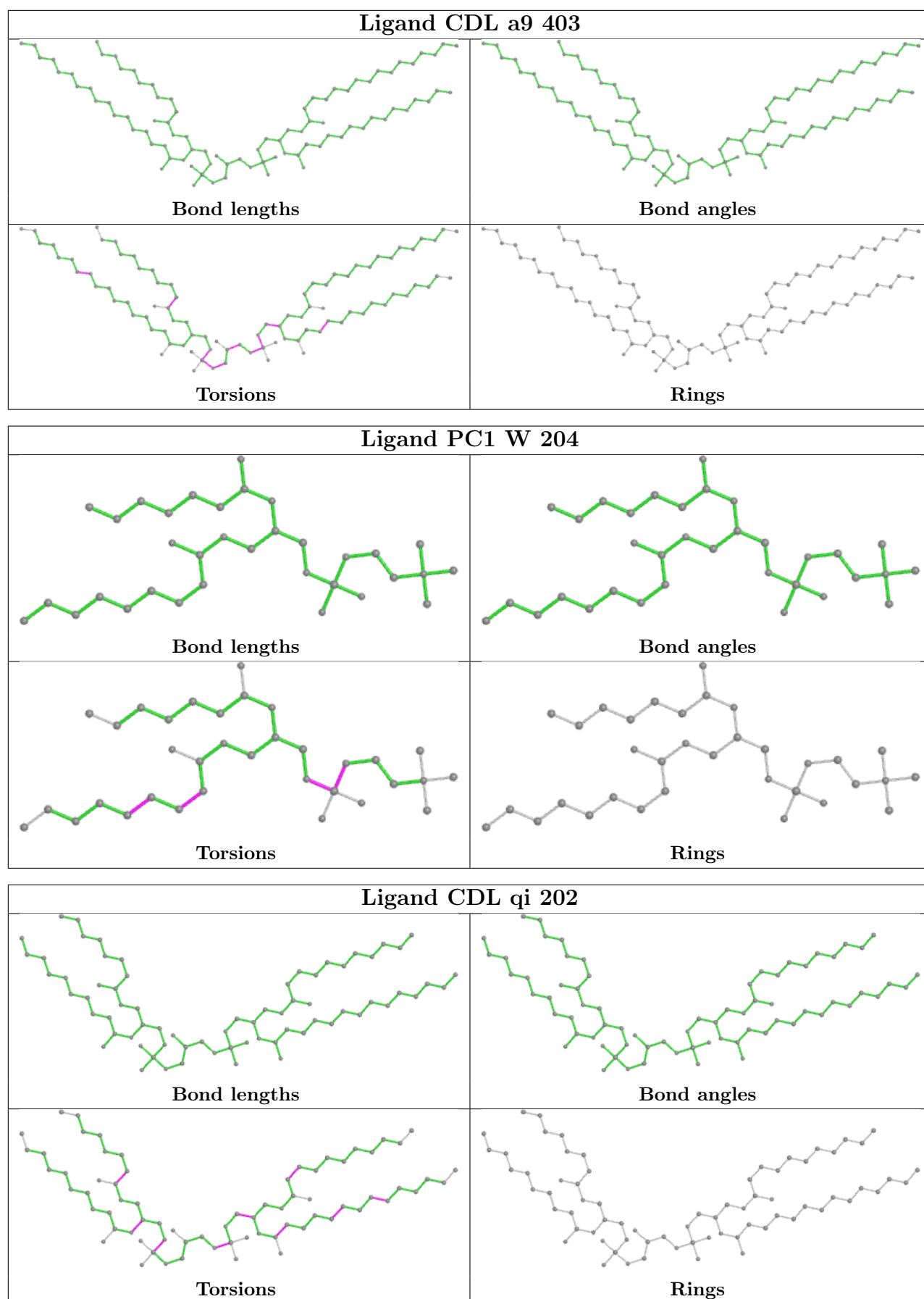


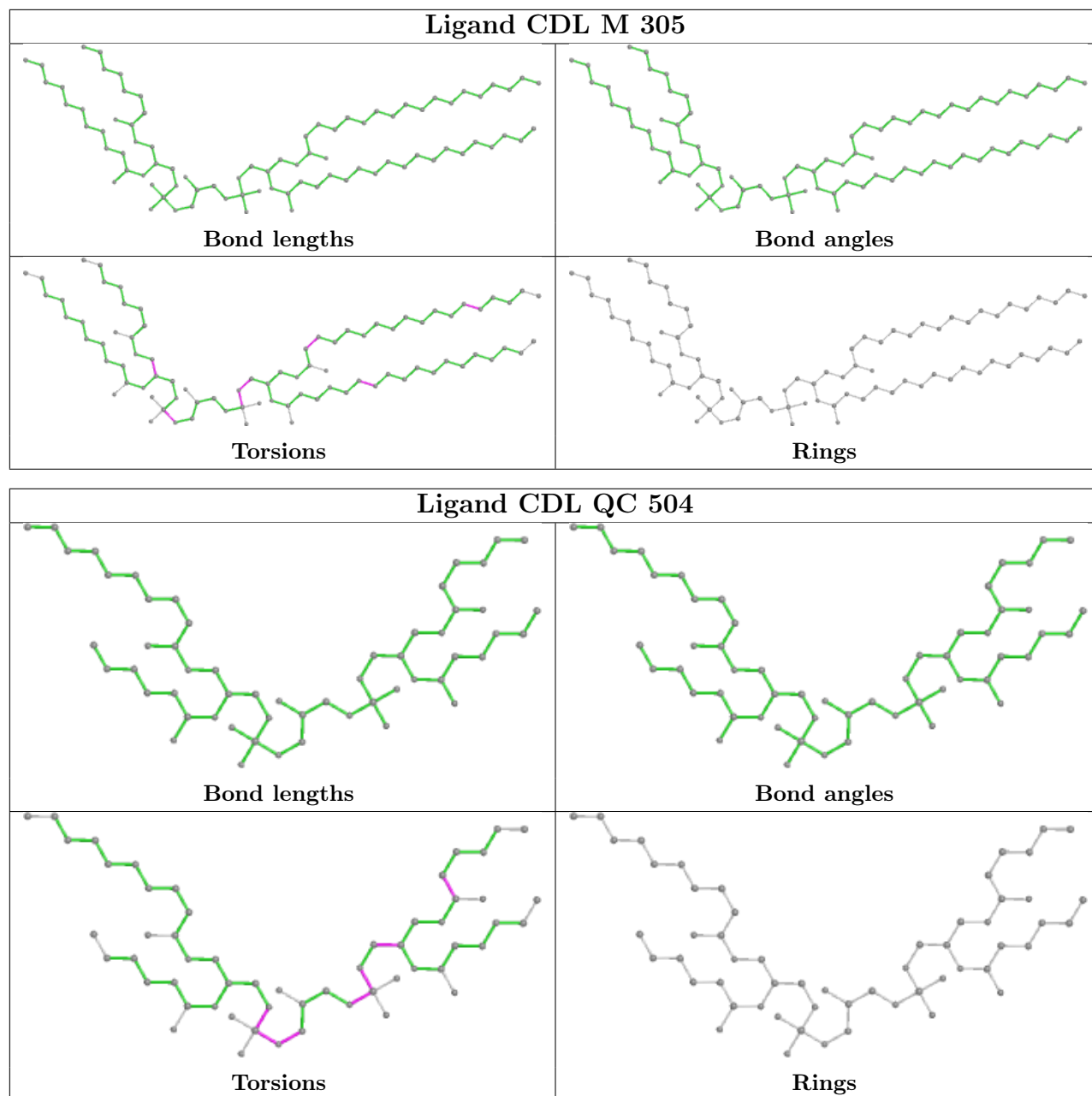


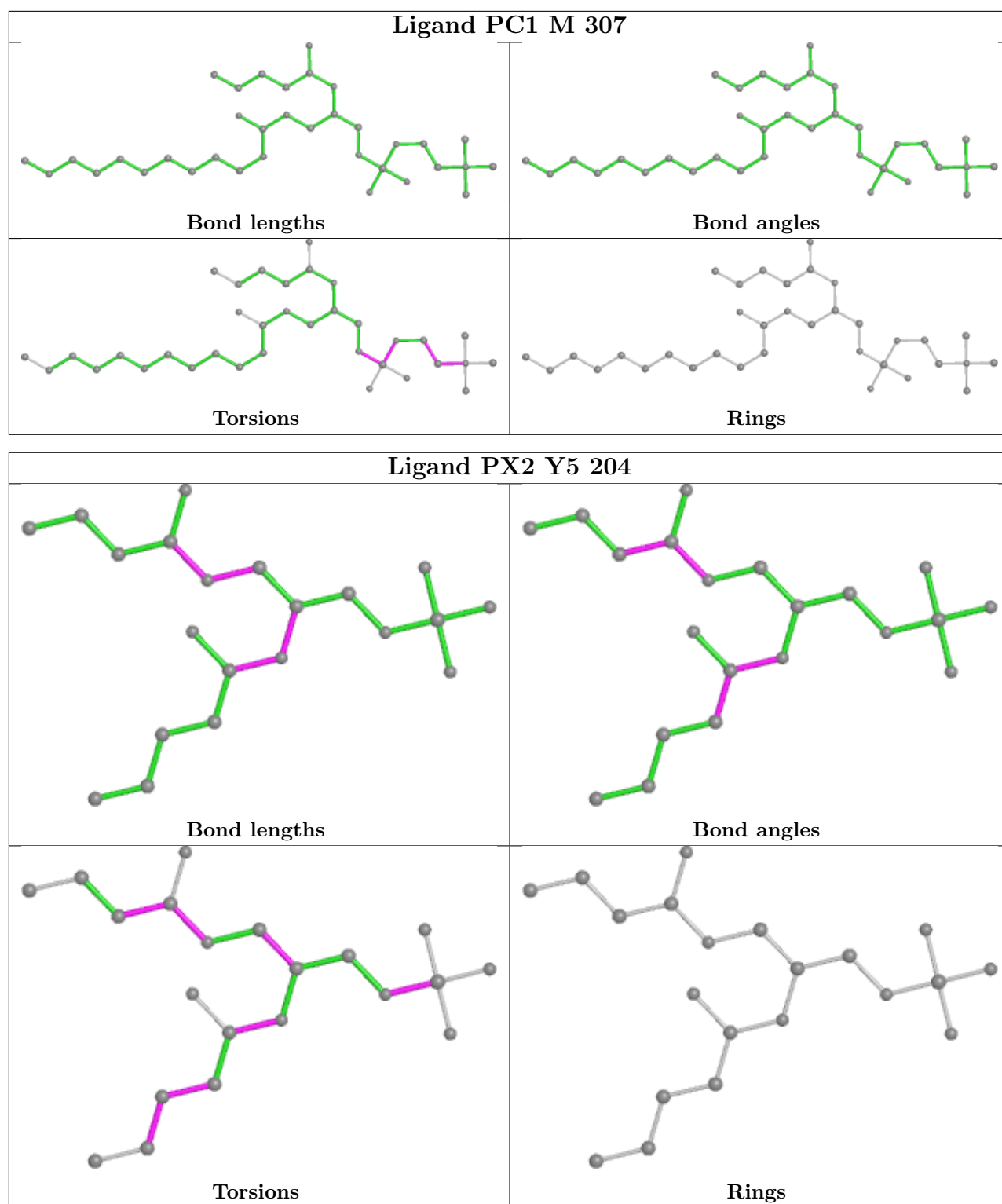


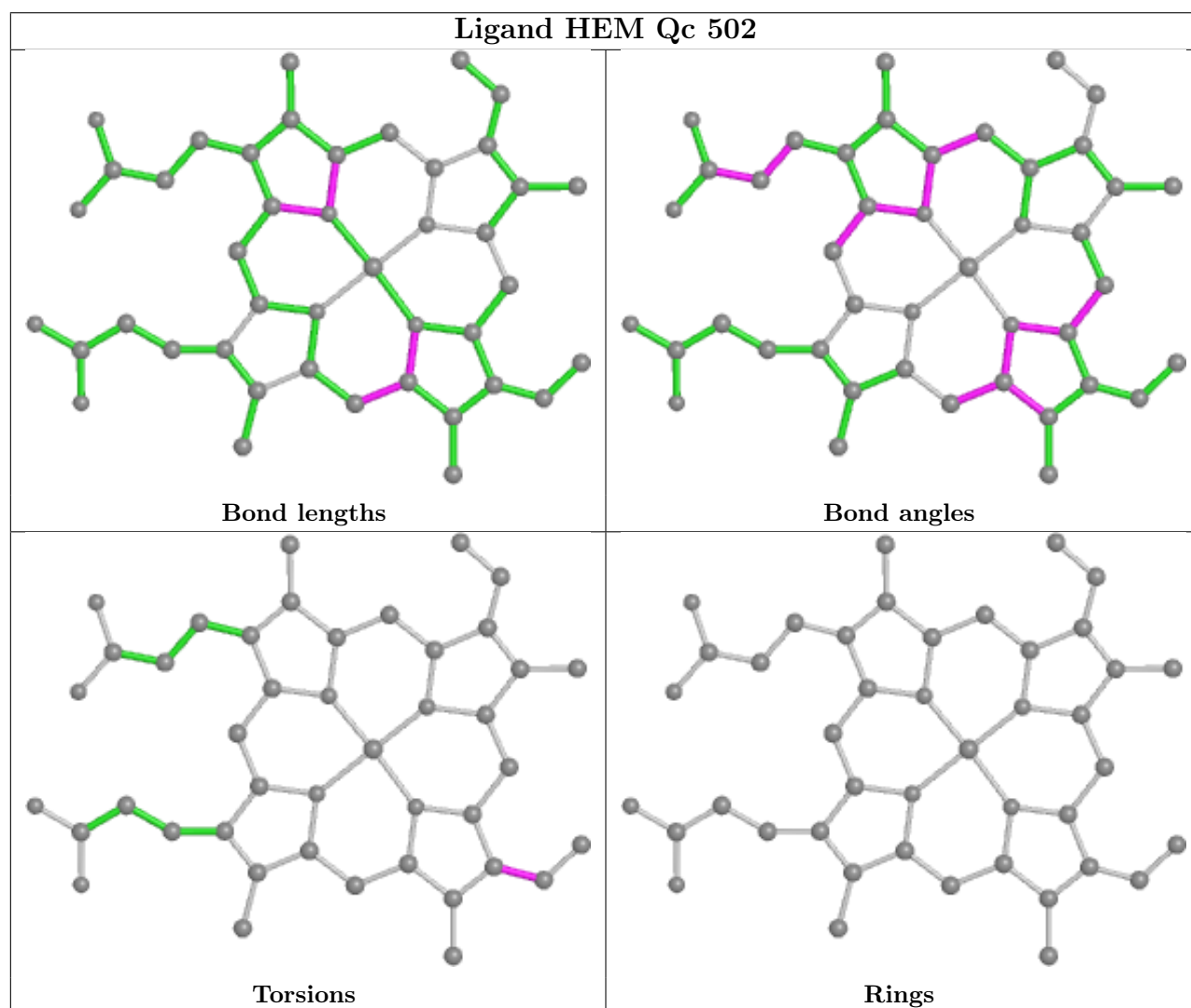
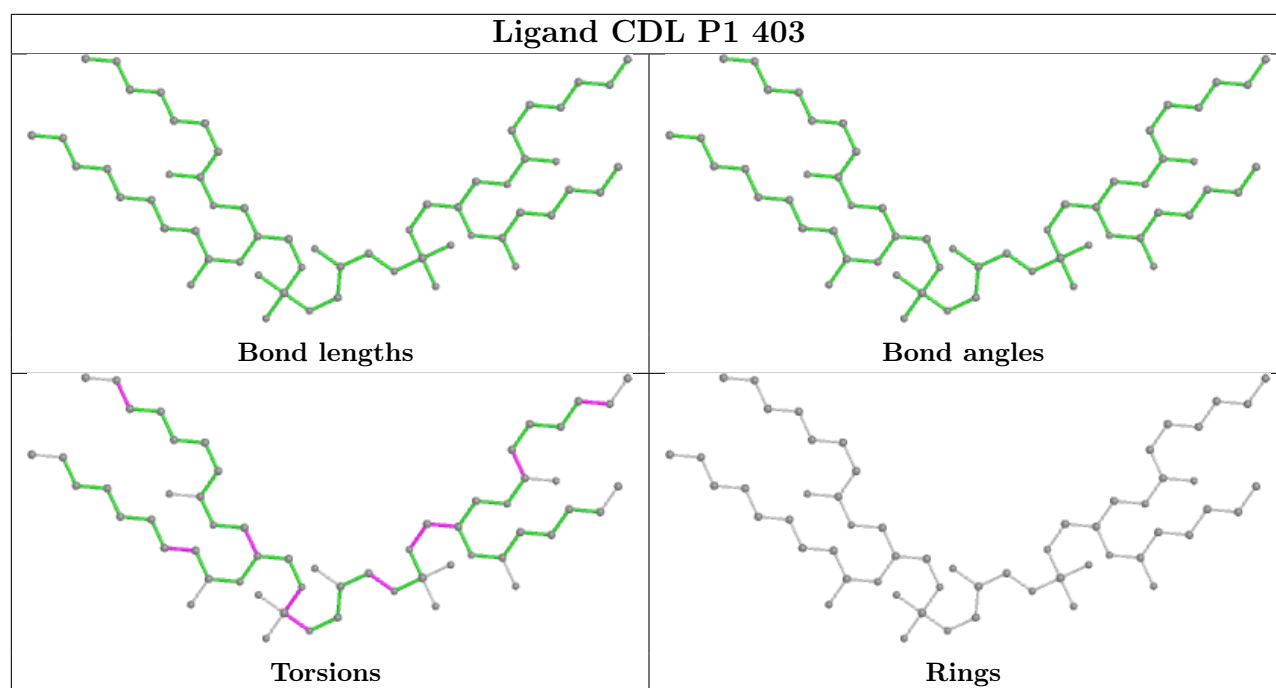


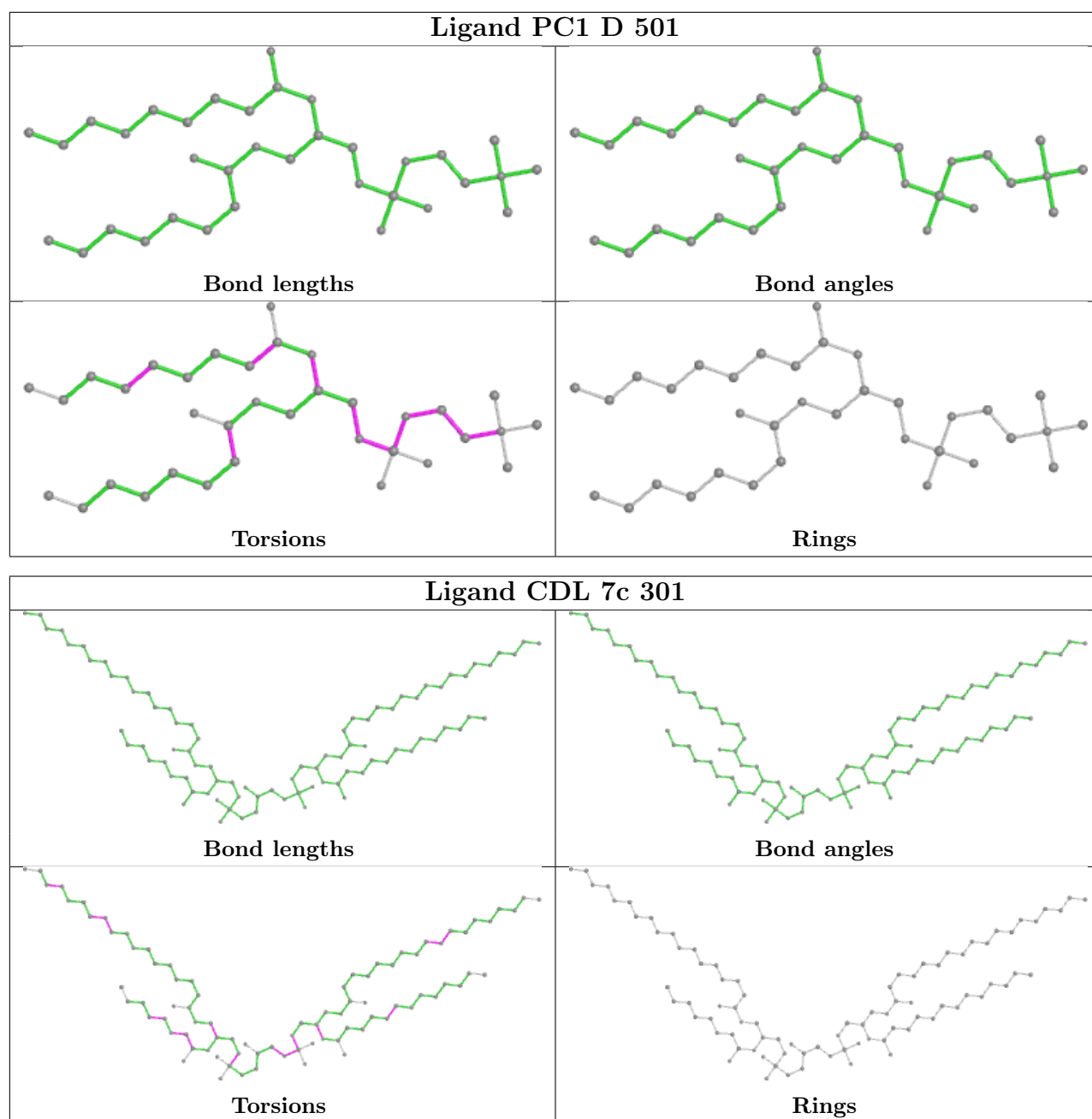


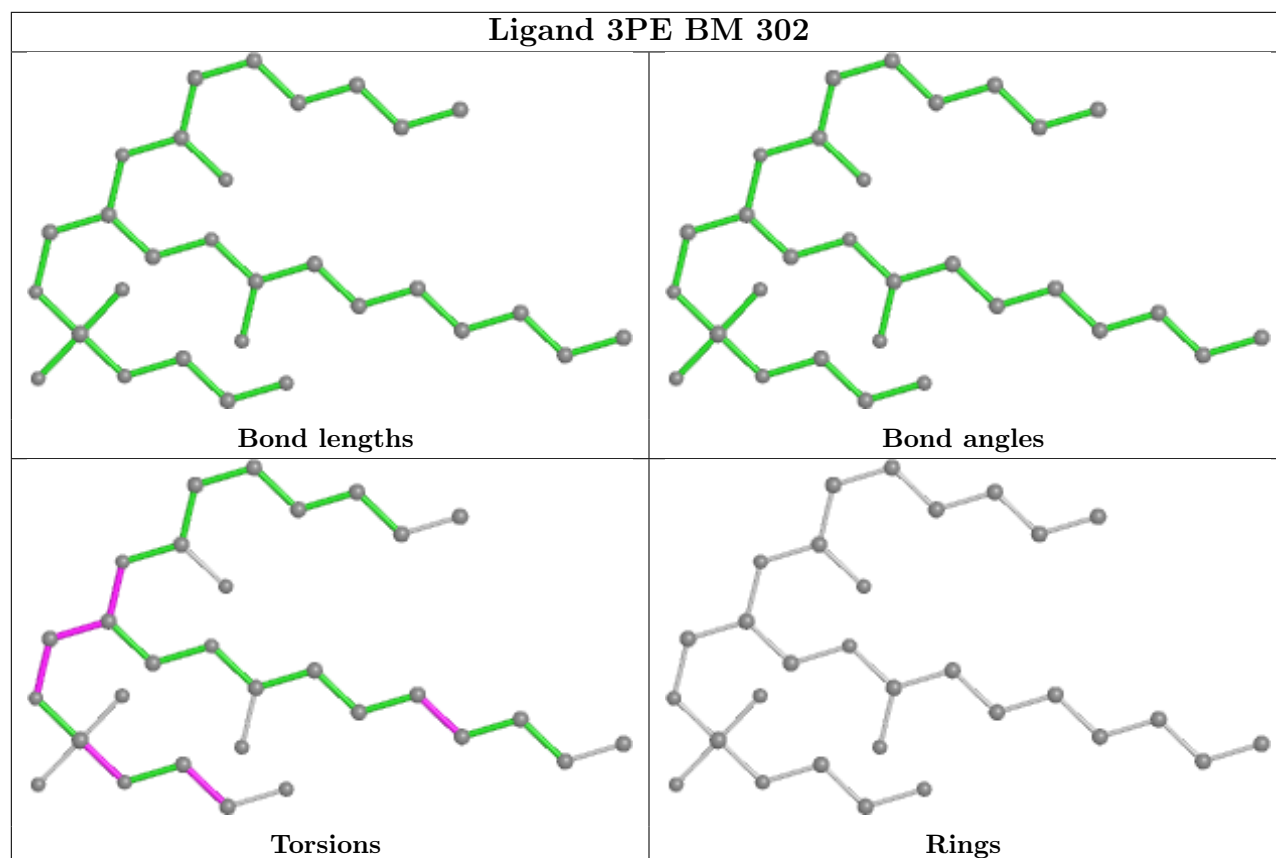
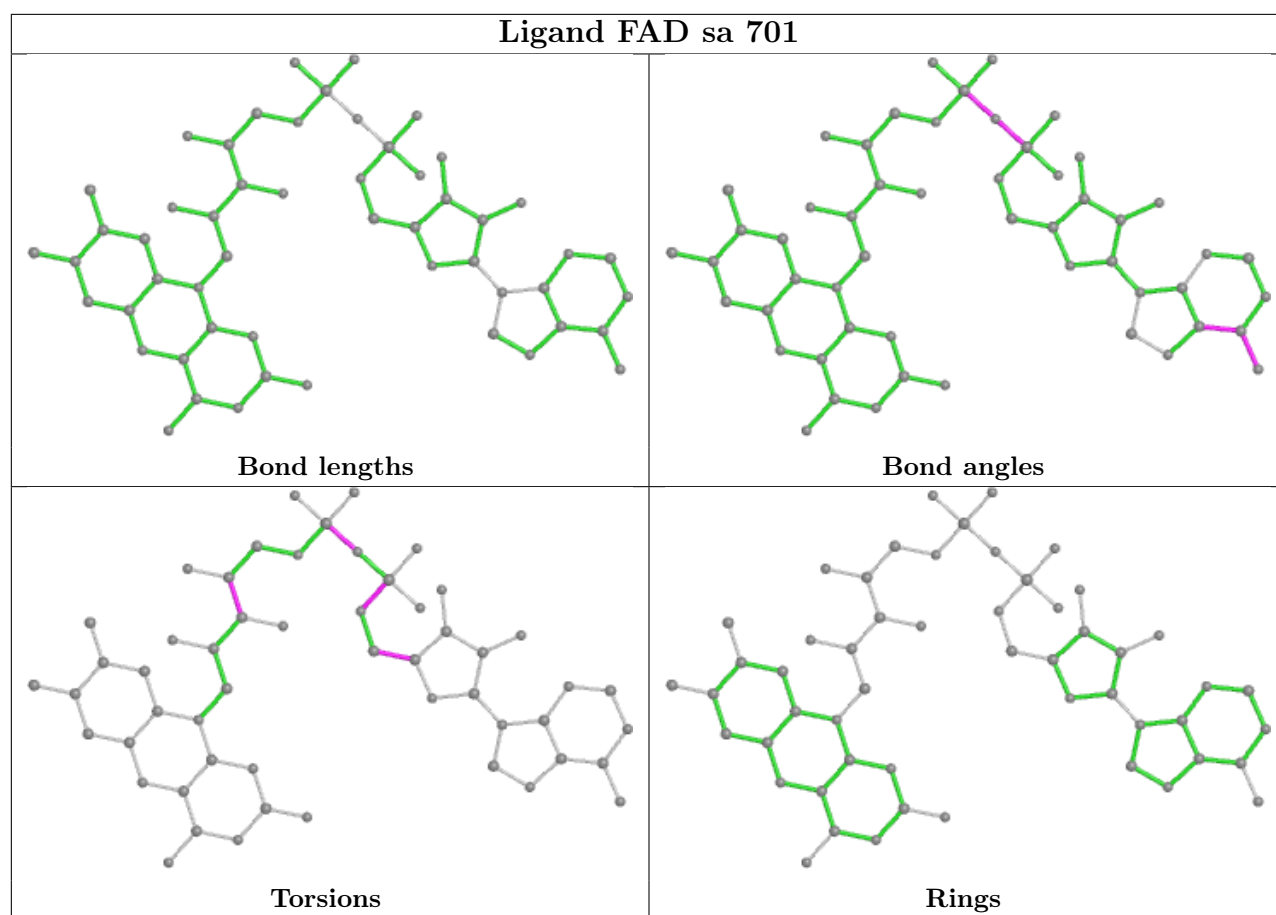


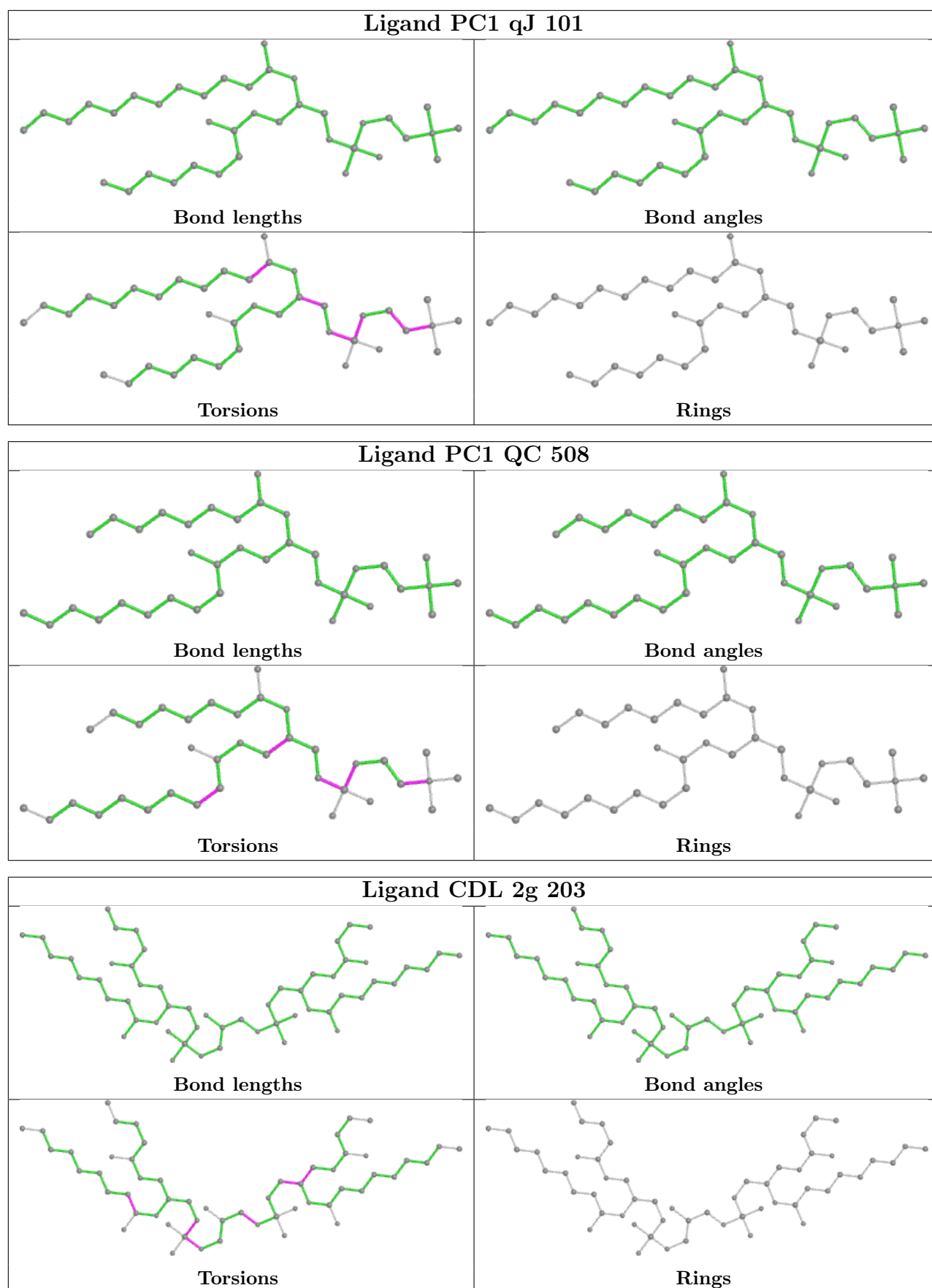


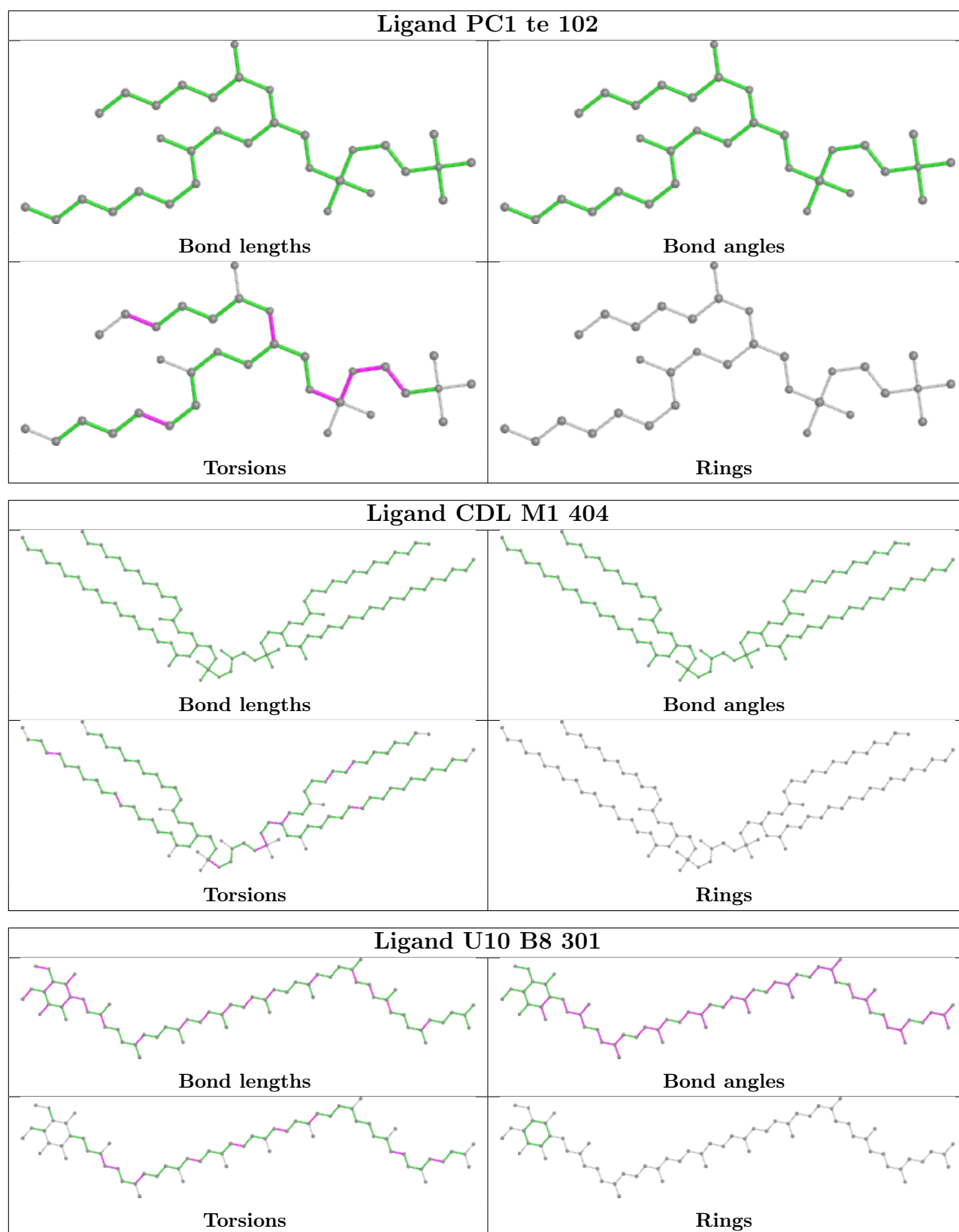


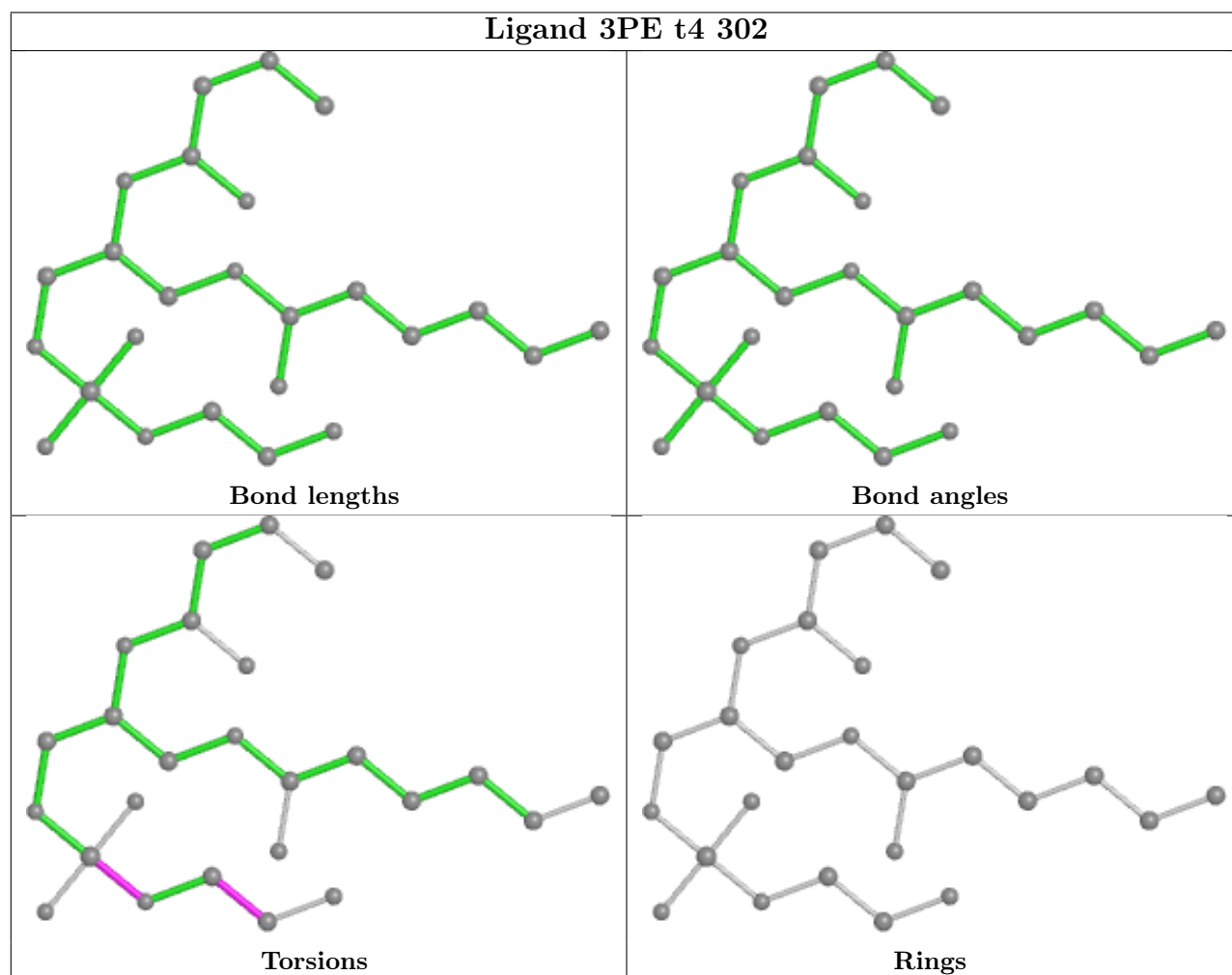
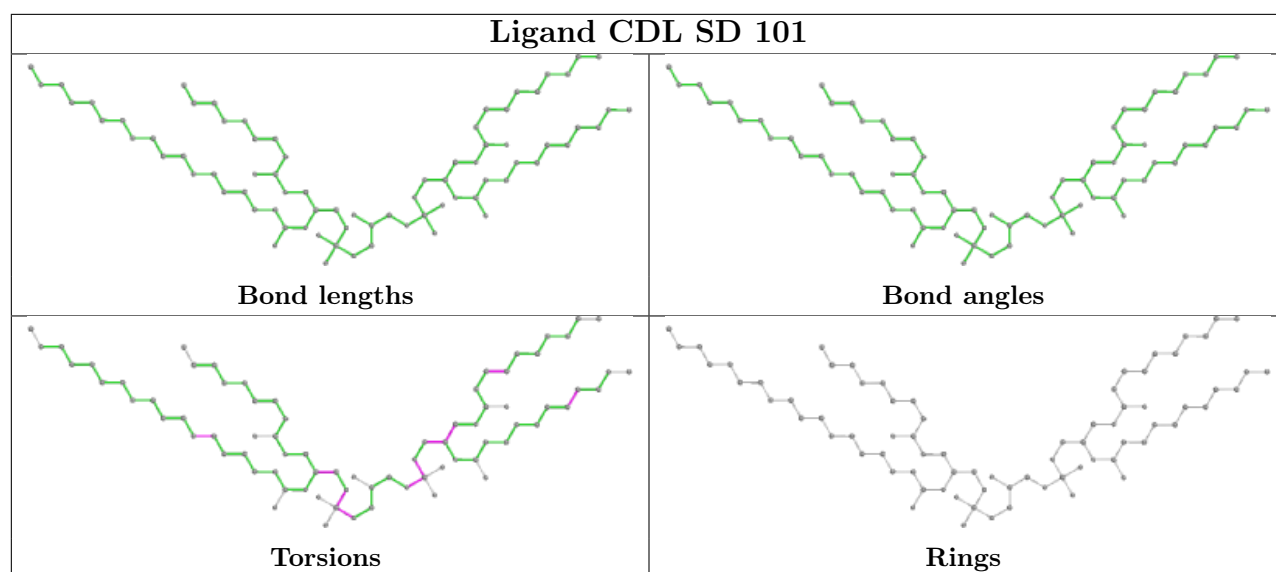


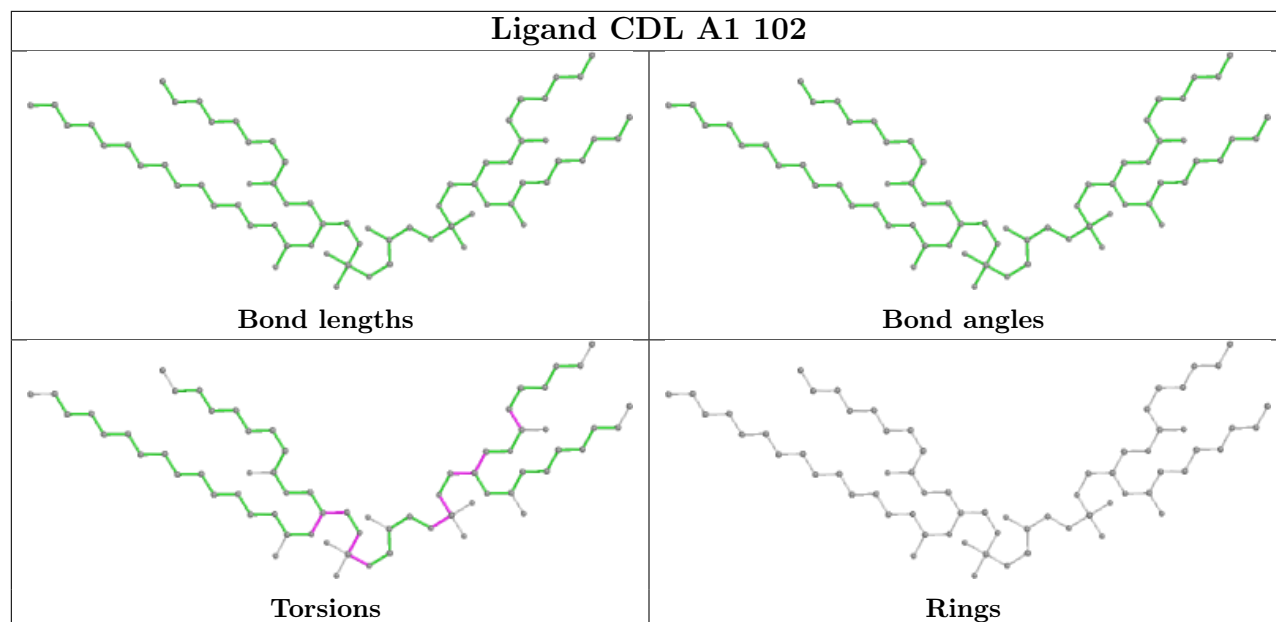
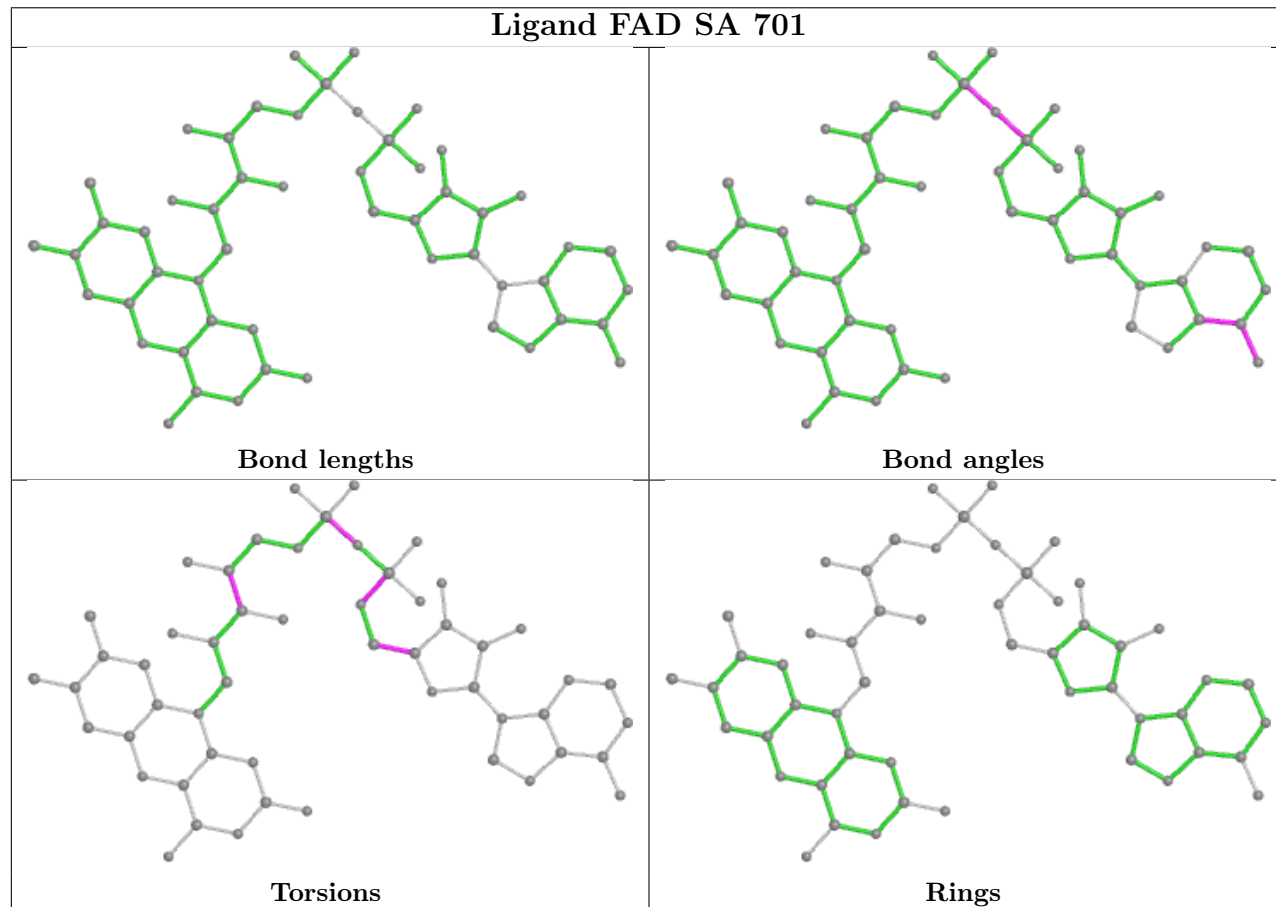


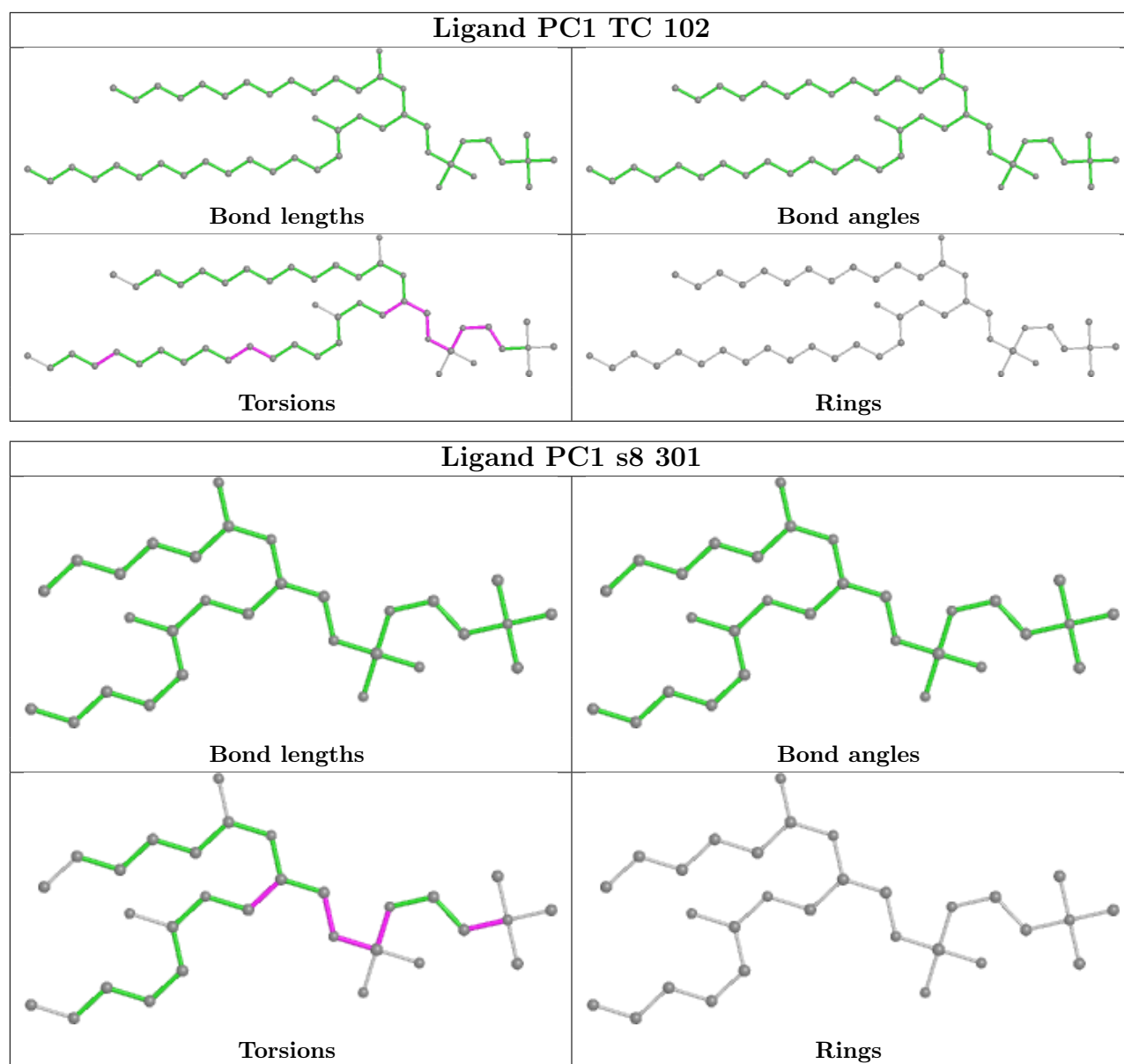


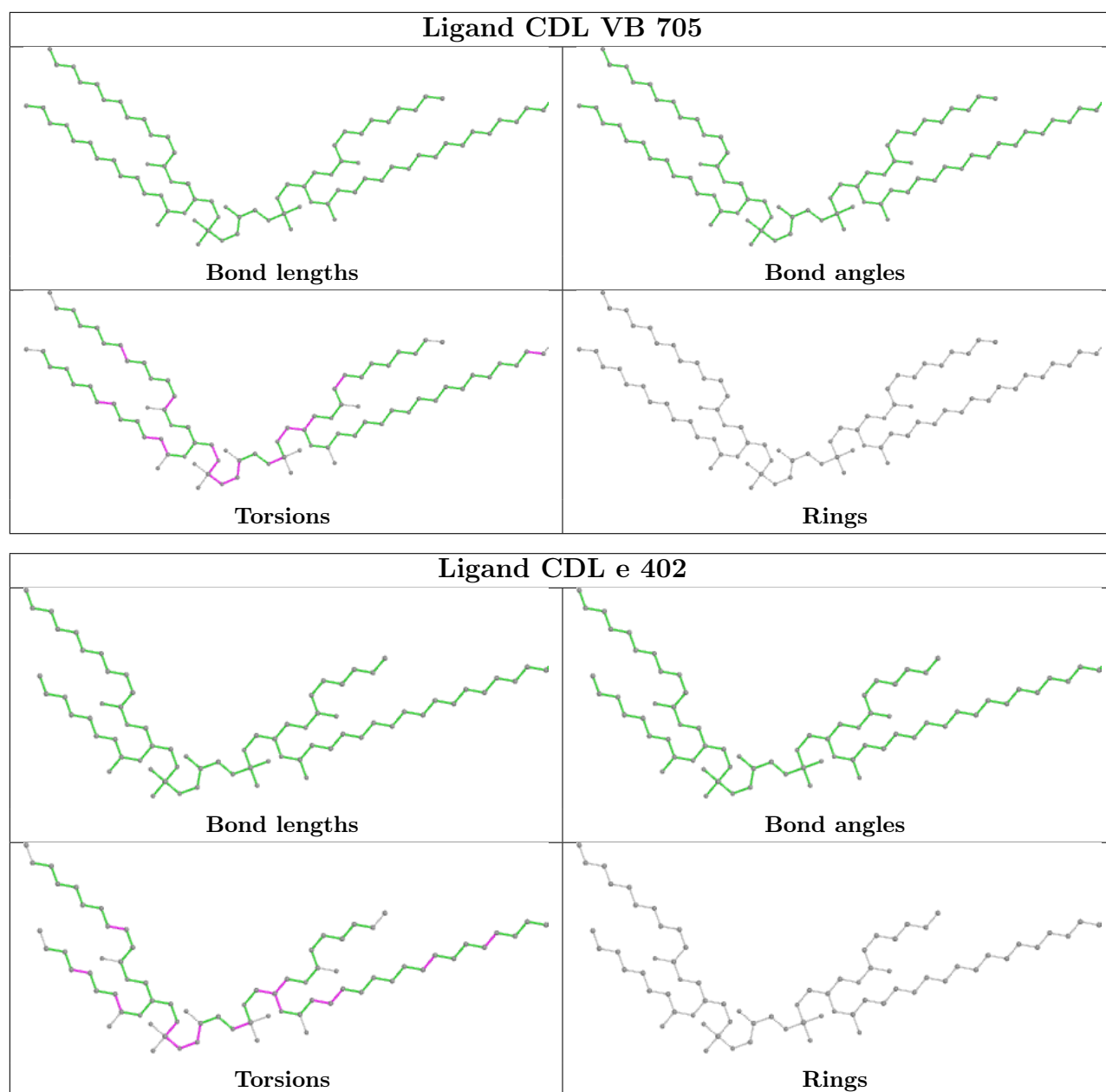


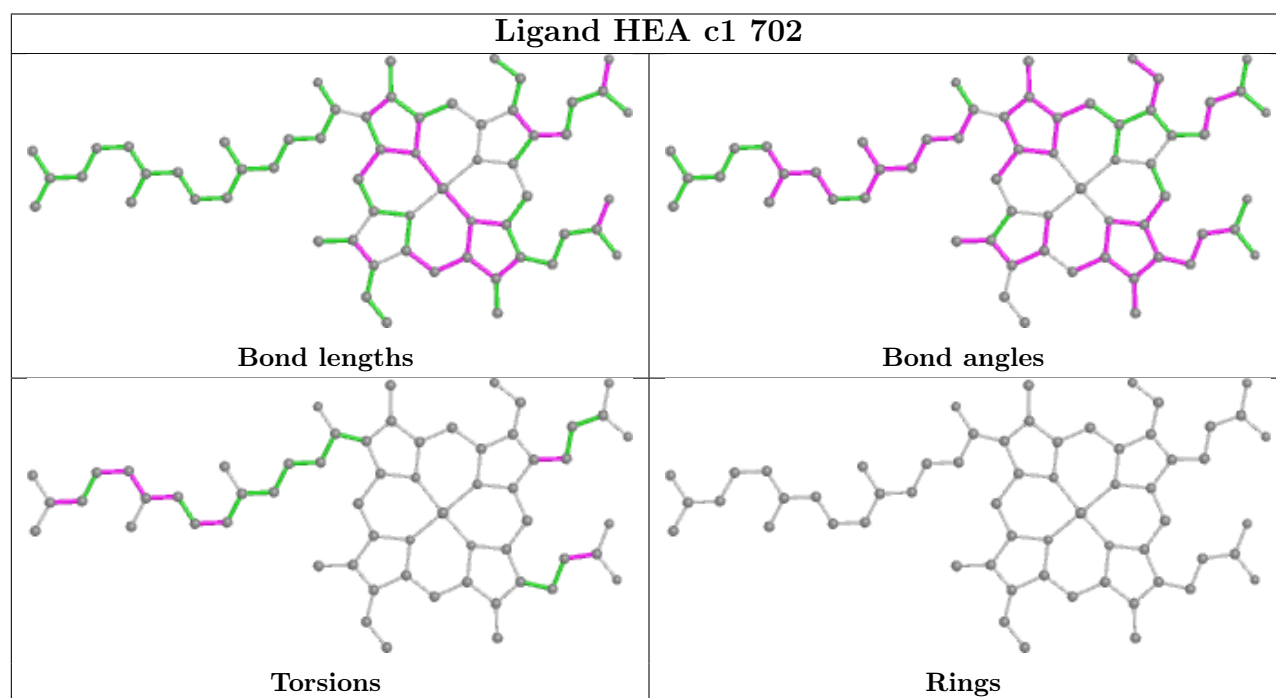
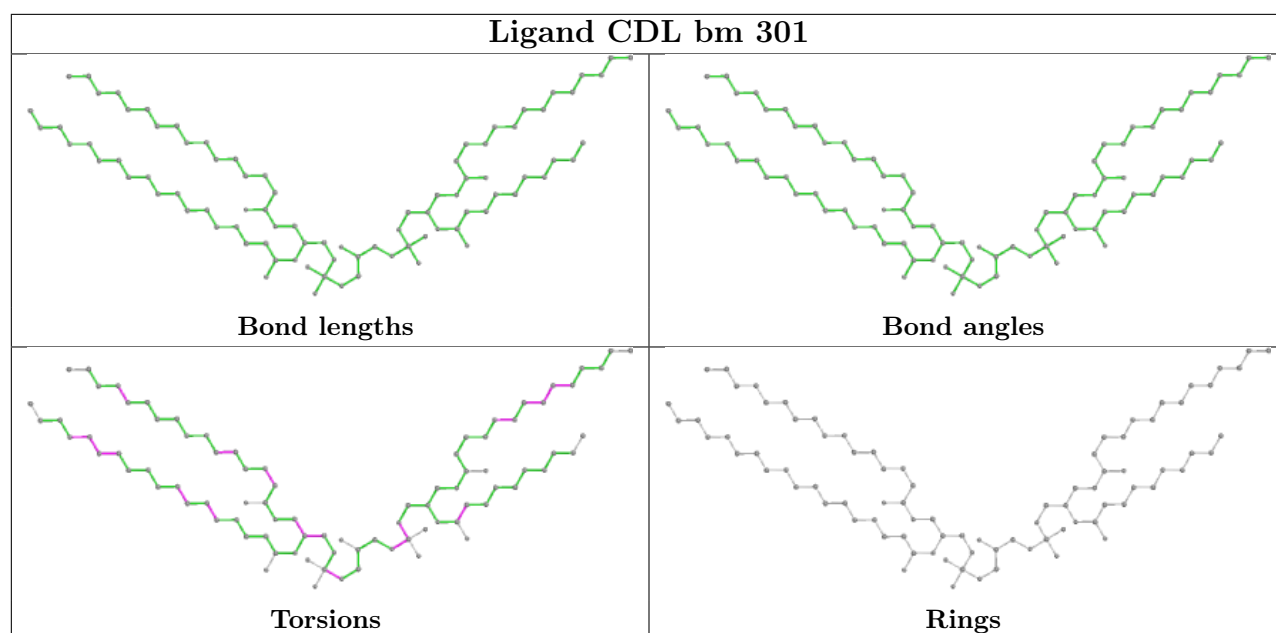


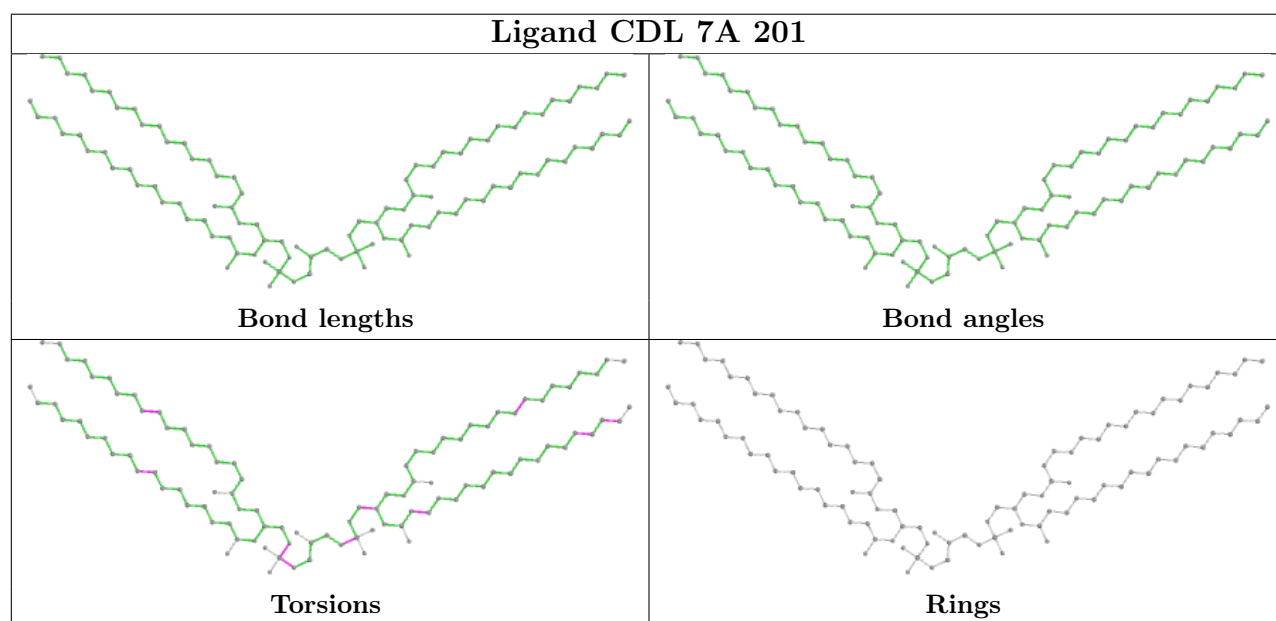
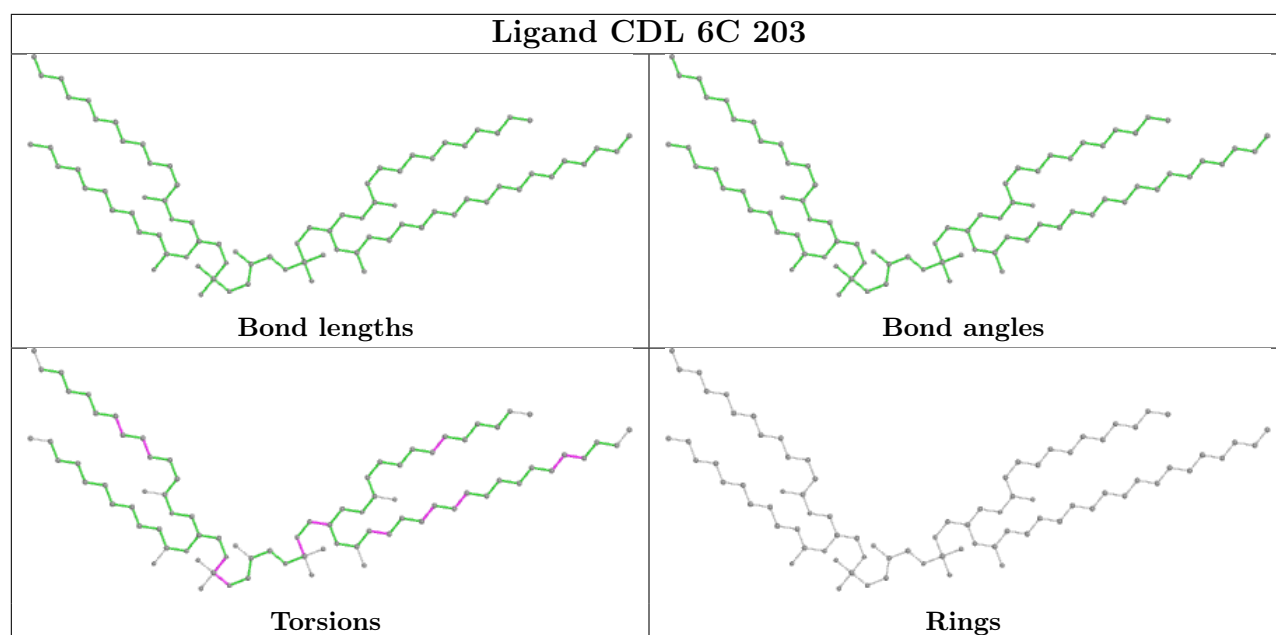


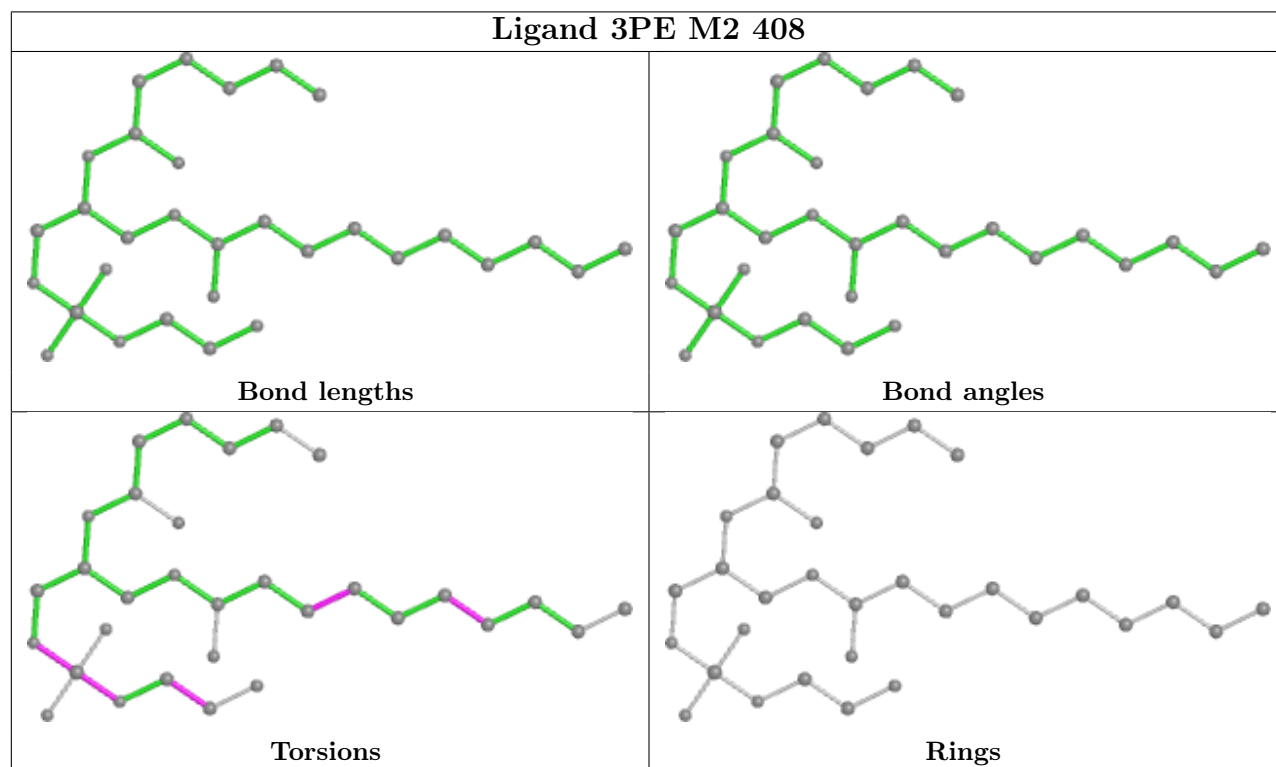
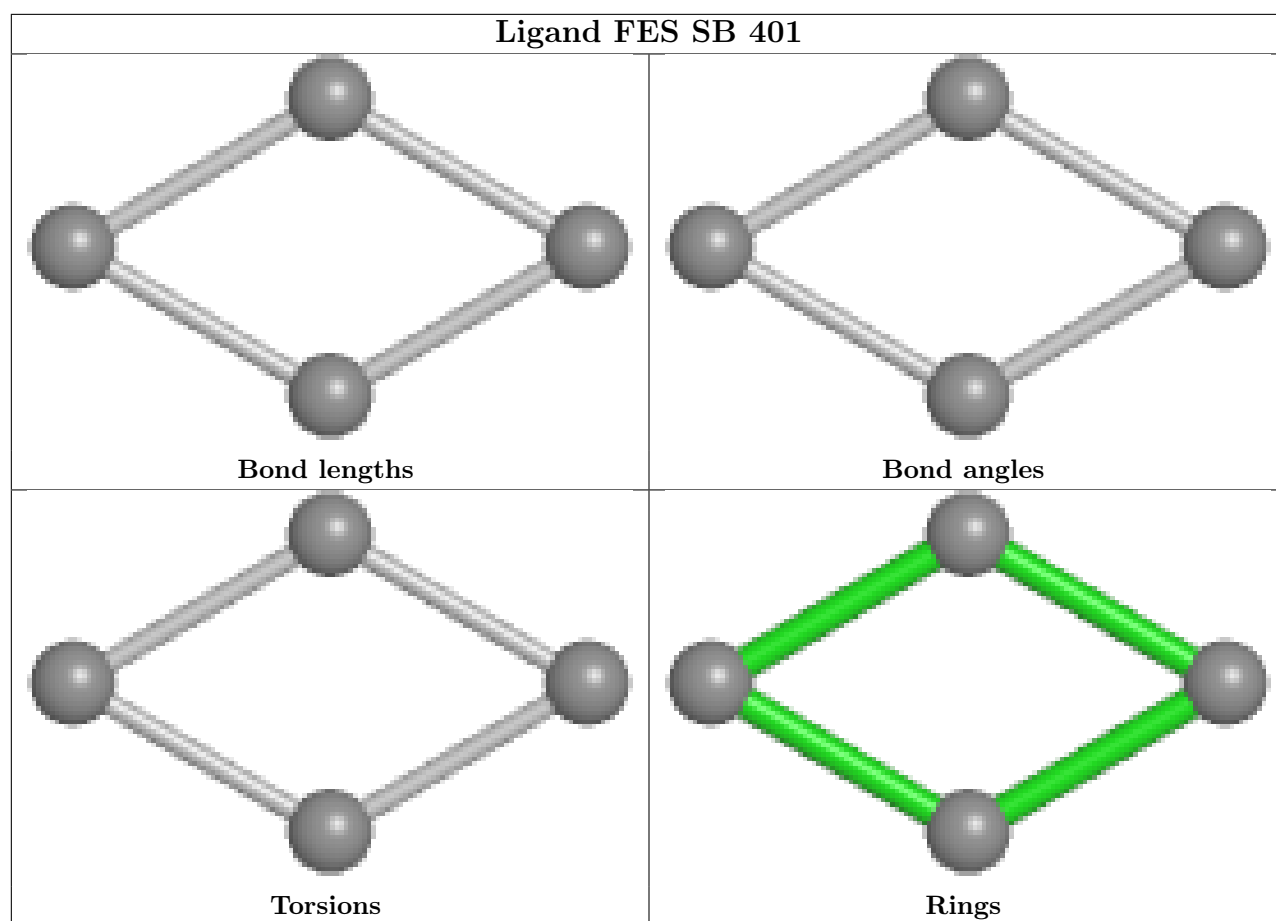
Ligand CDL A1 102**Ligand FAD SA 701**

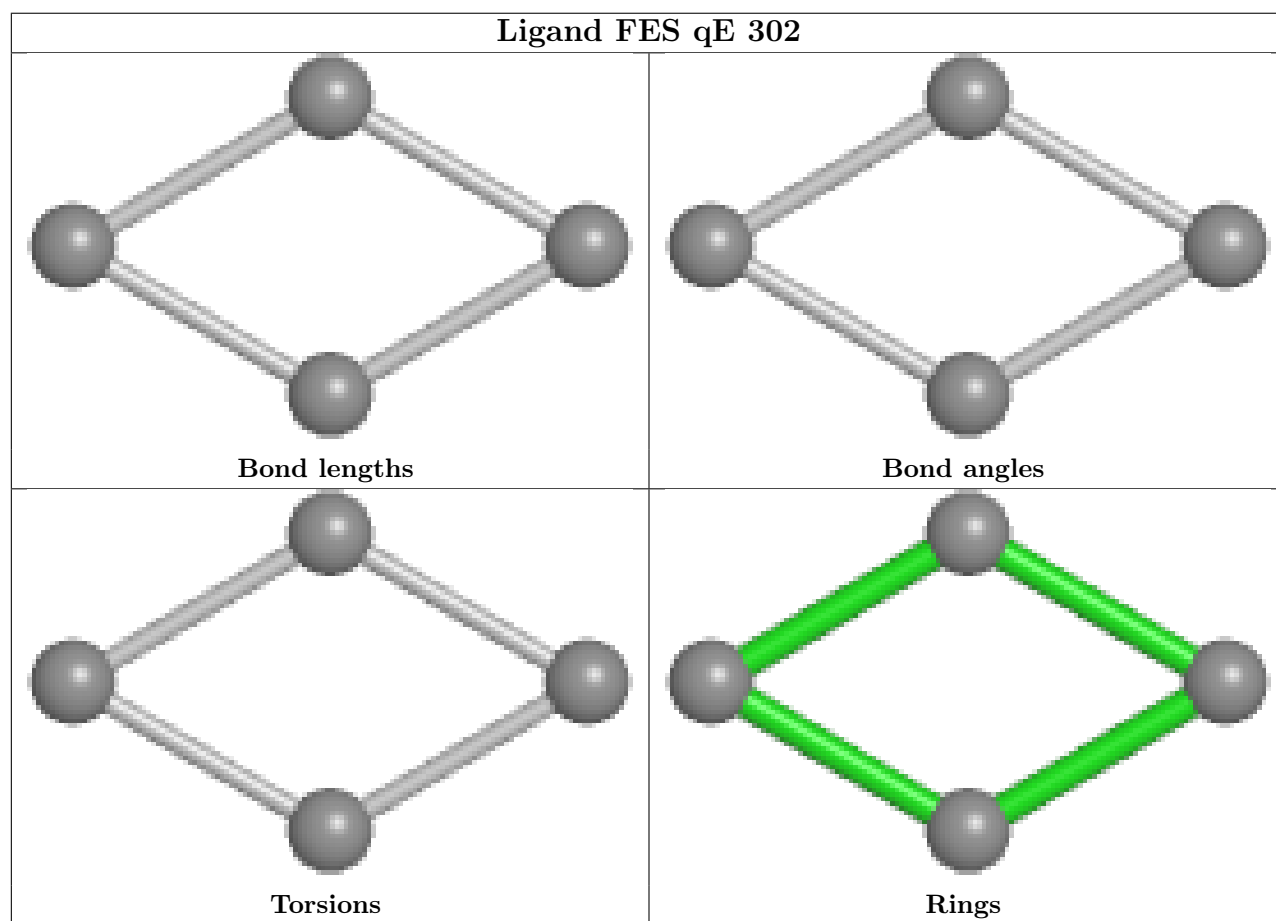
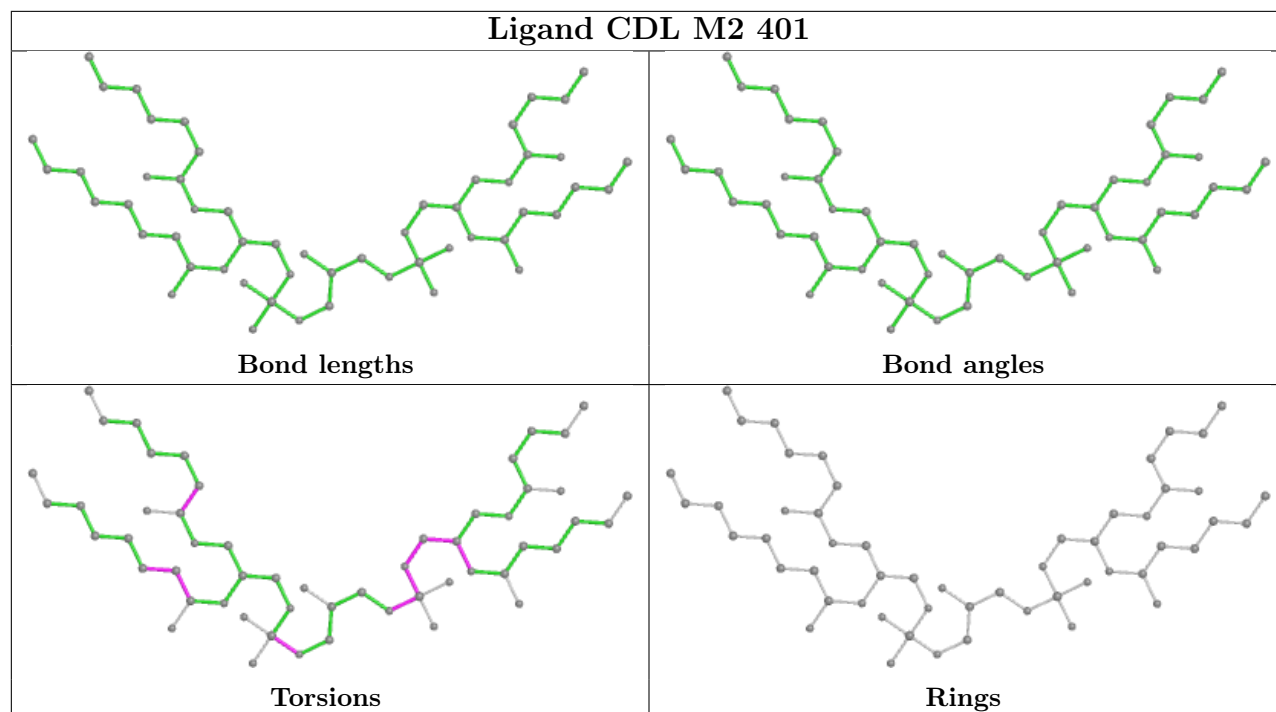


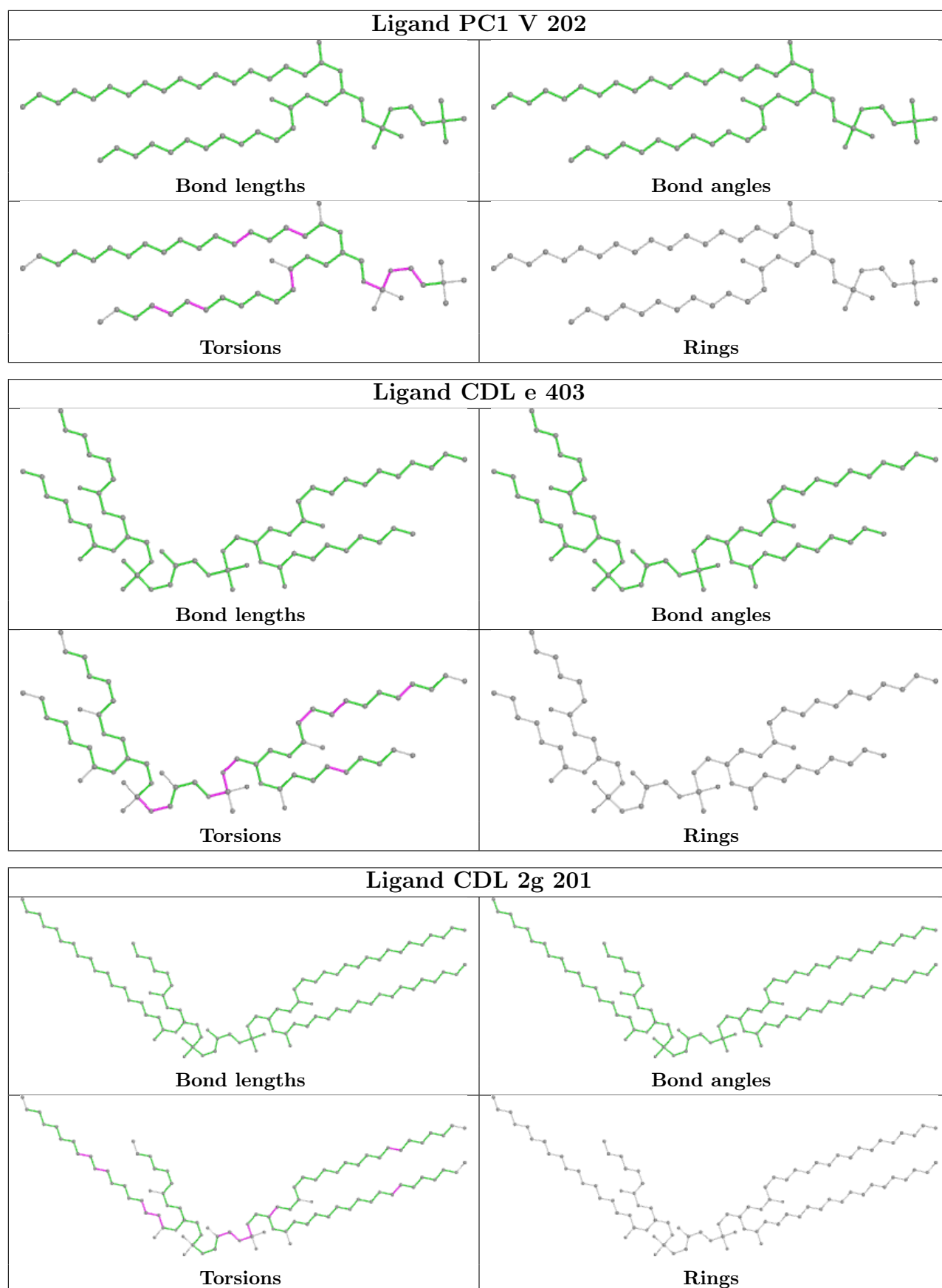




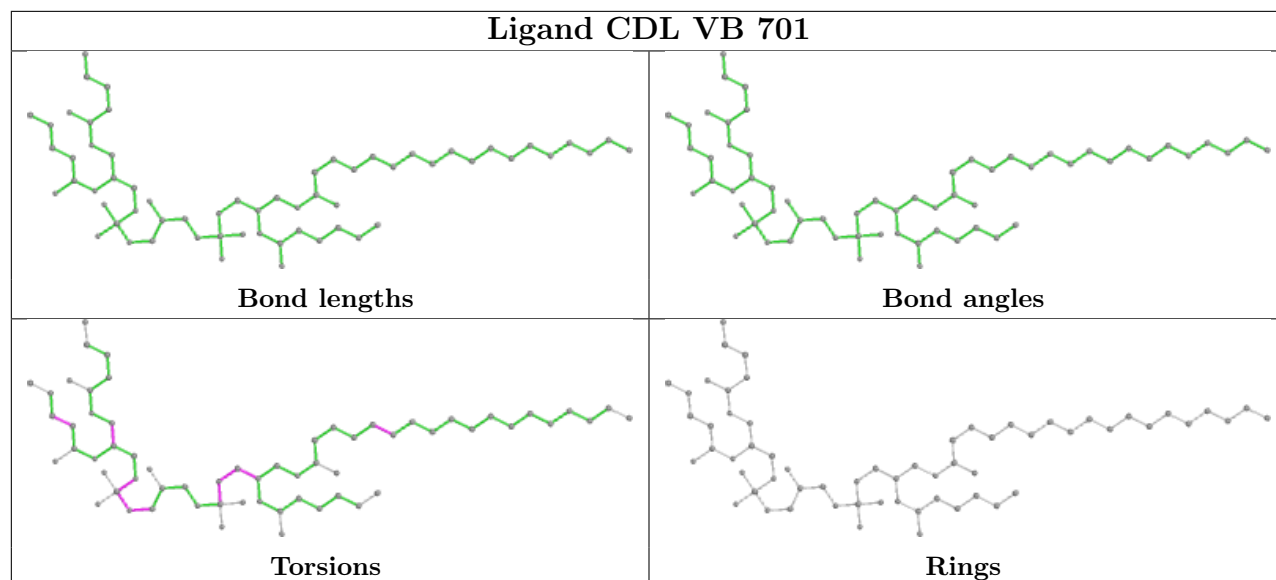




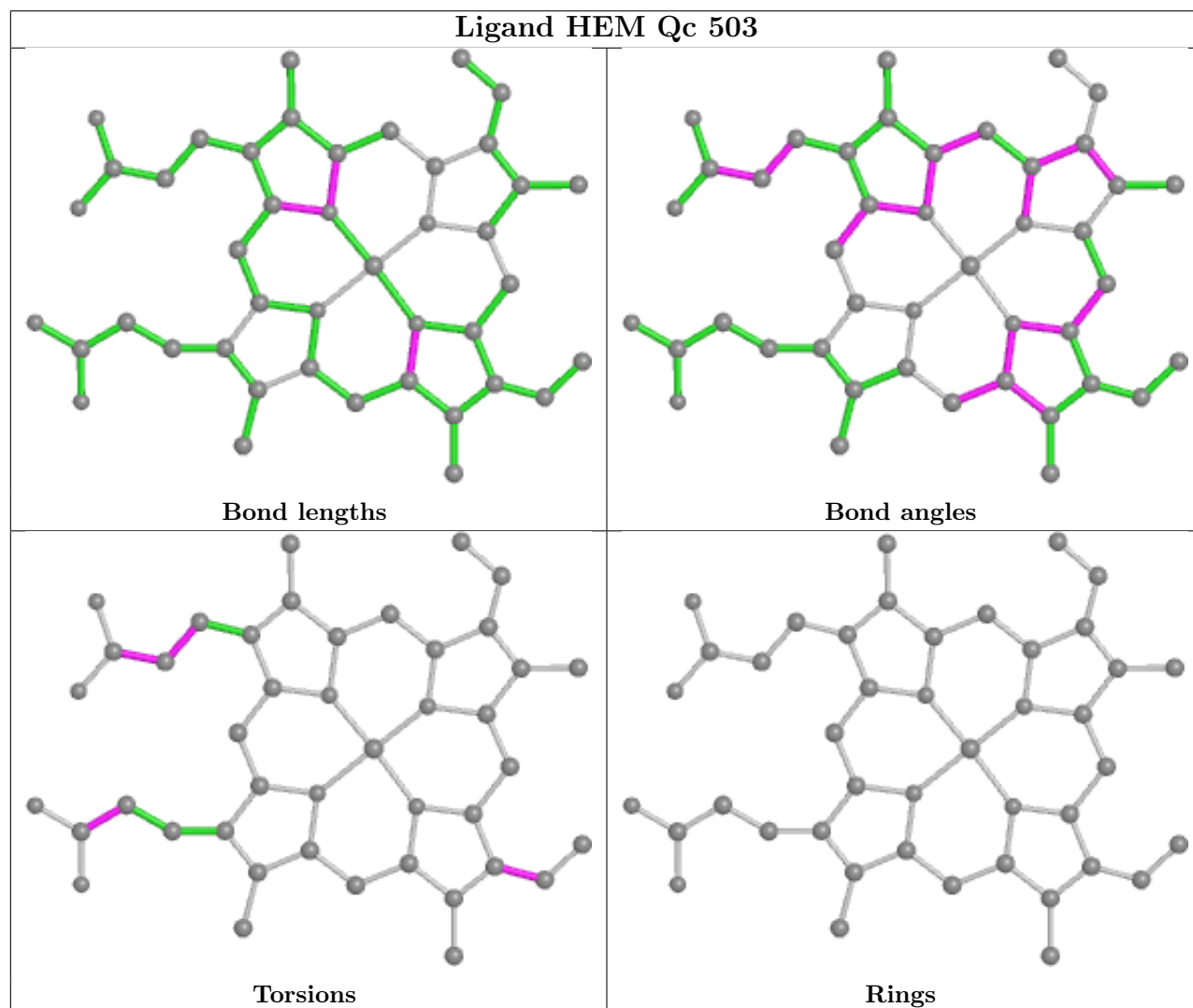


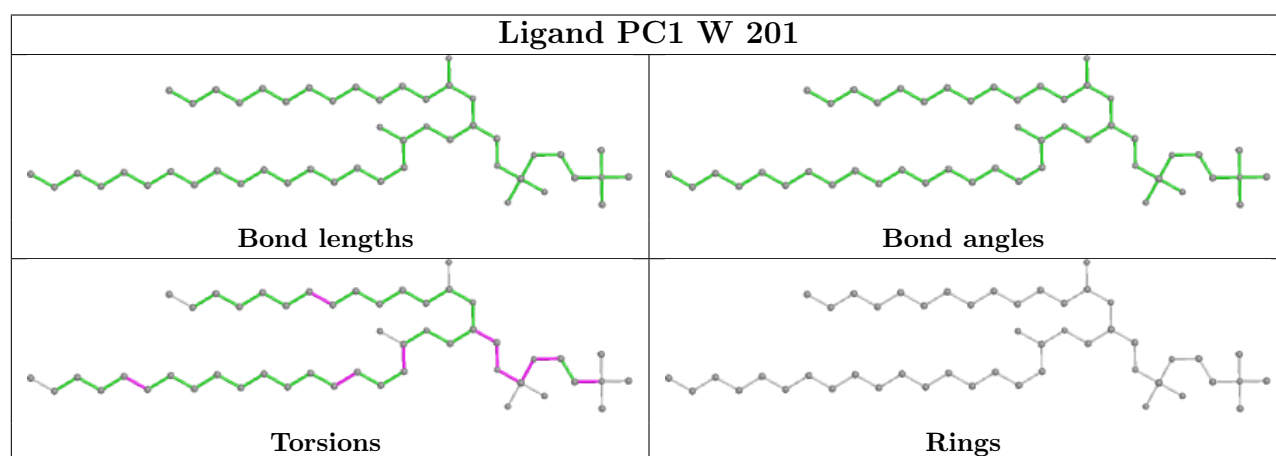
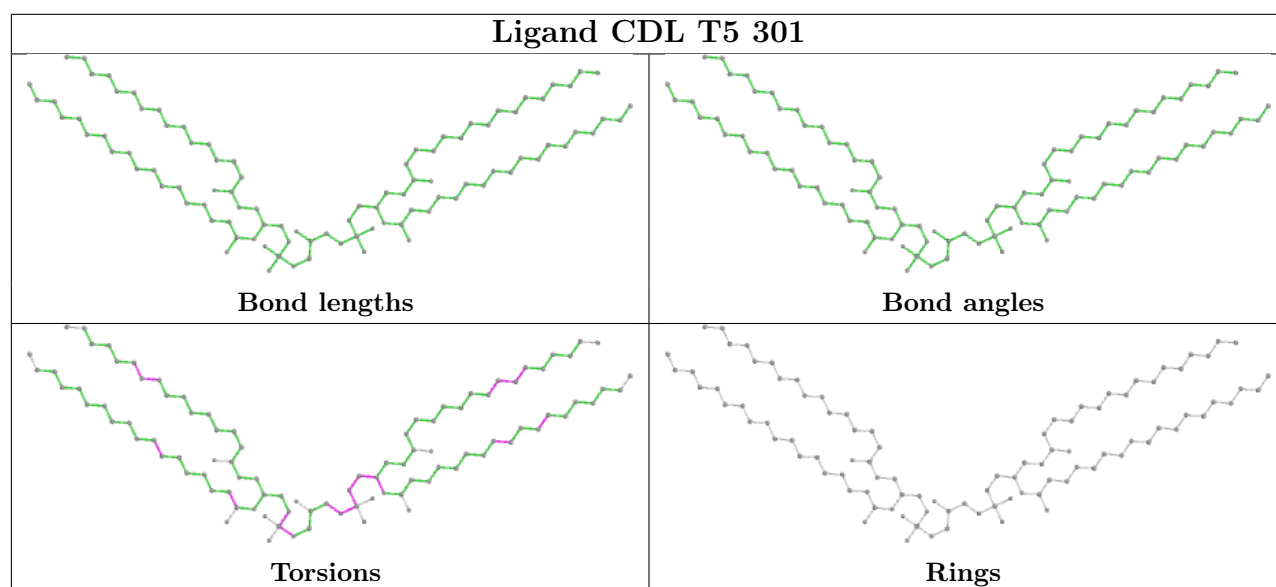


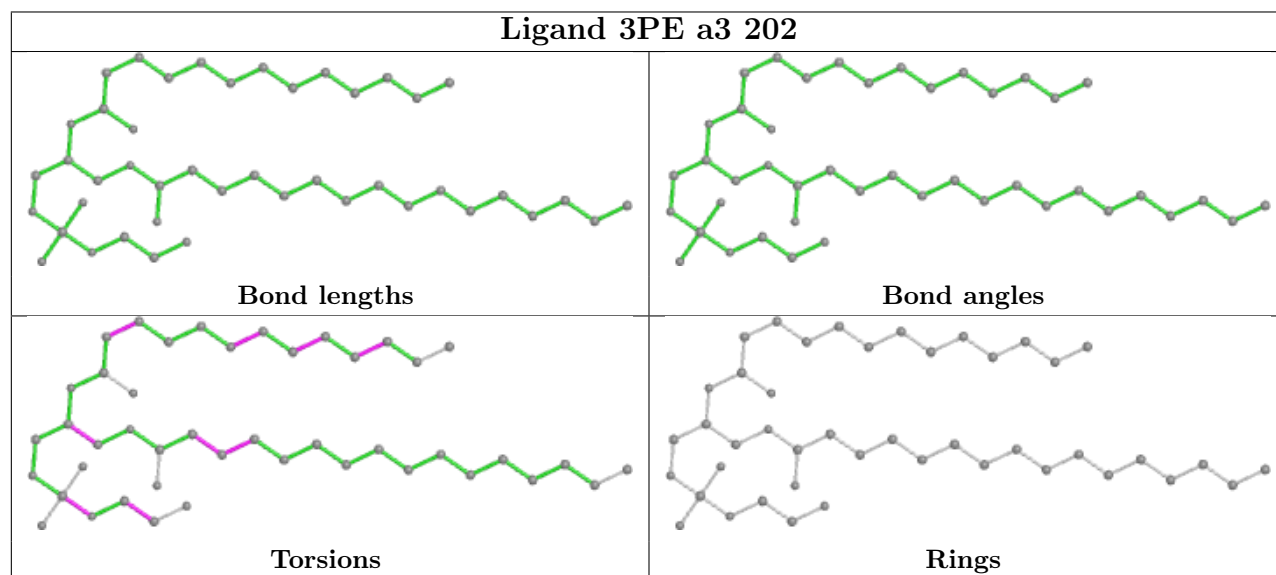
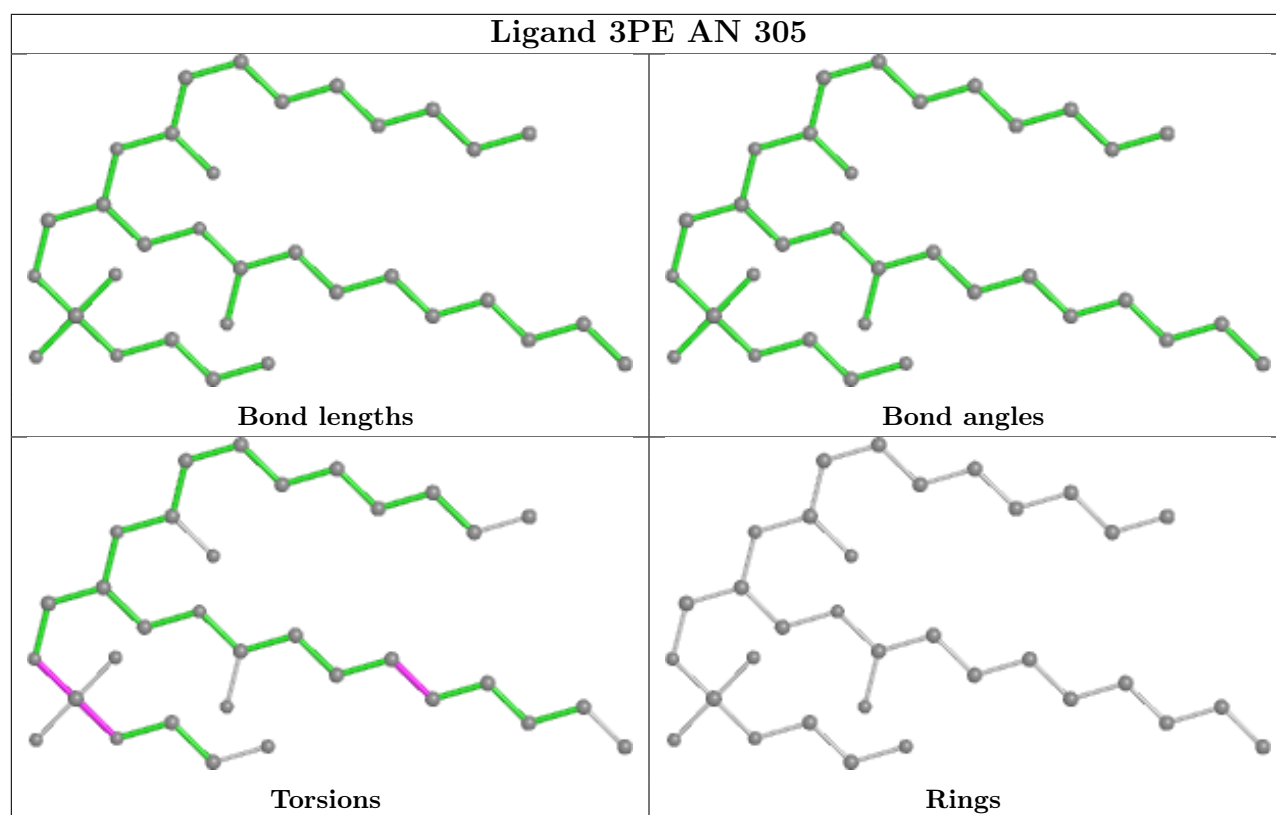
Ligand CDL VB 701

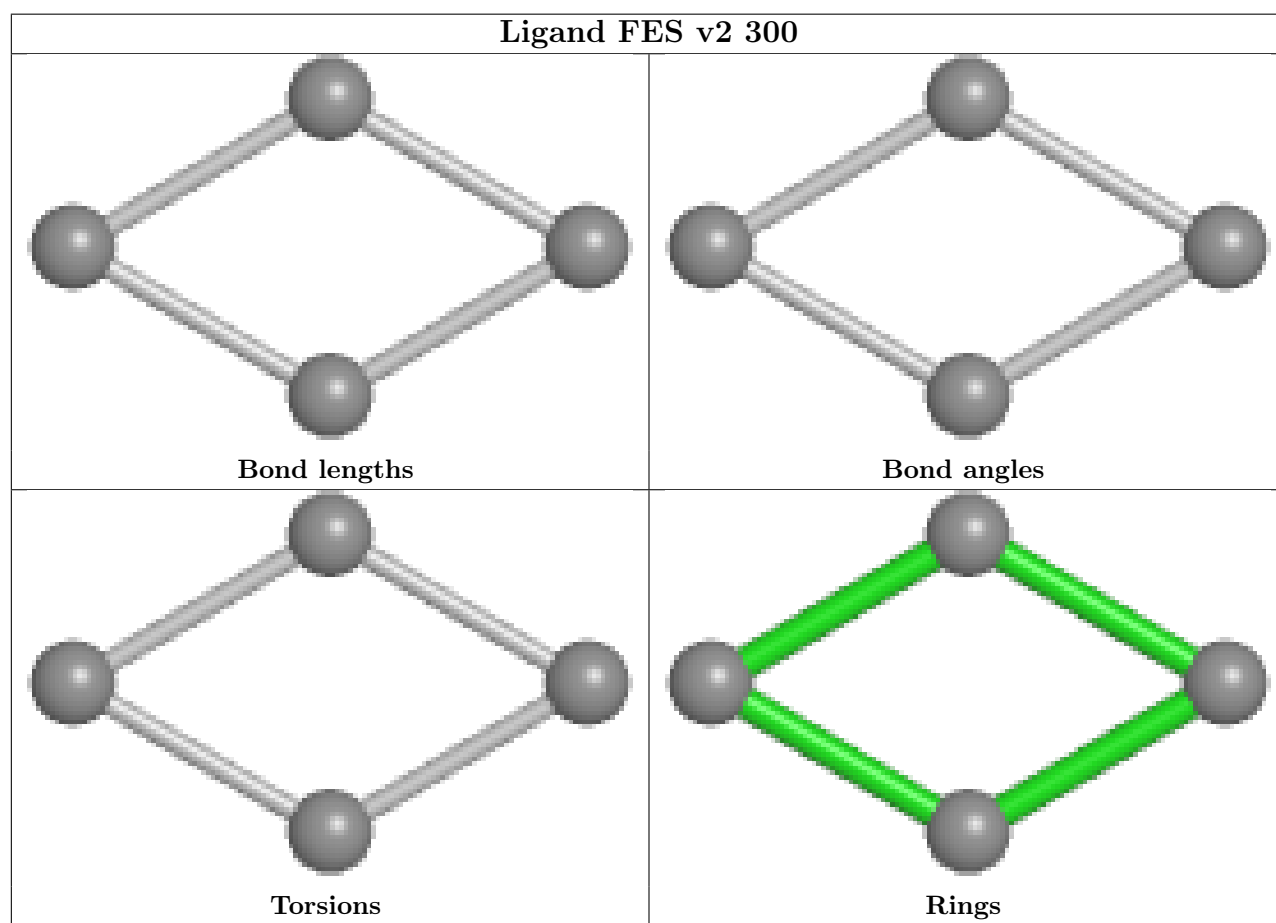
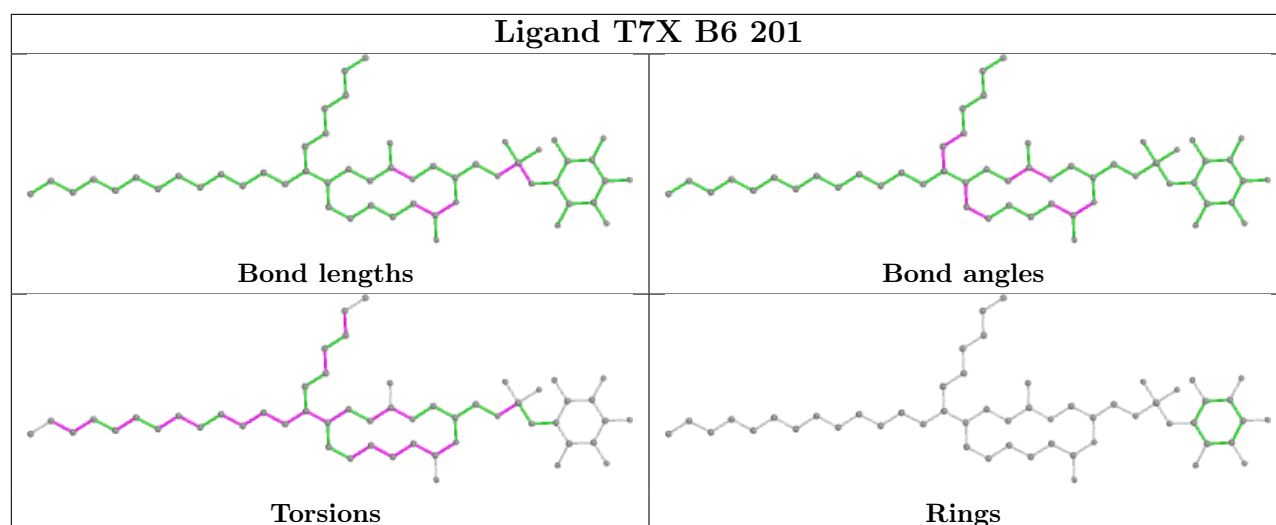


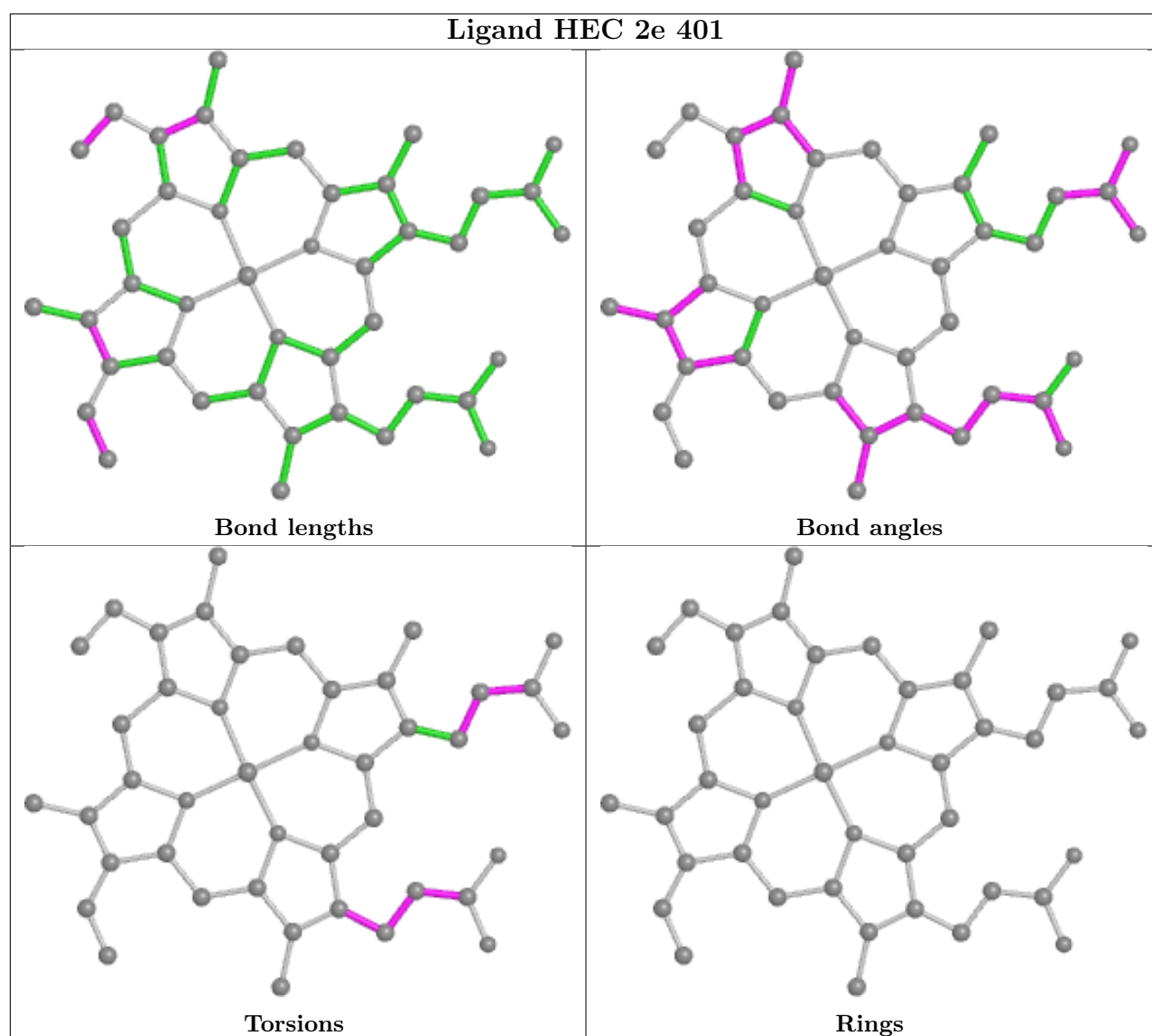
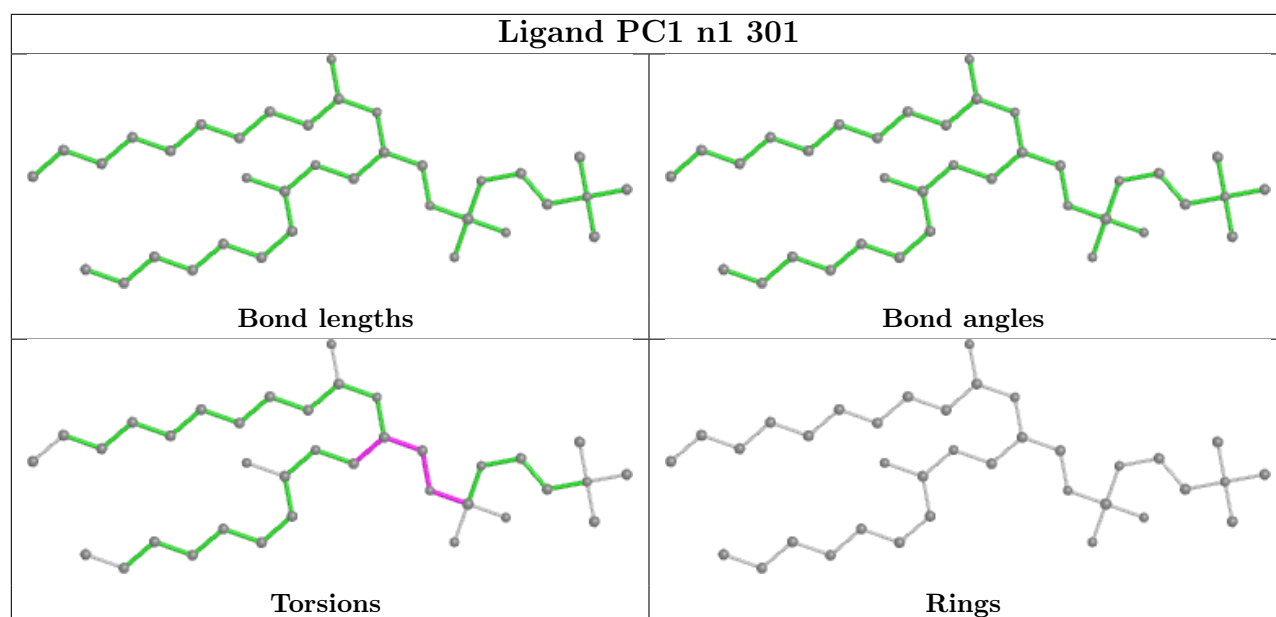
Ligand HEM Qc 503

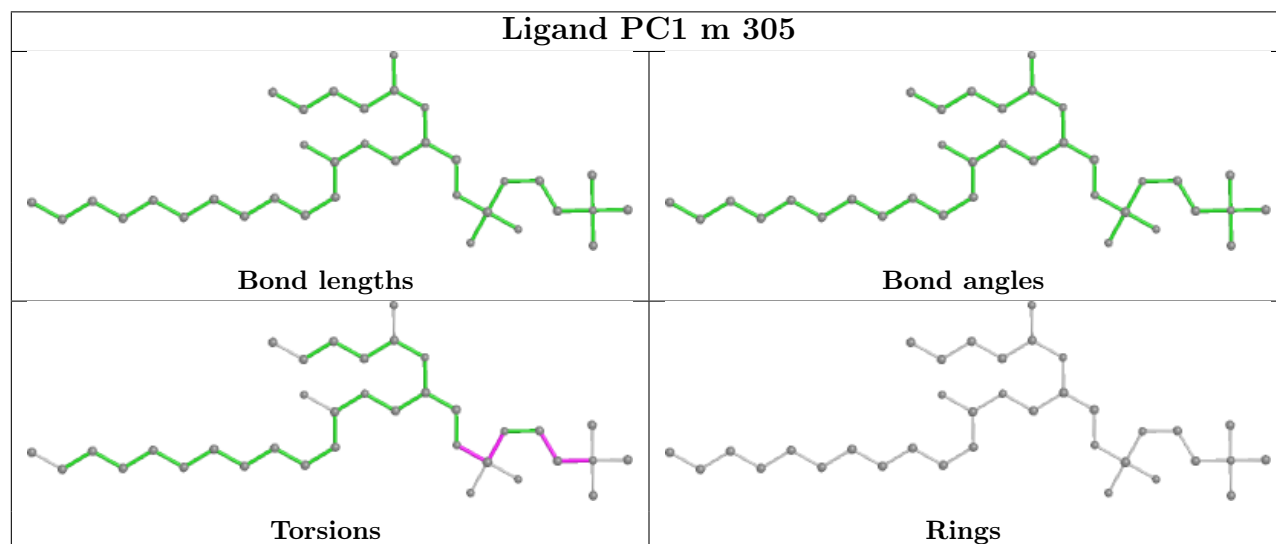
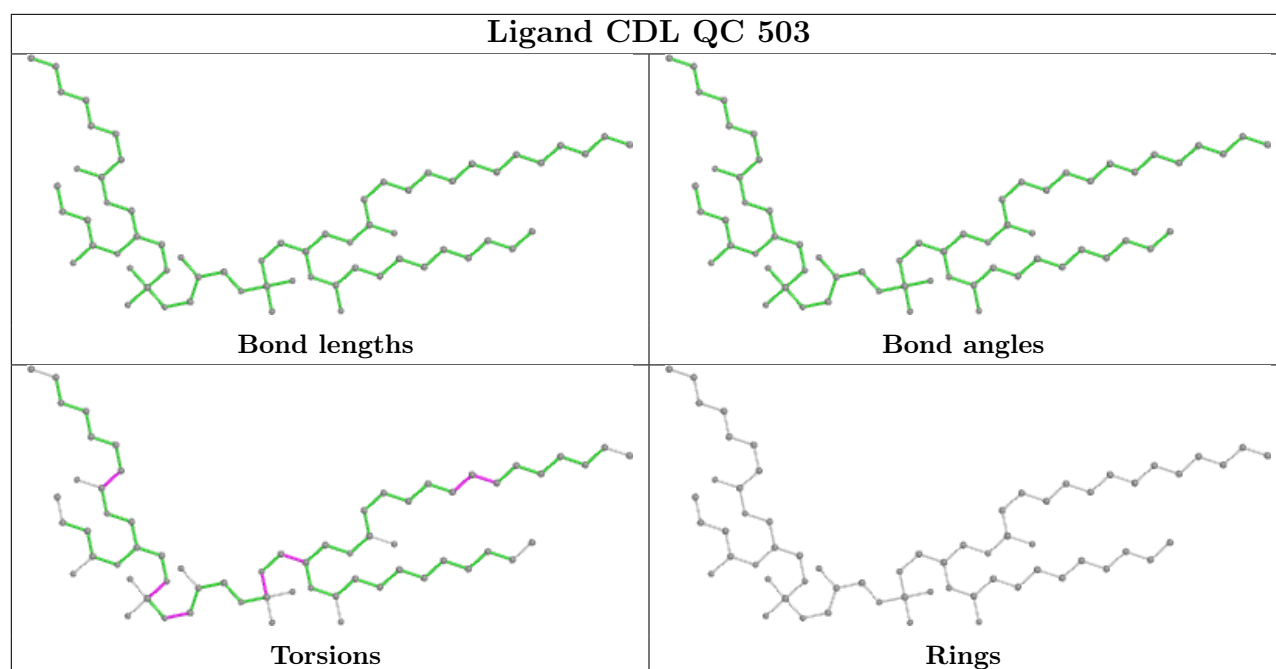


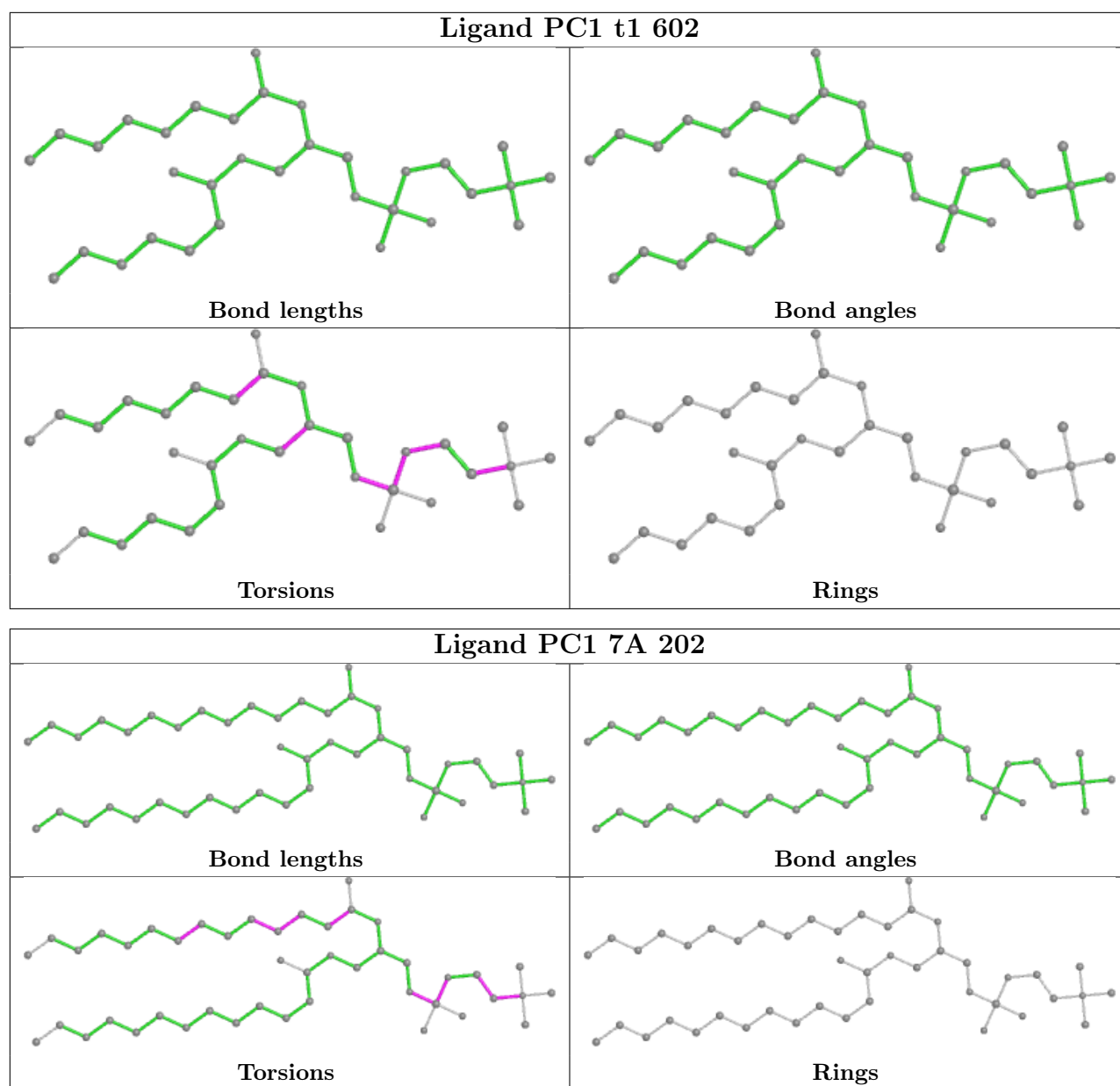


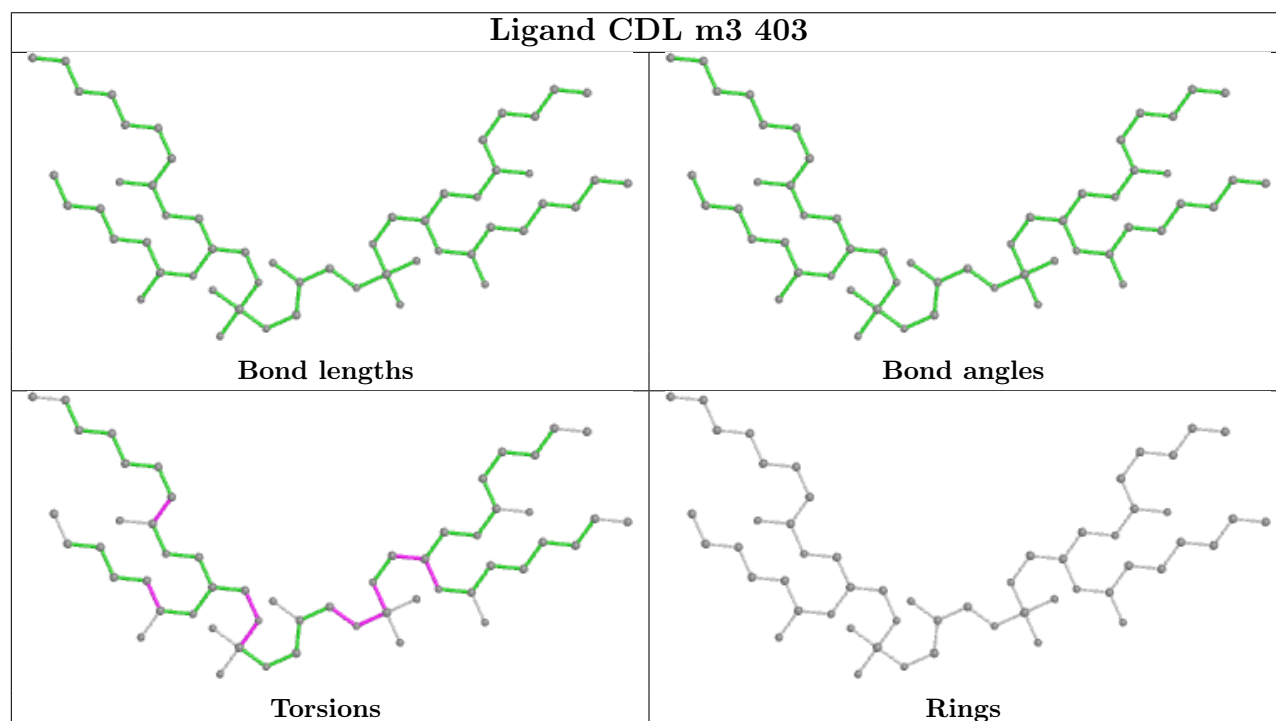
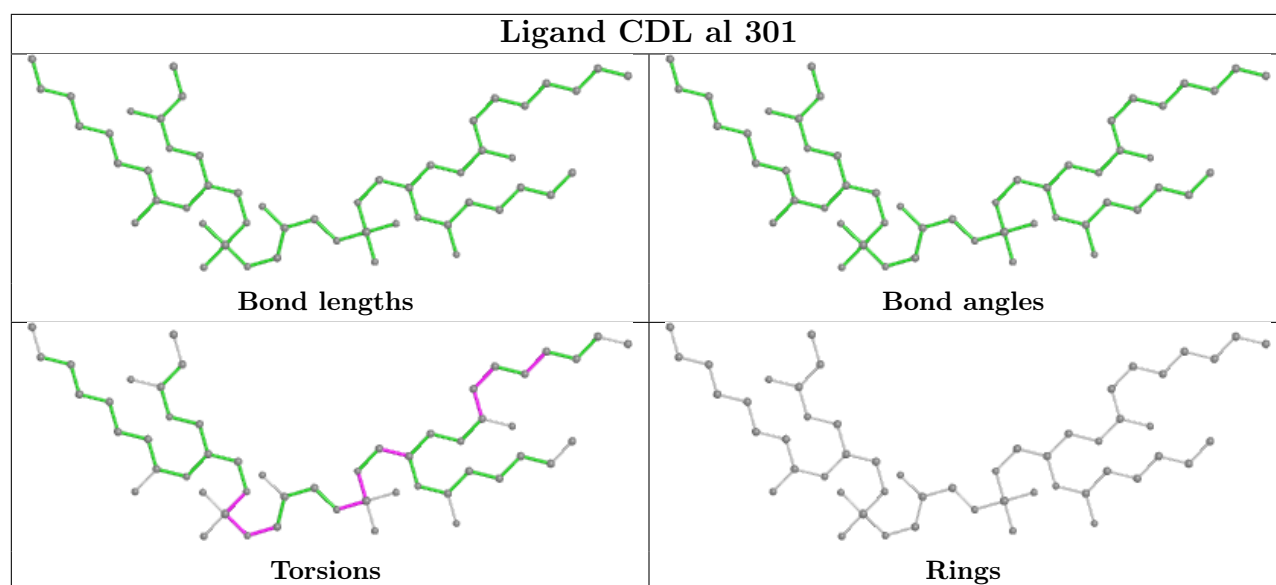


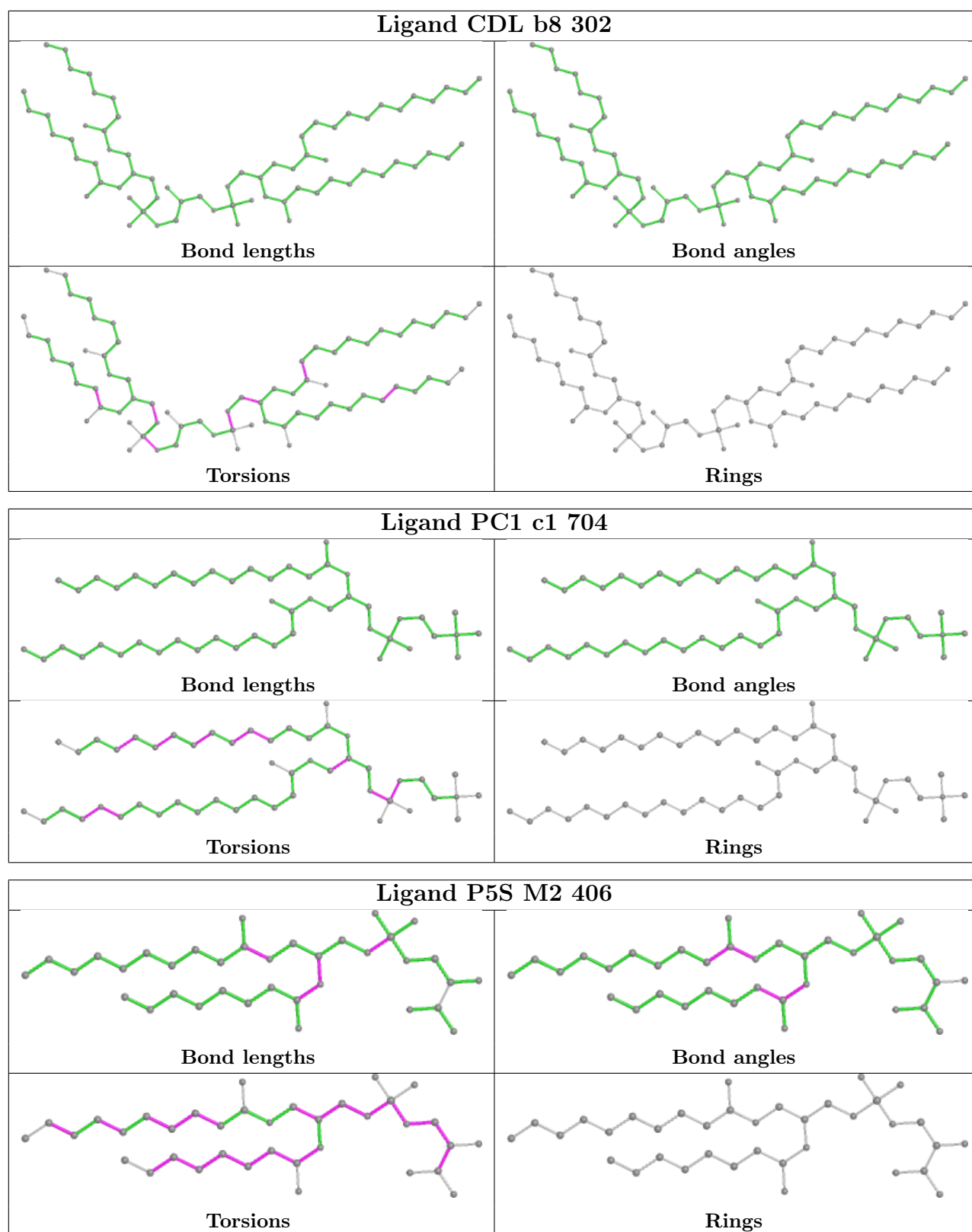


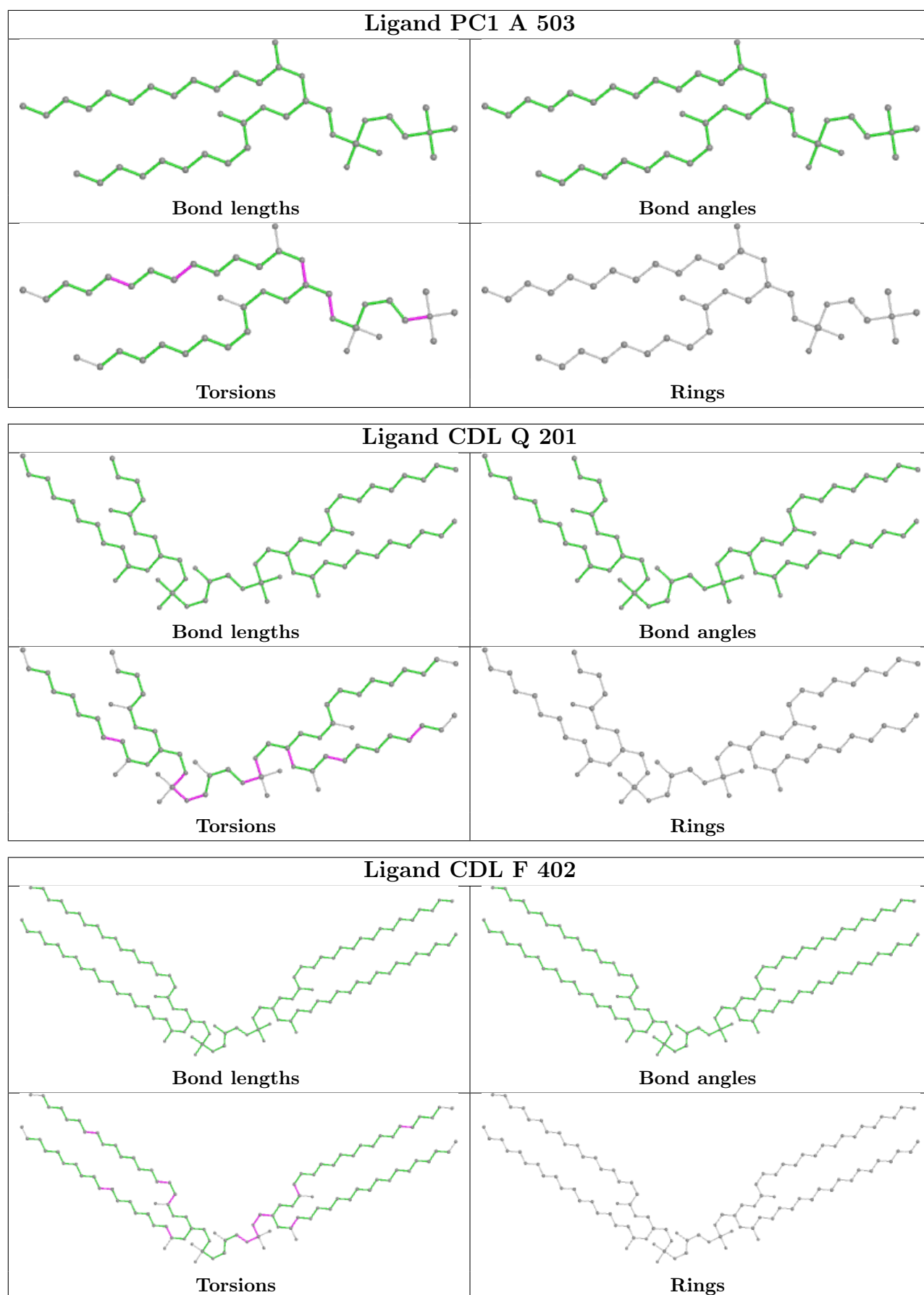


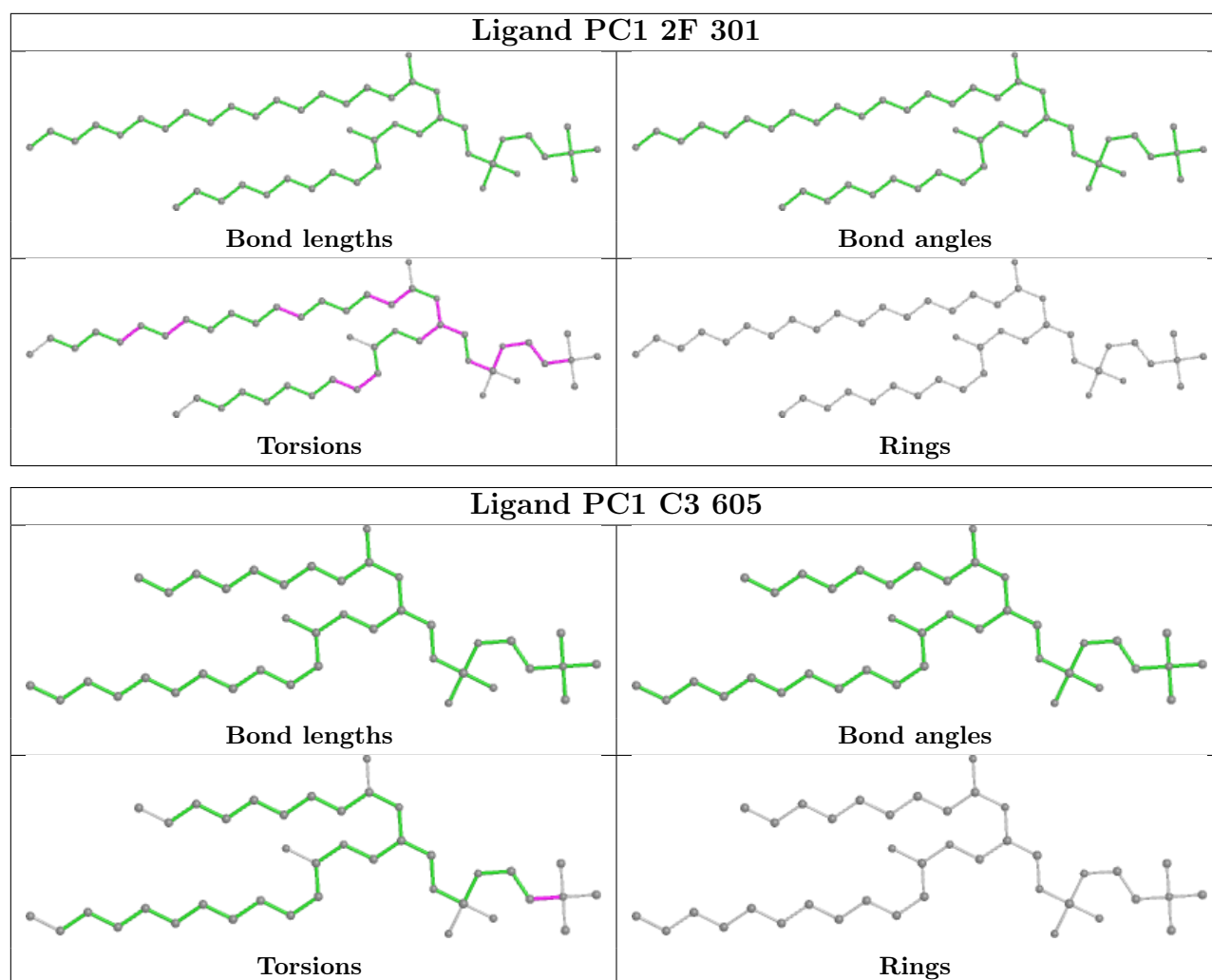




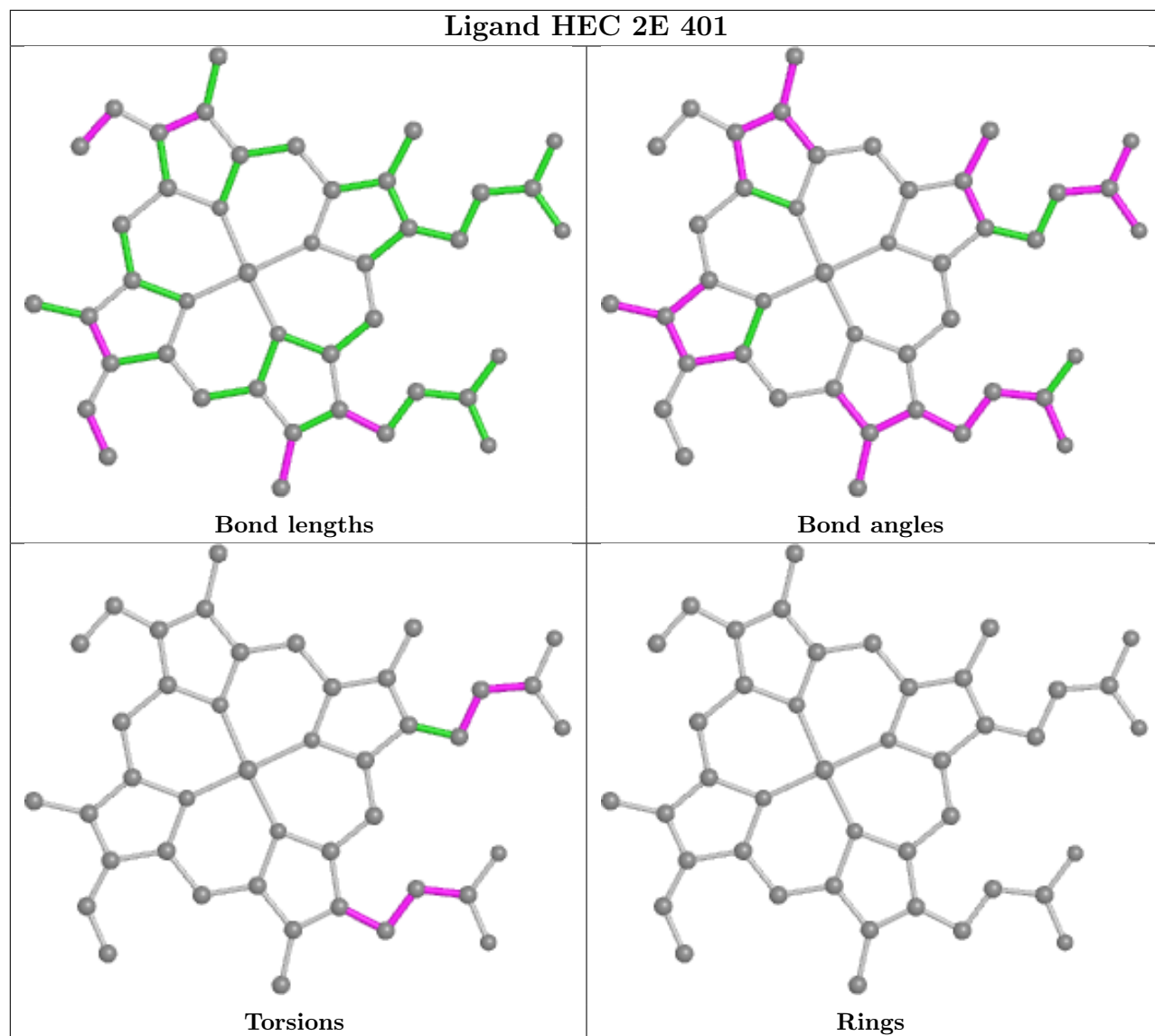




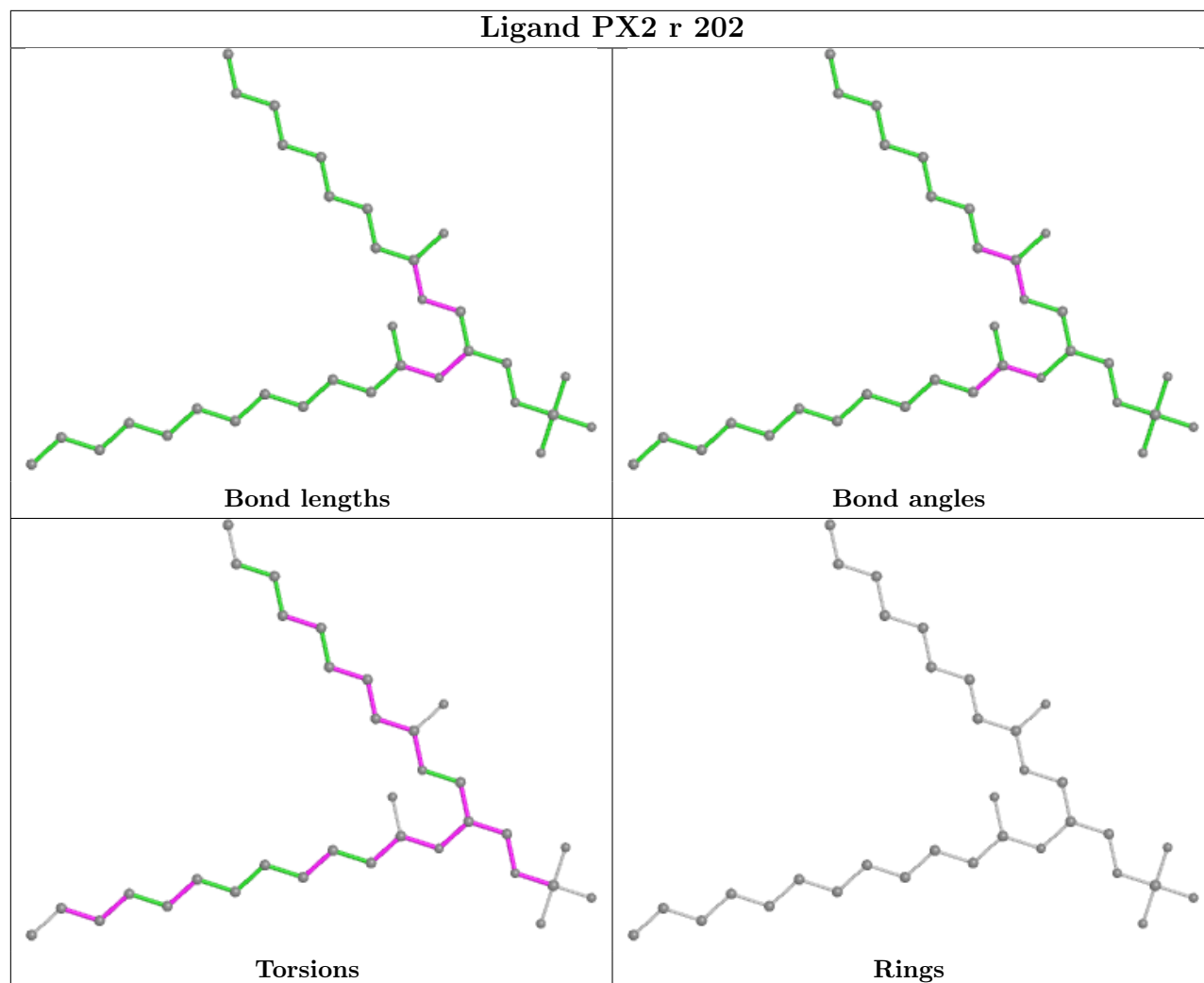




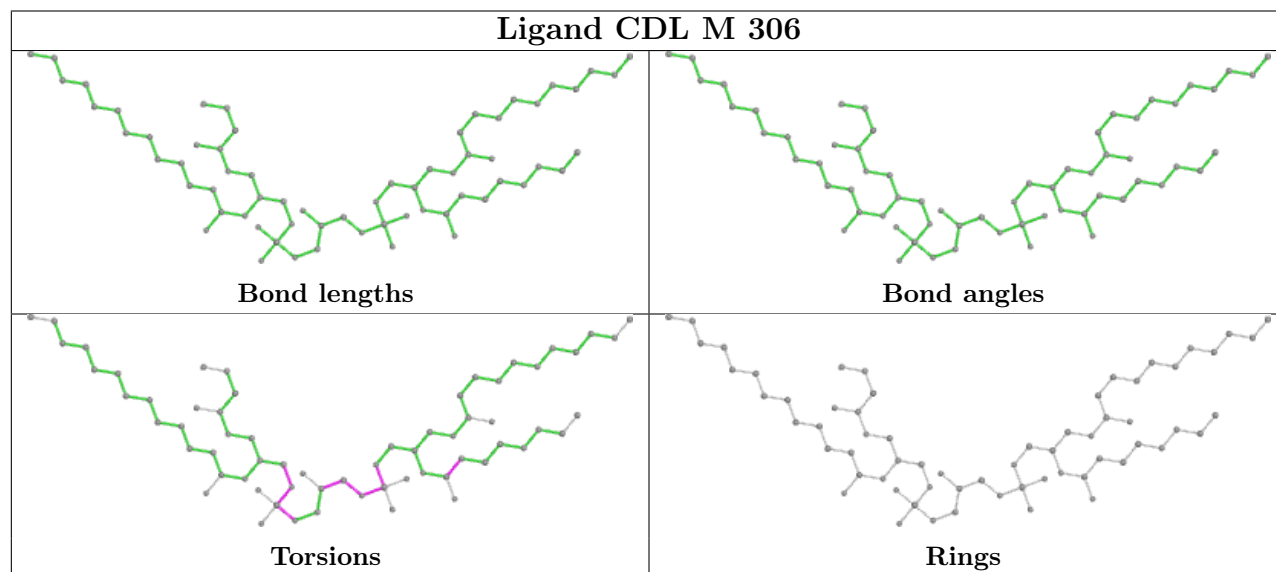
Ligand HEC 2E 401

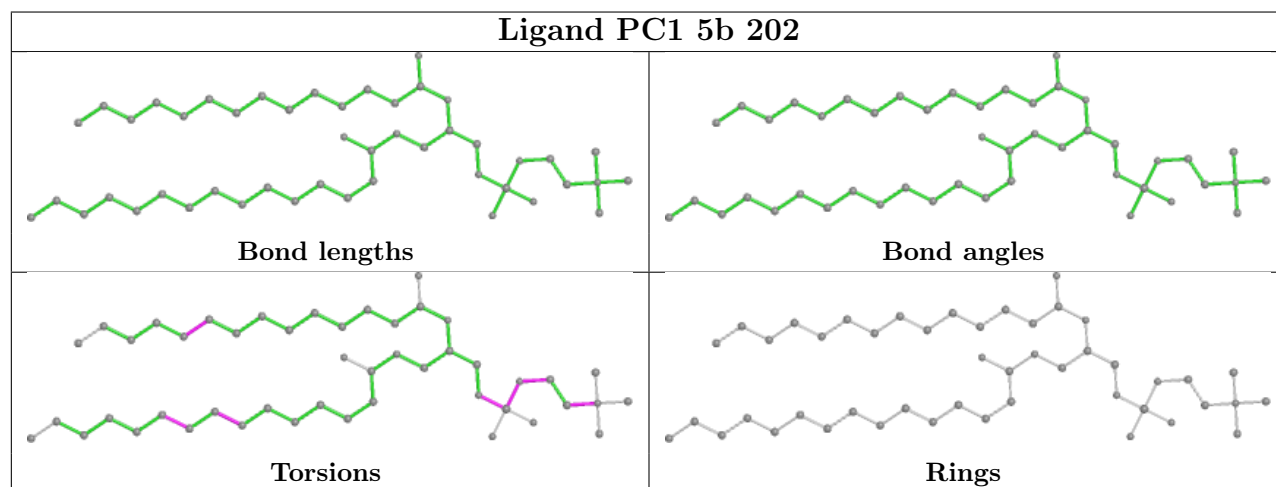
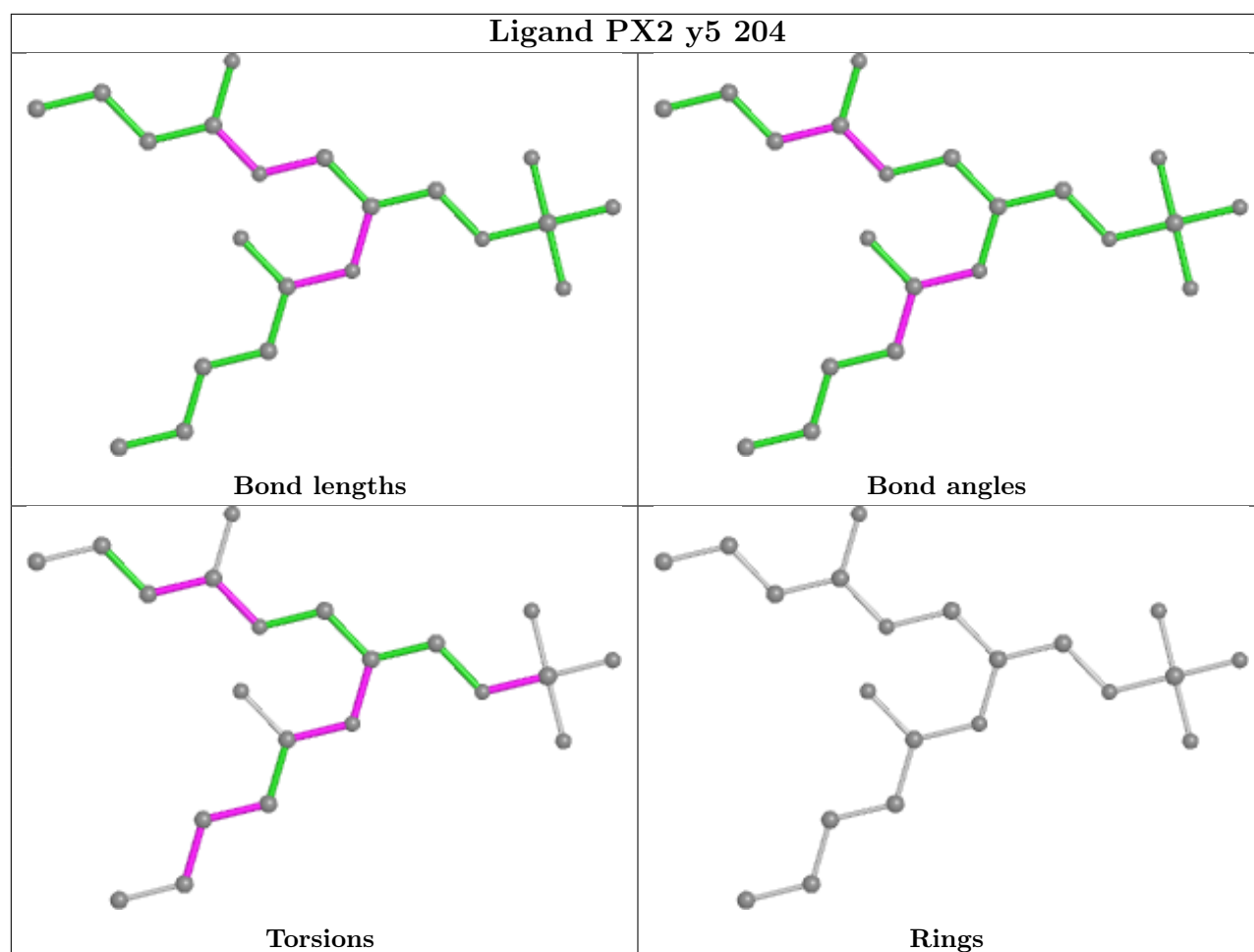


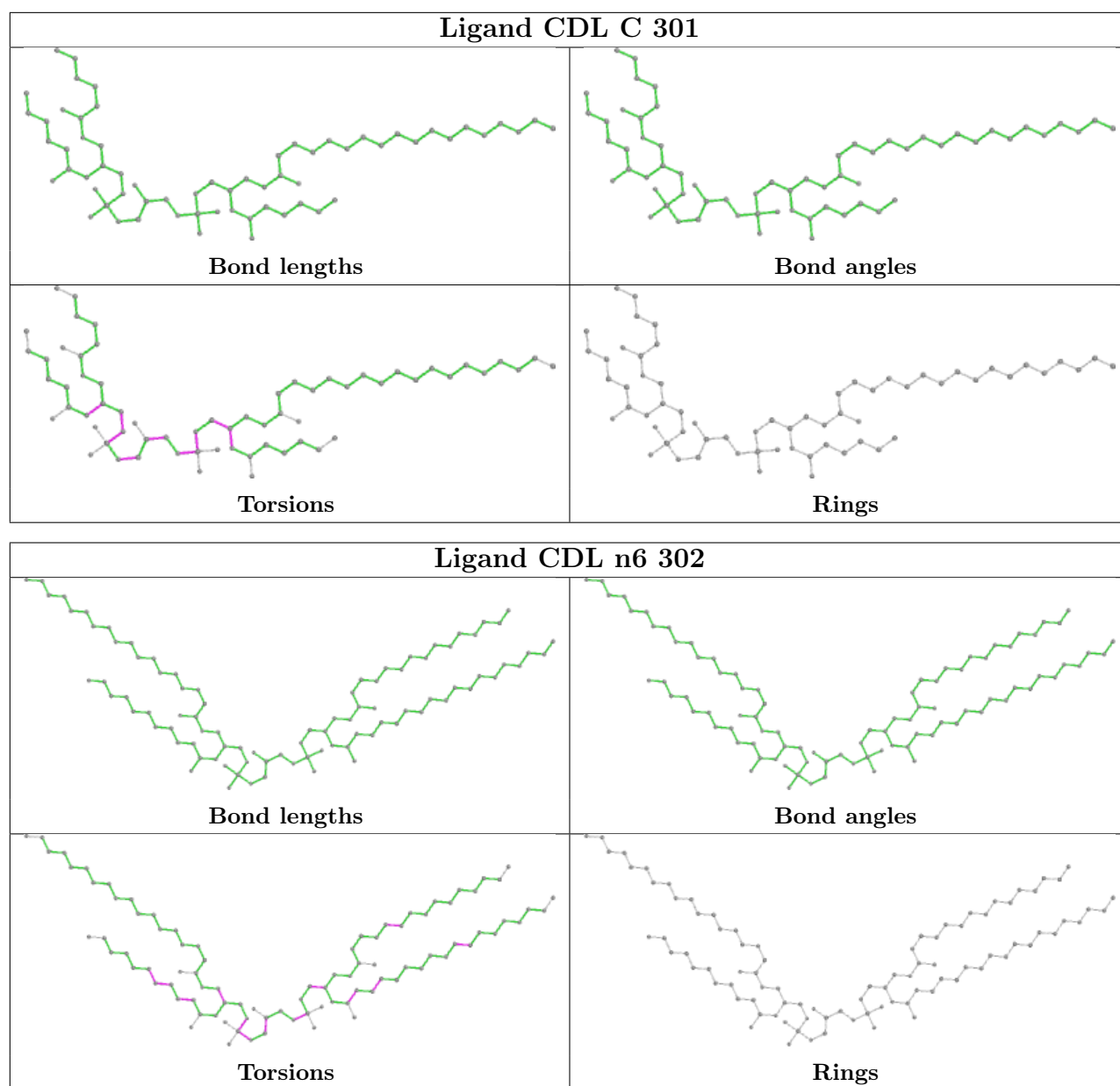
Ligand PX2 r 202

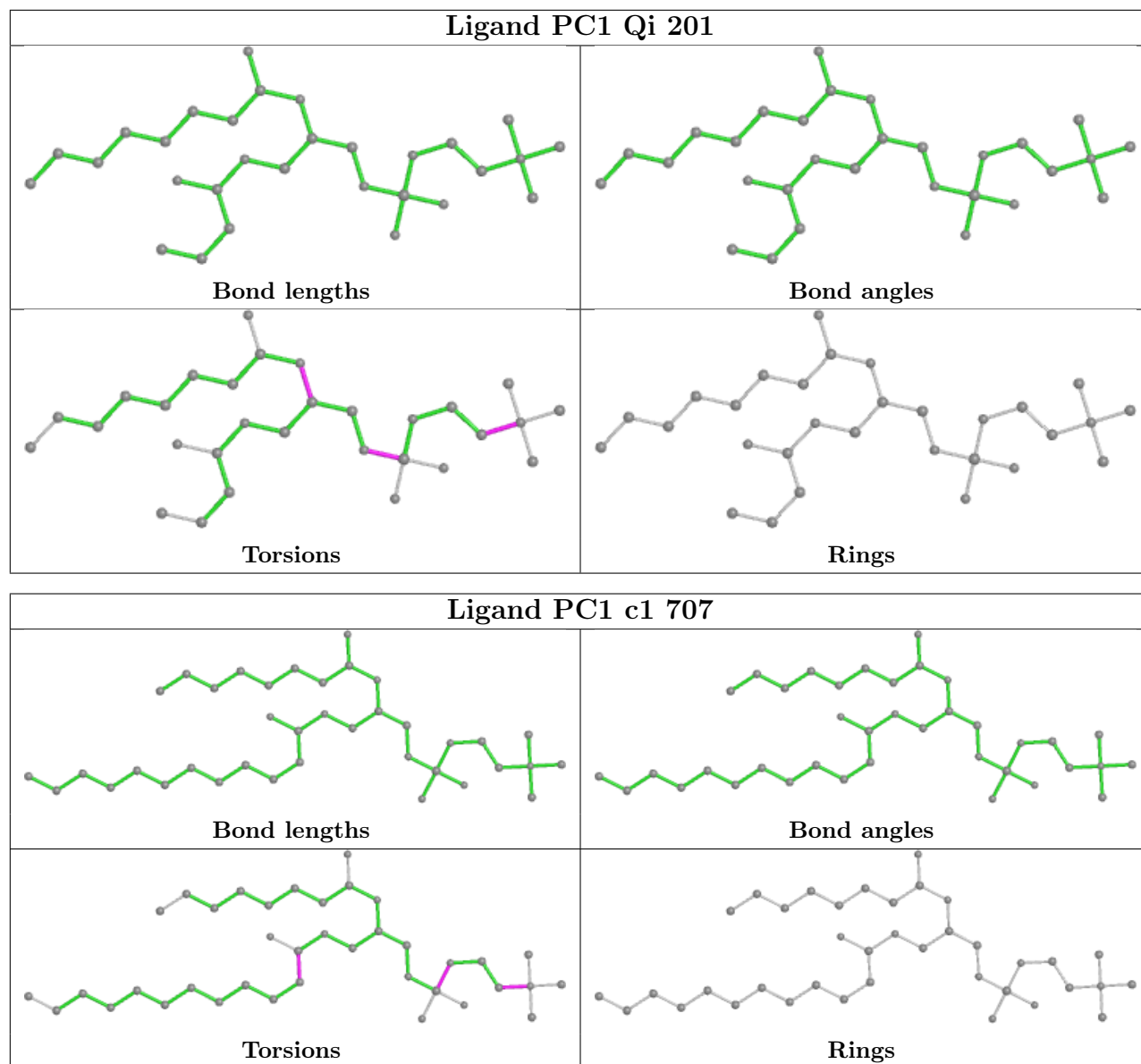


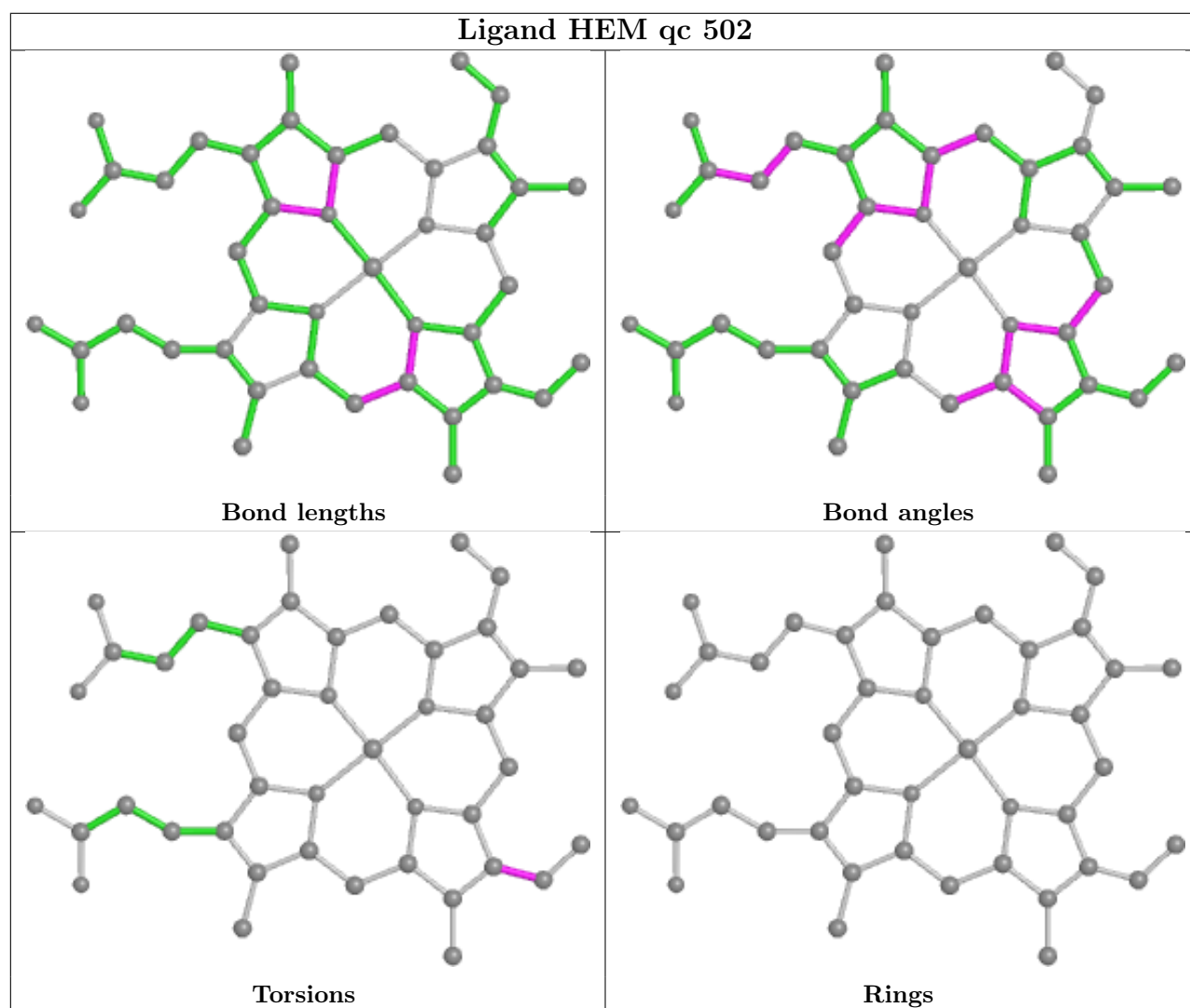
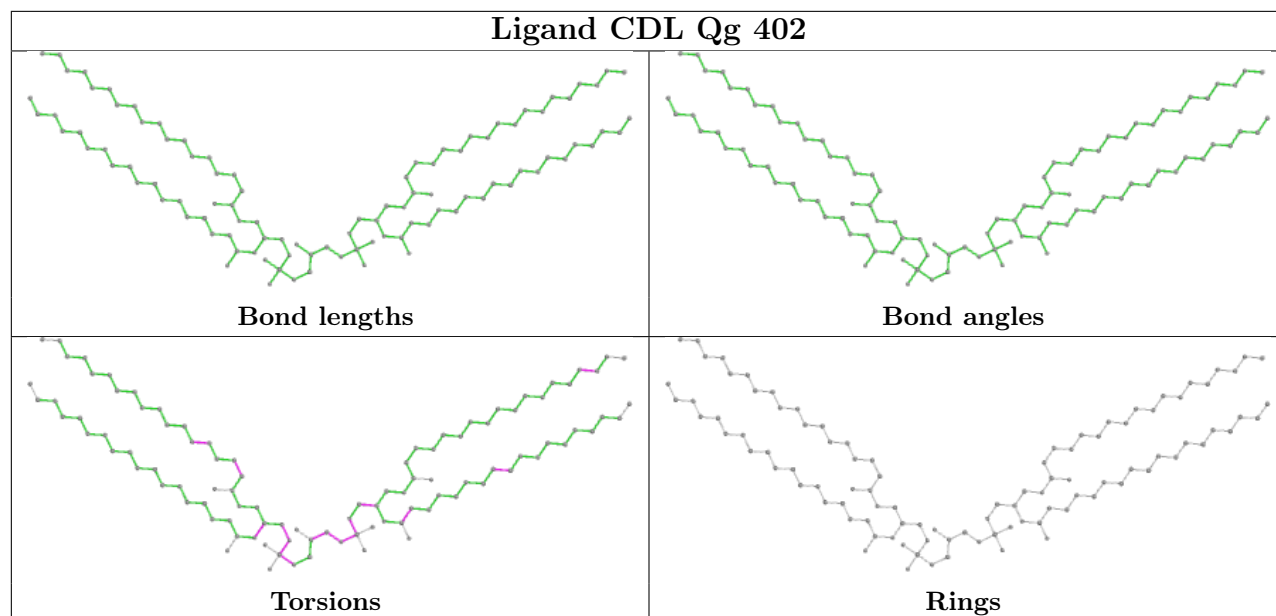
Ligand CDL M 306

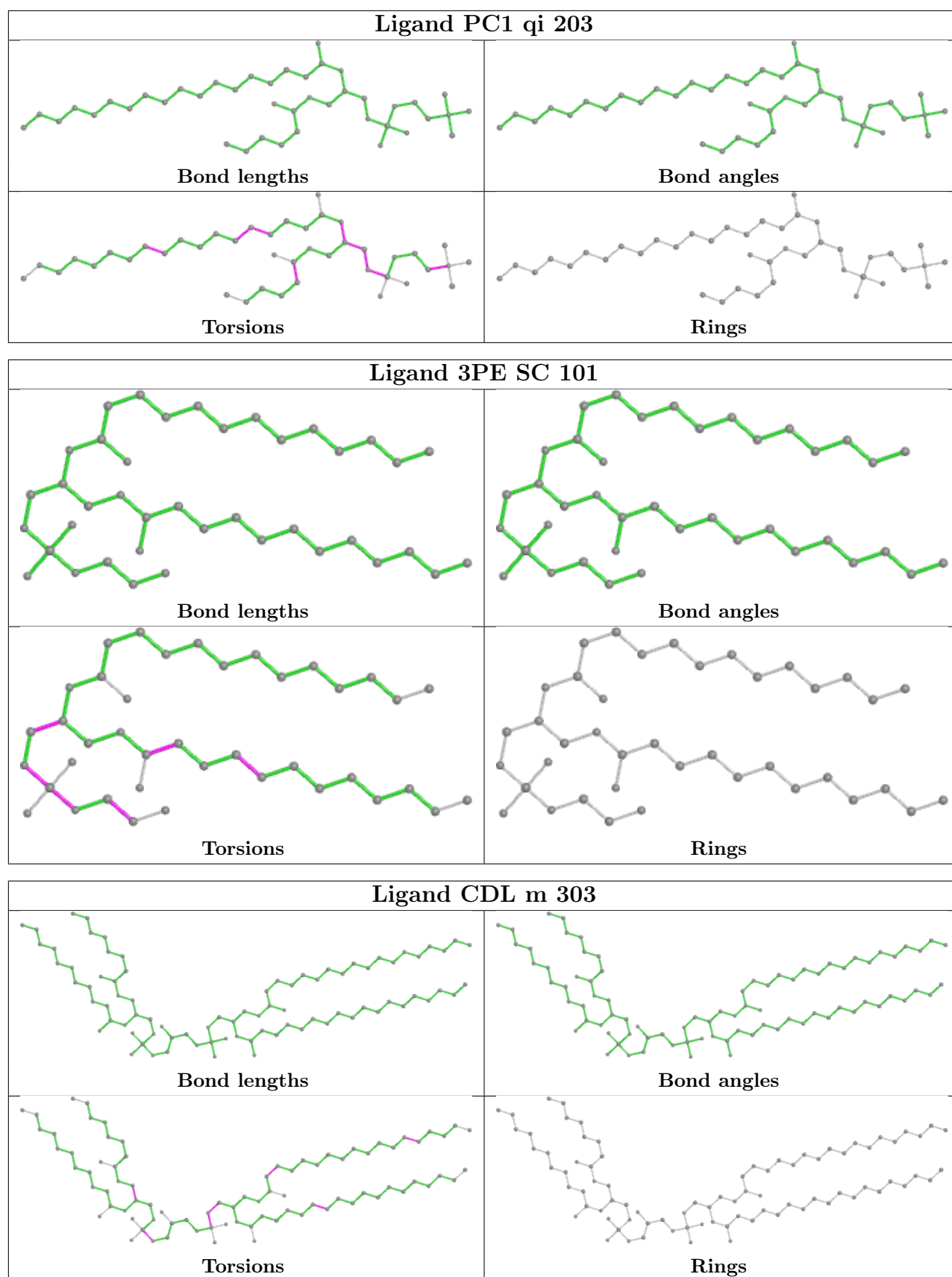


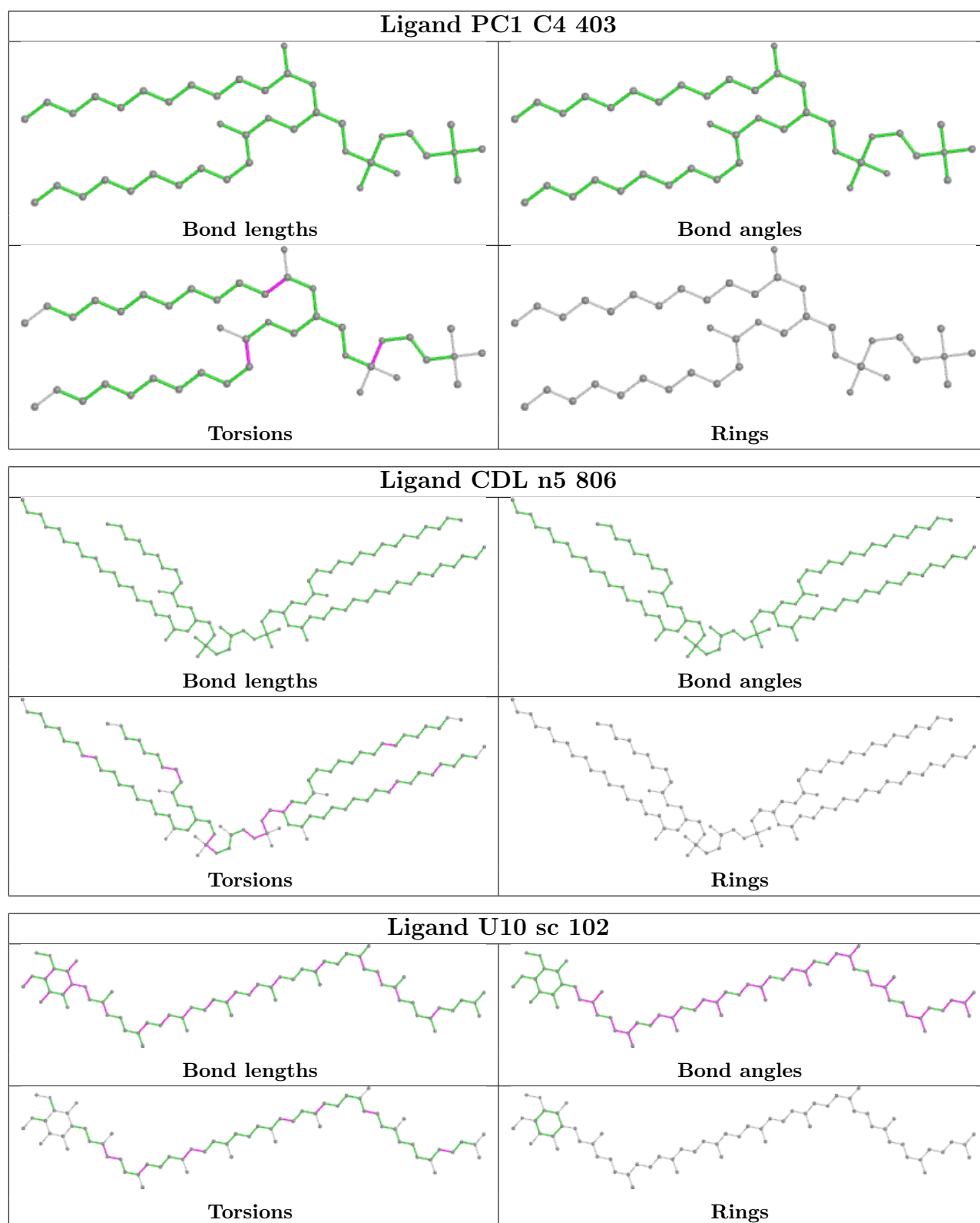


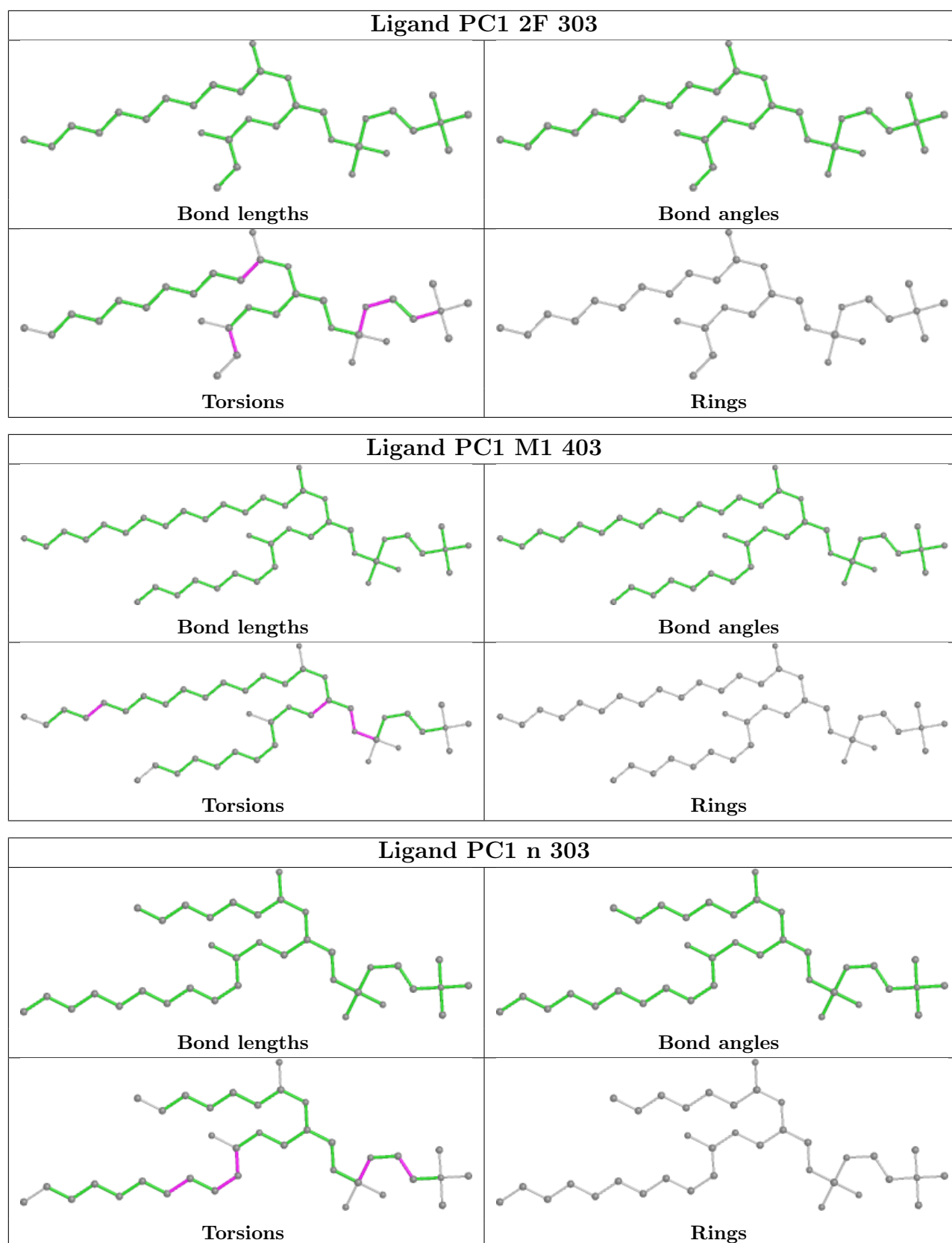


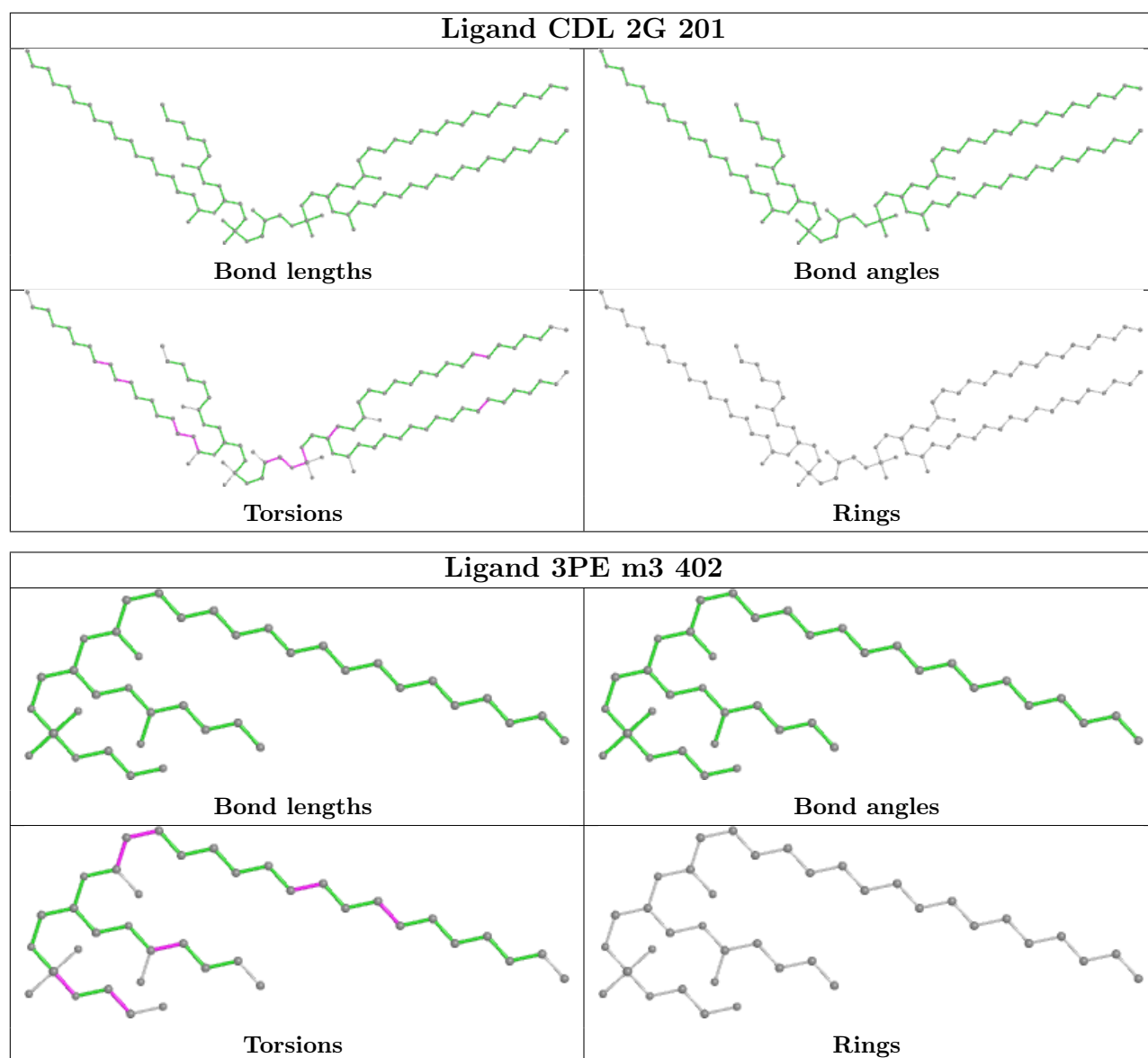


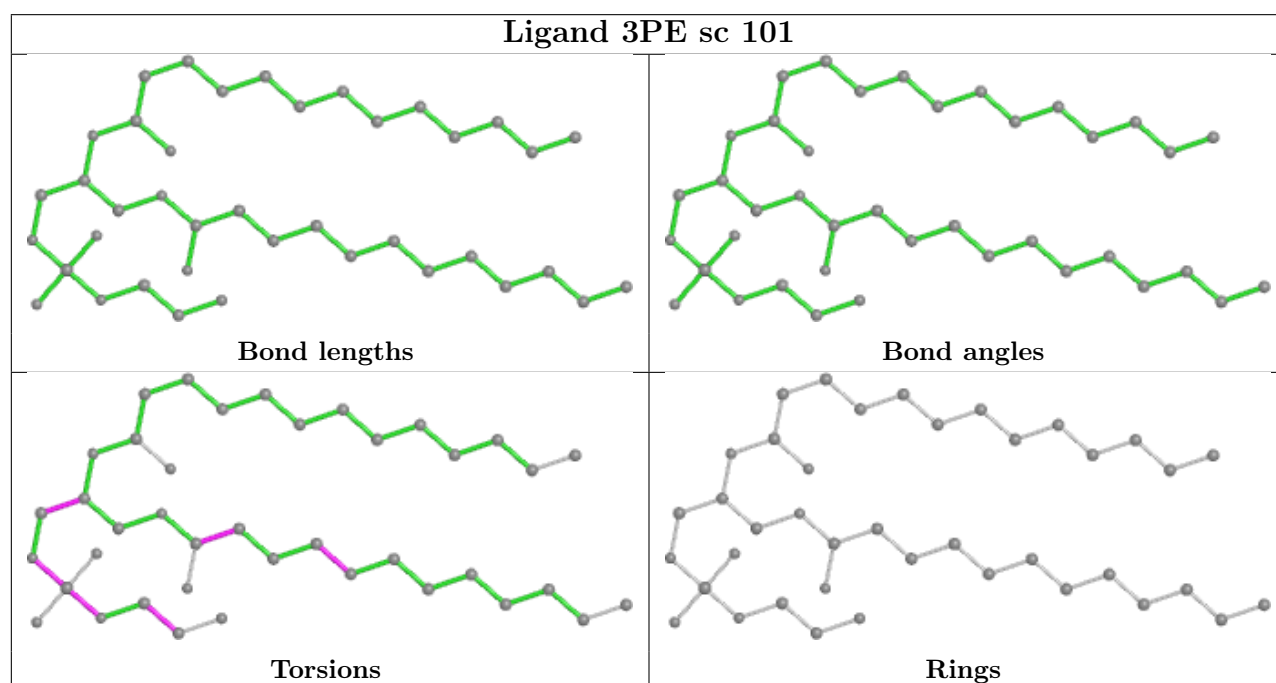
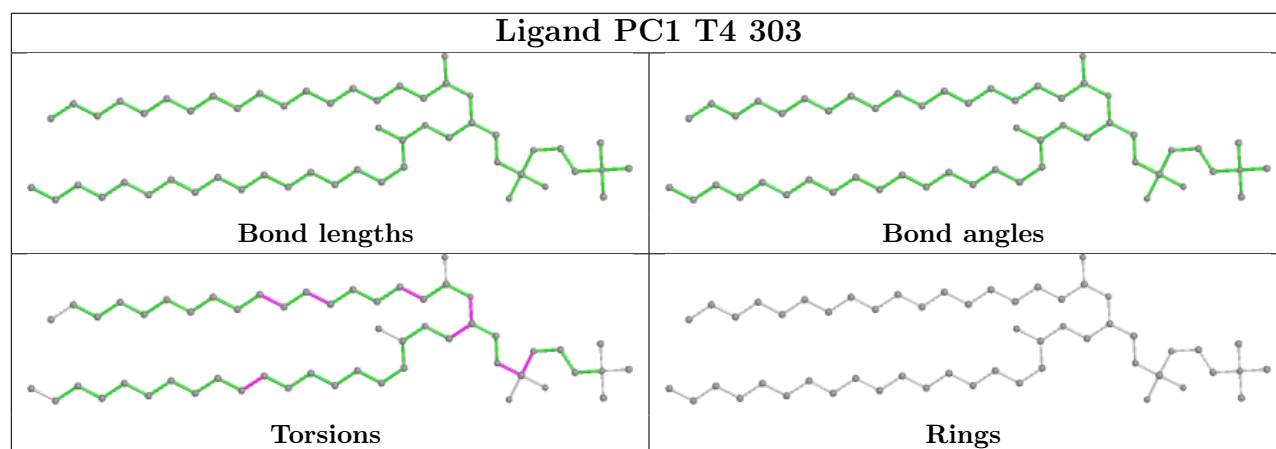
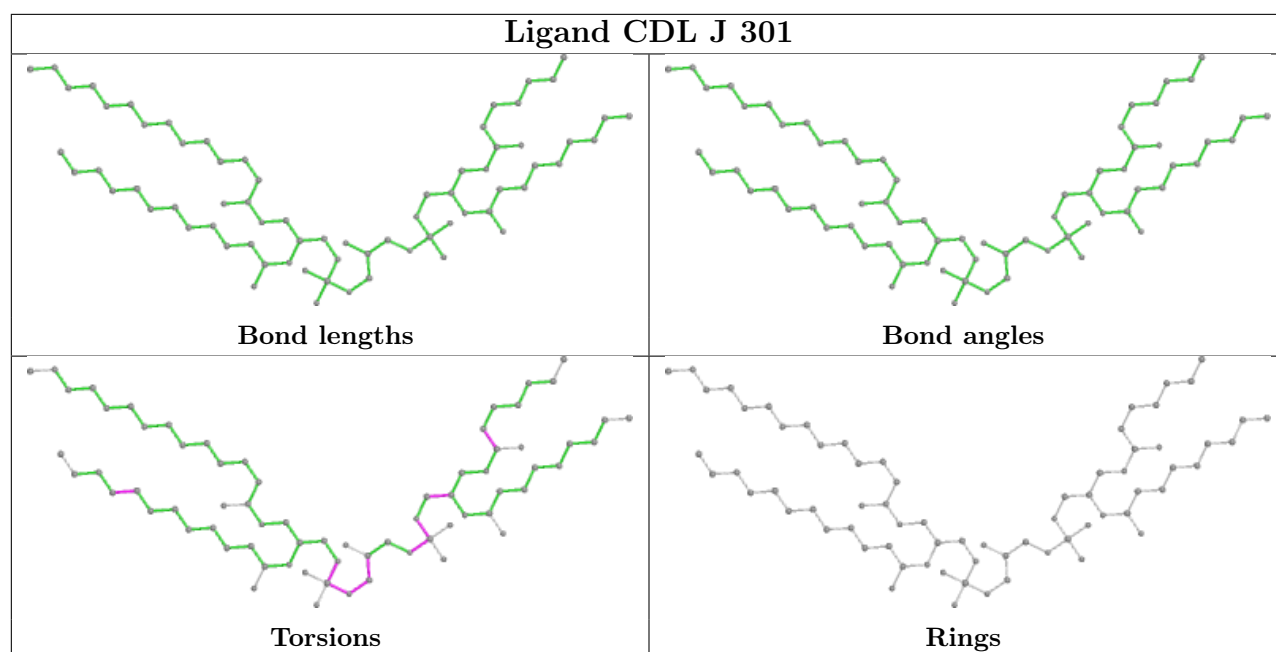


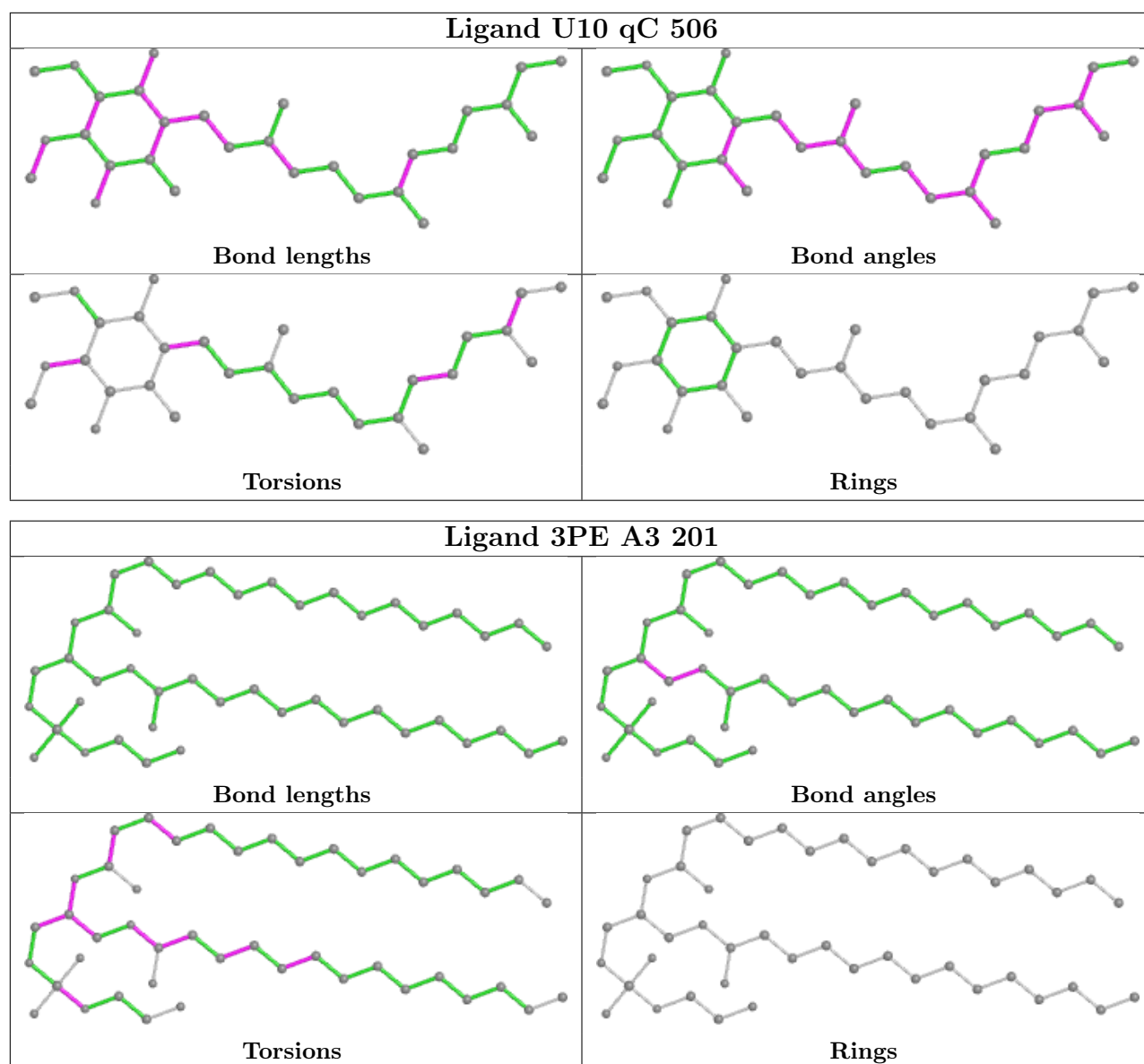


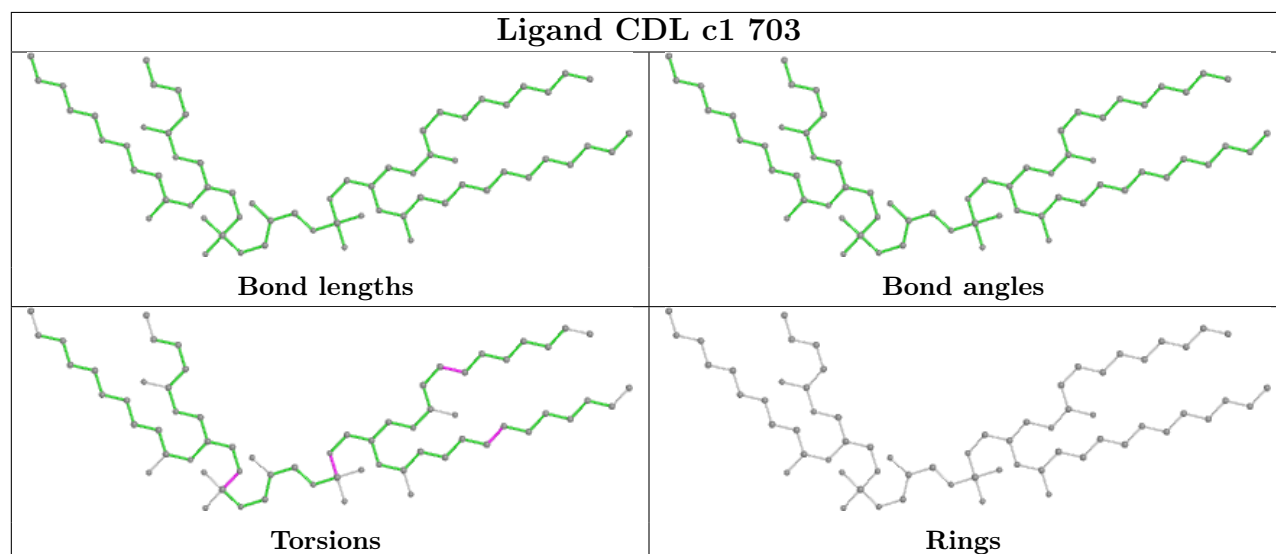
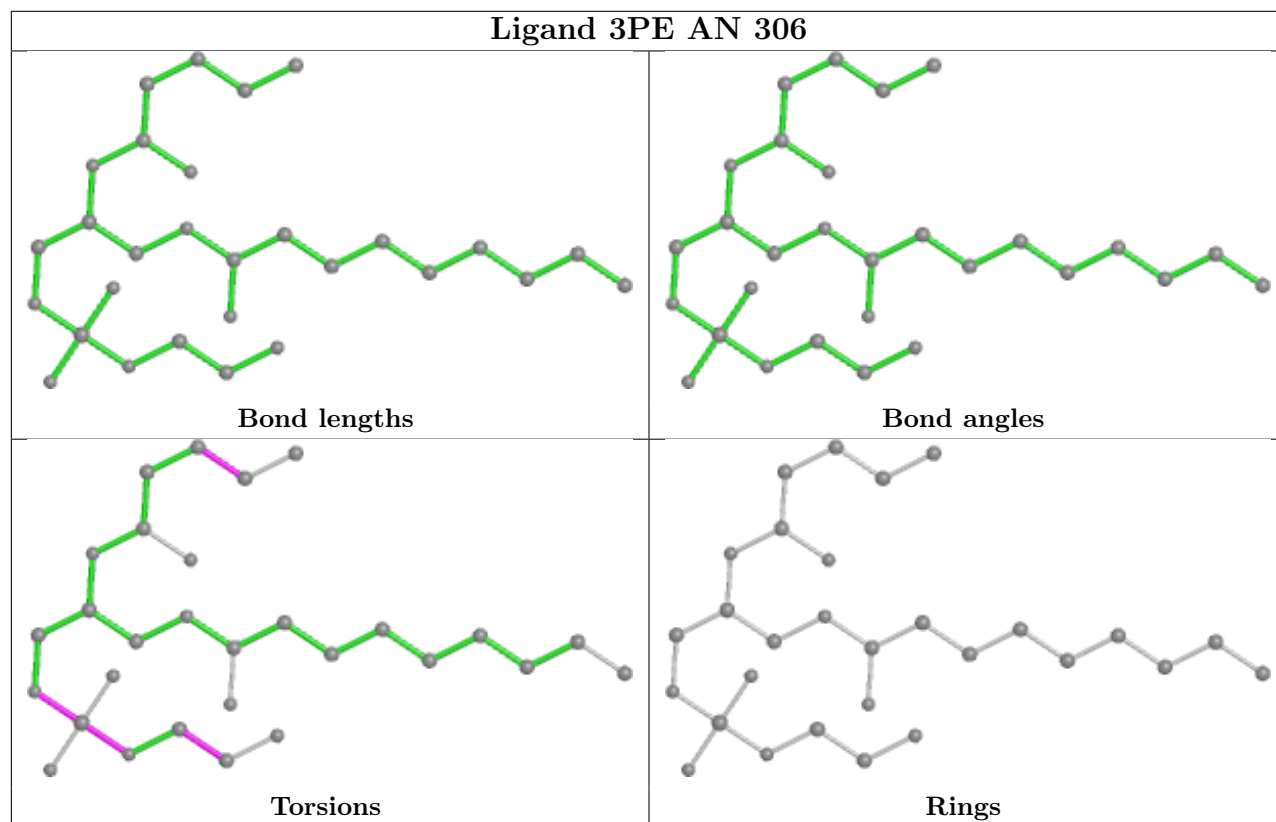


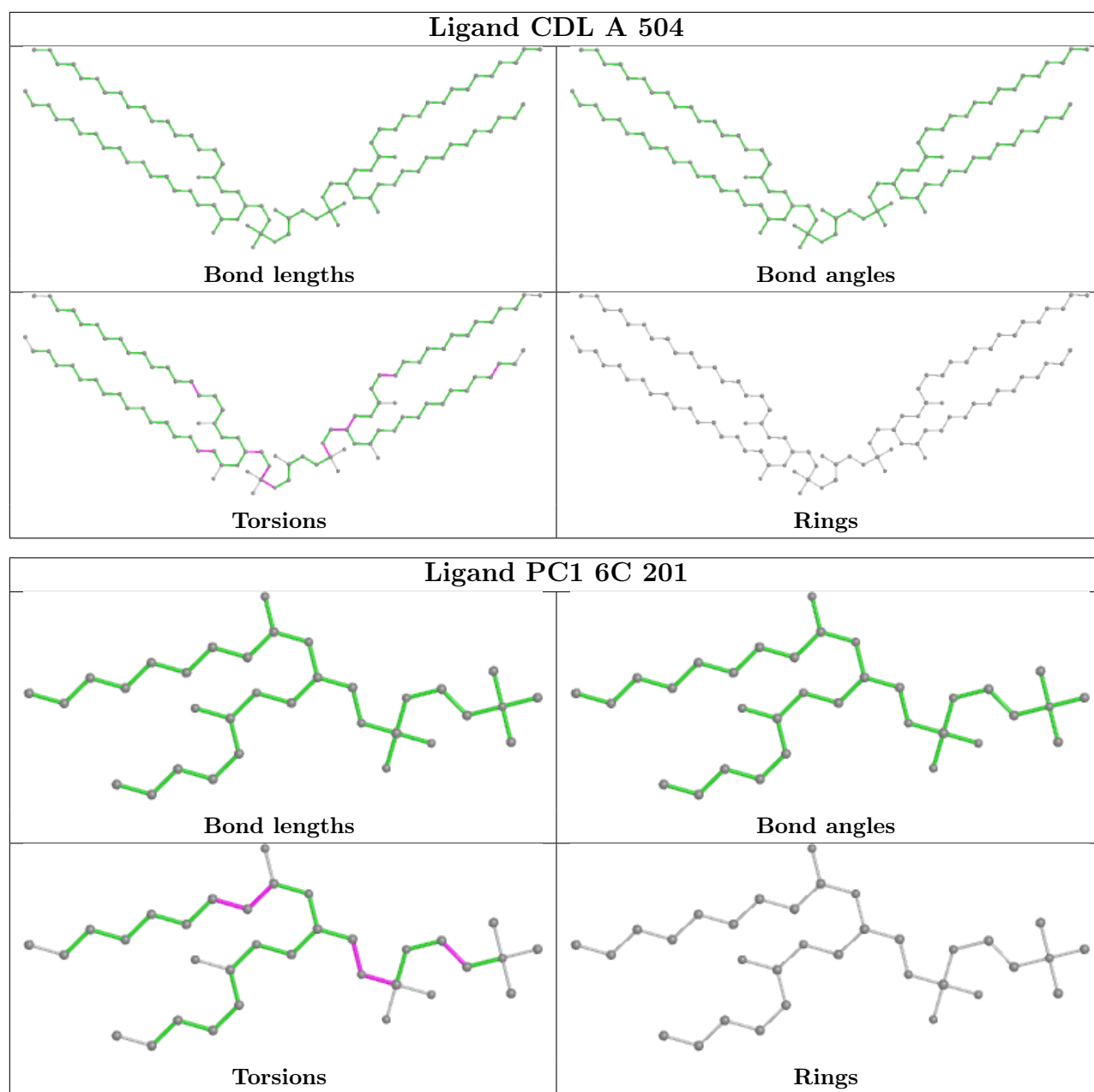


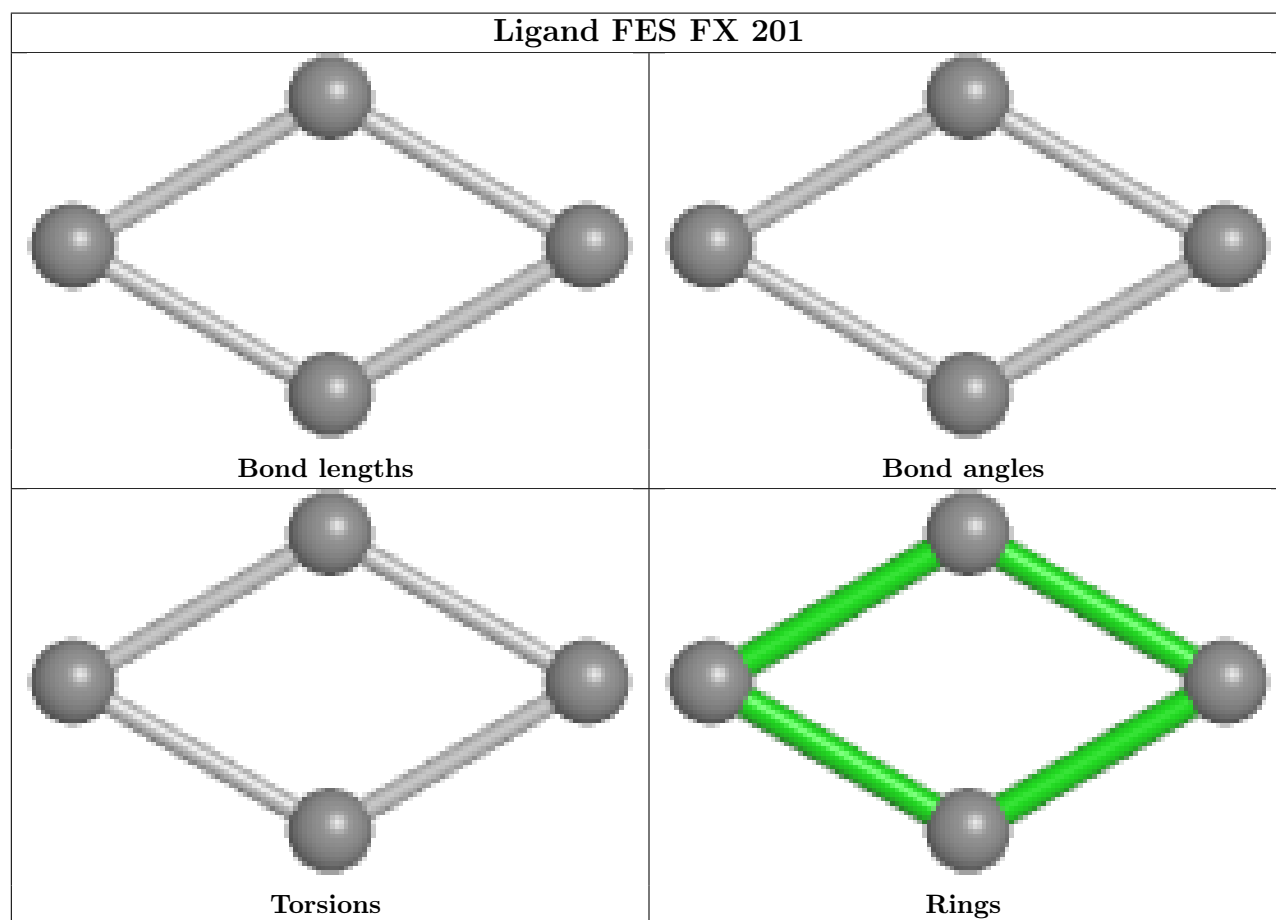
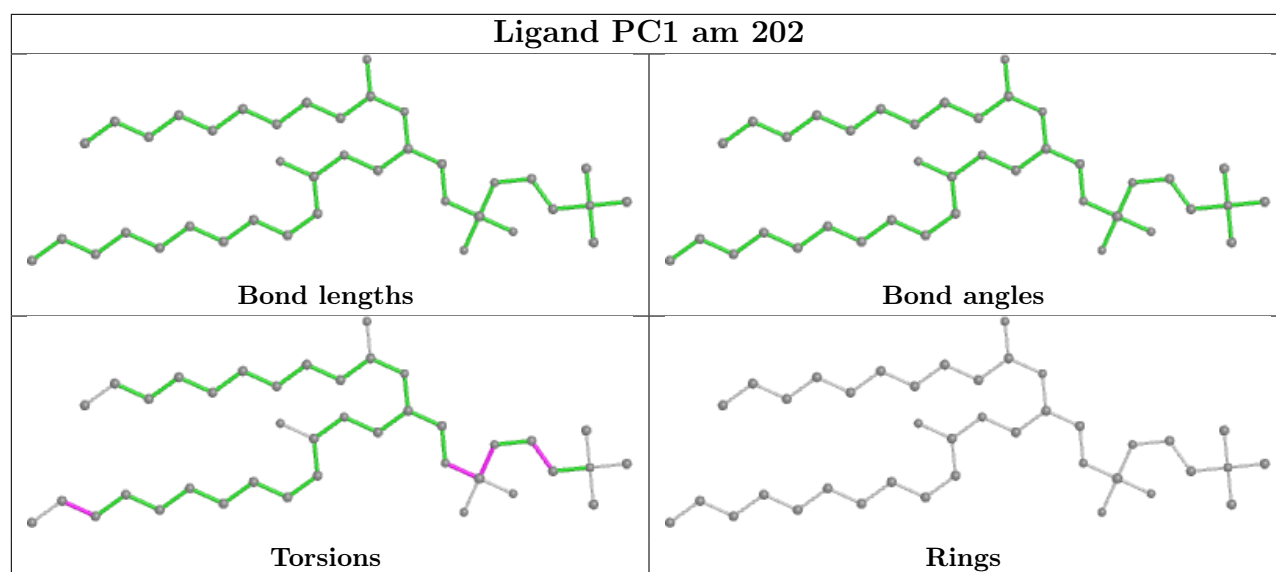


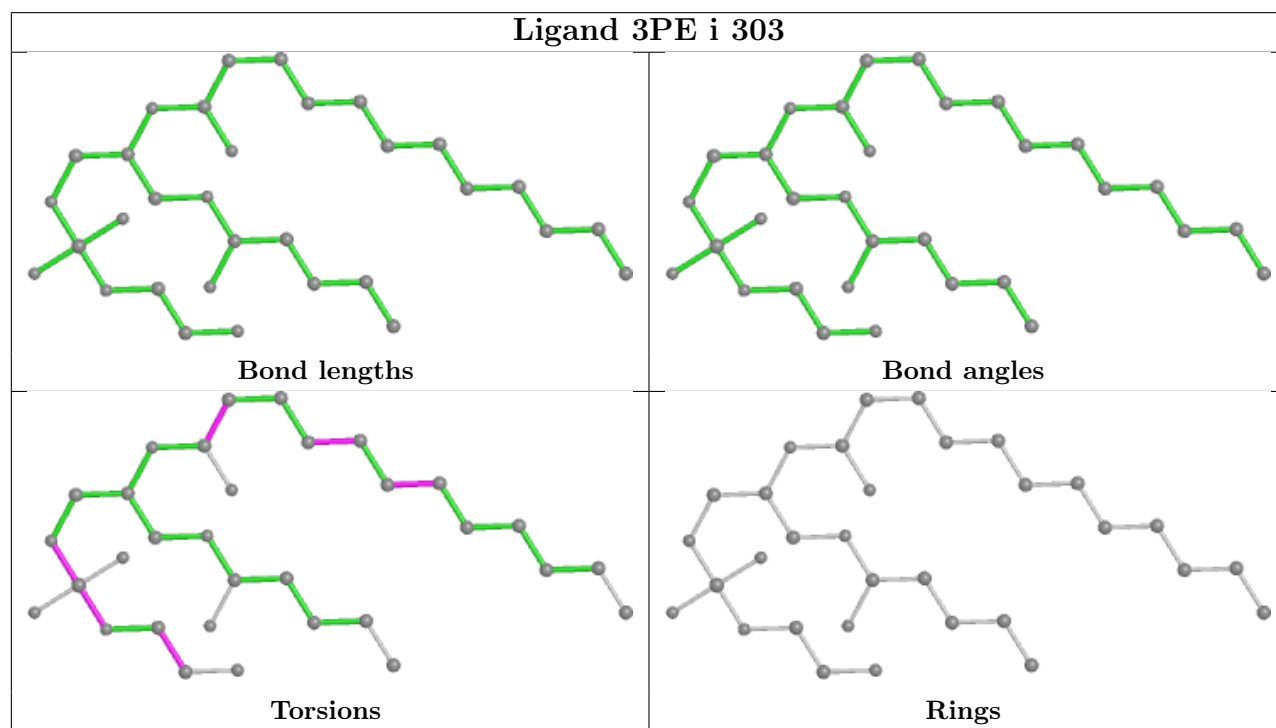
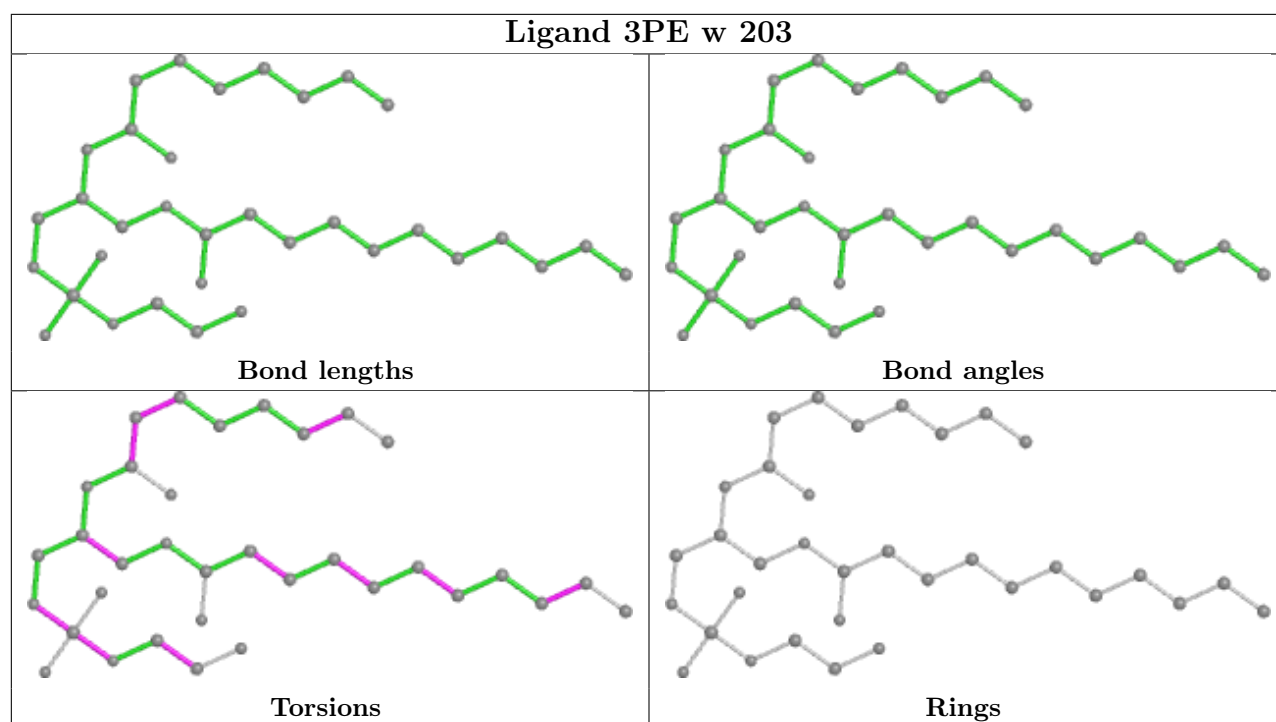


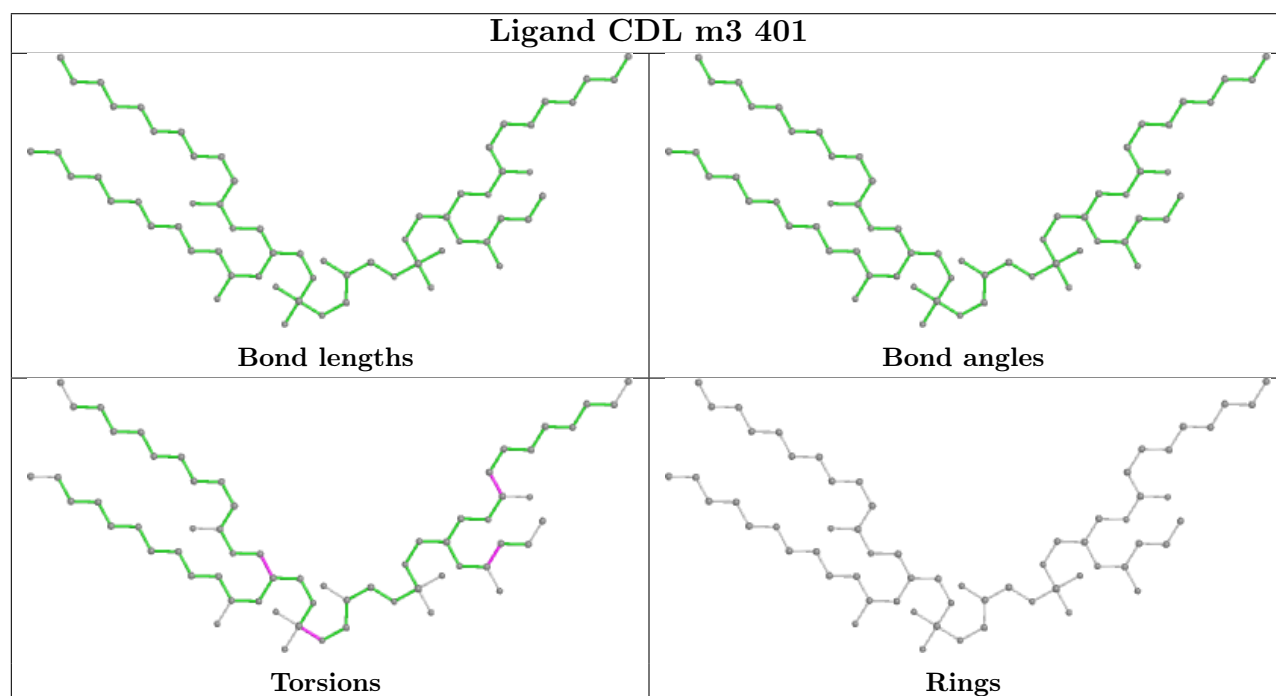
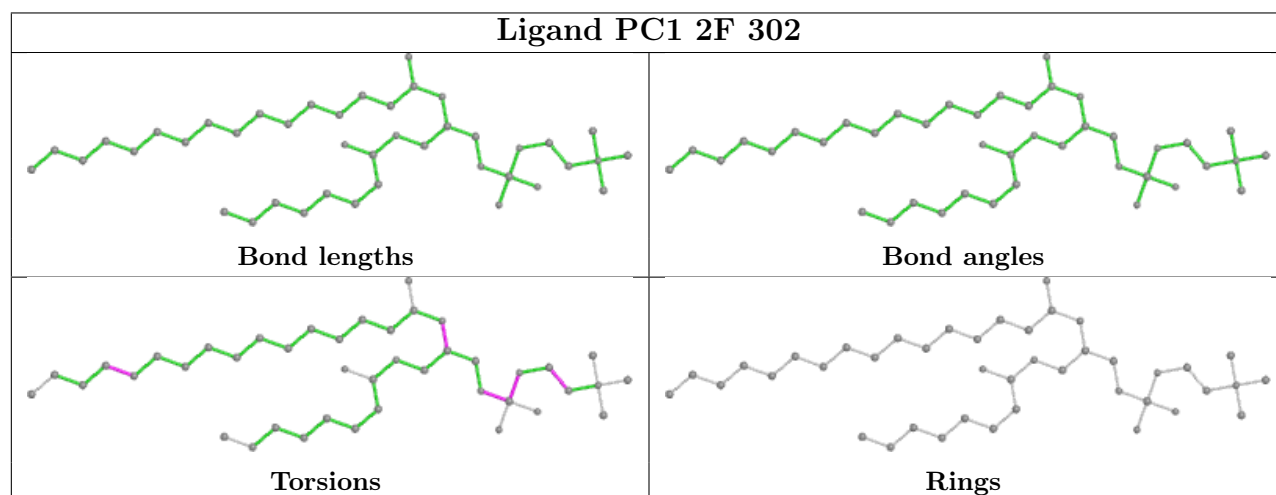
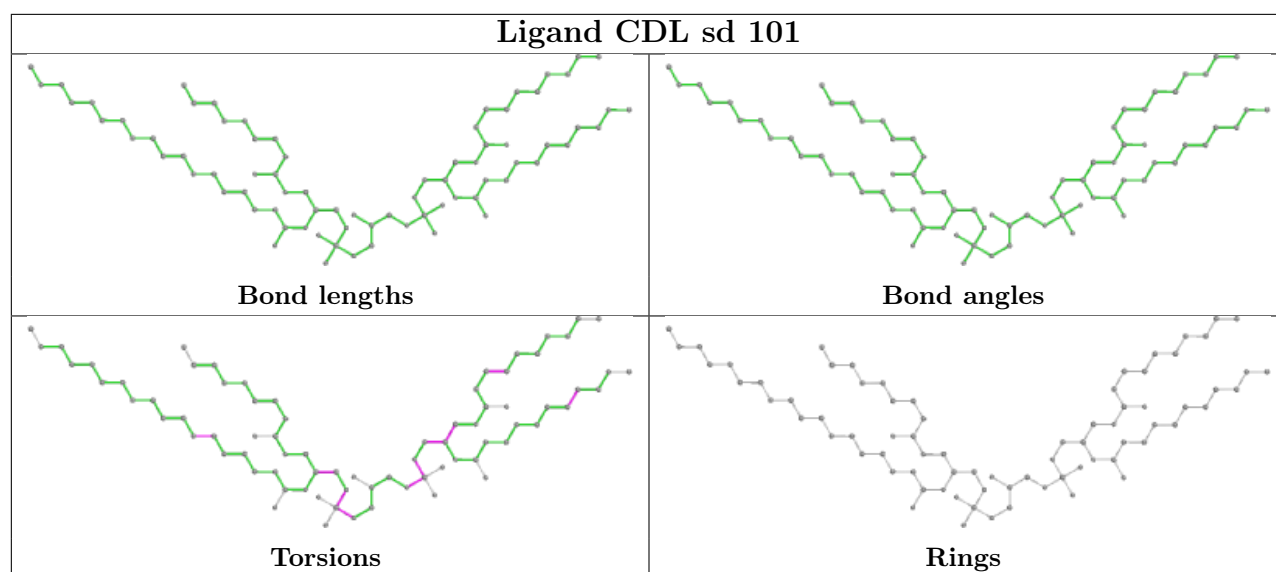


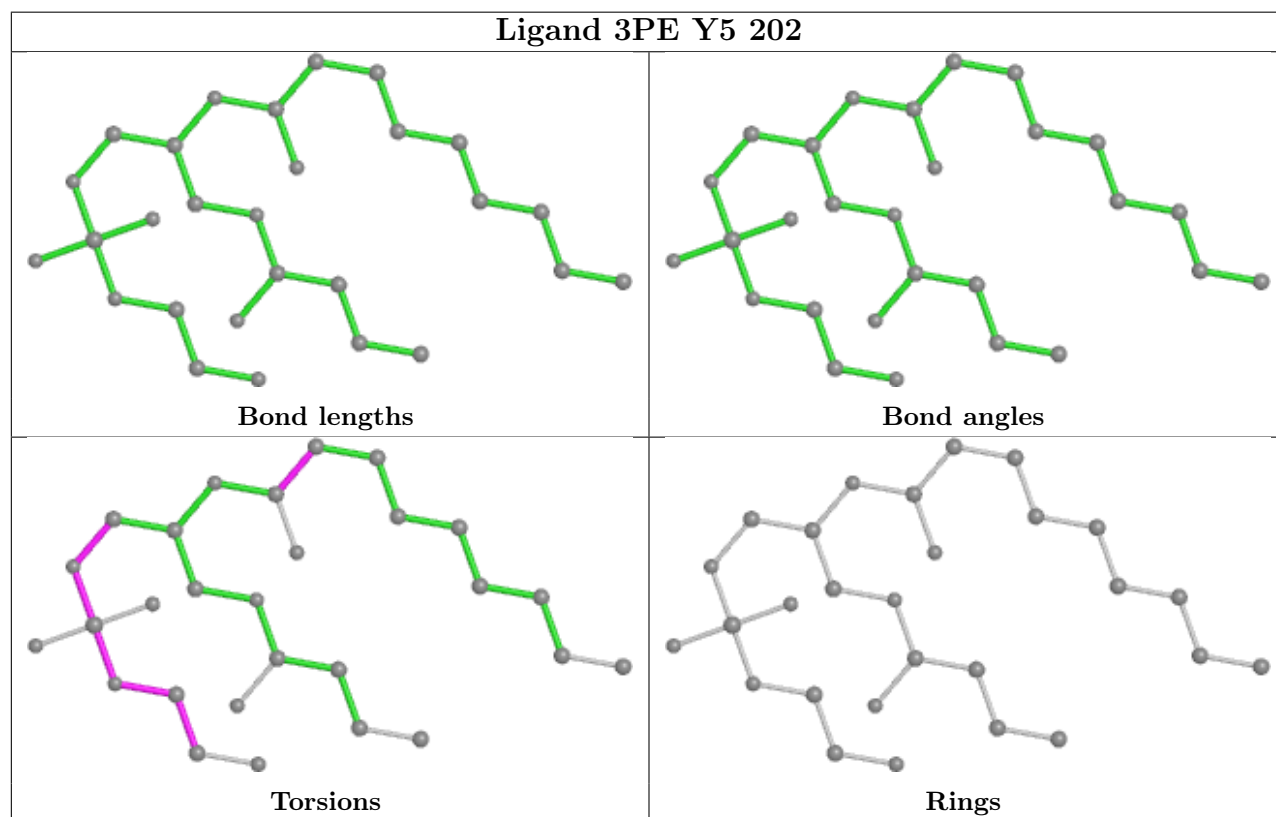
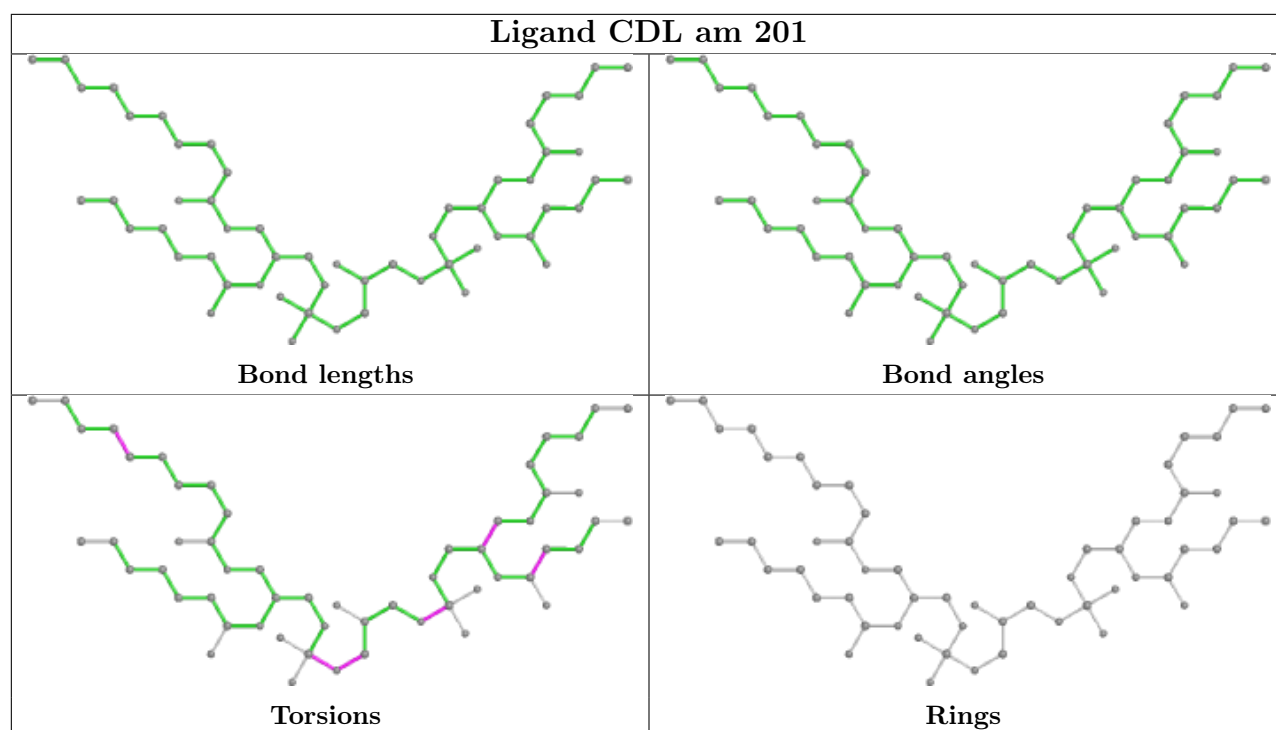


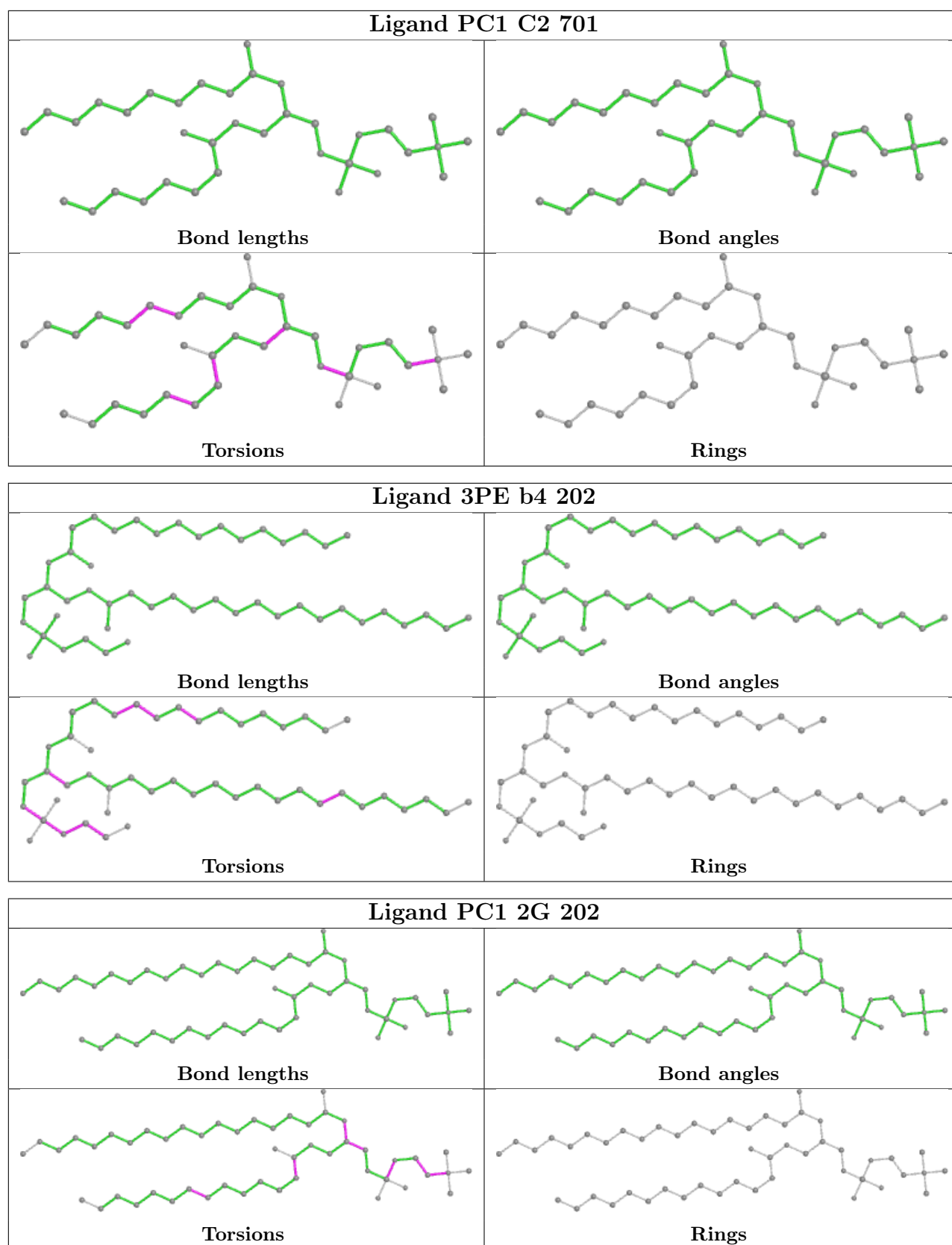


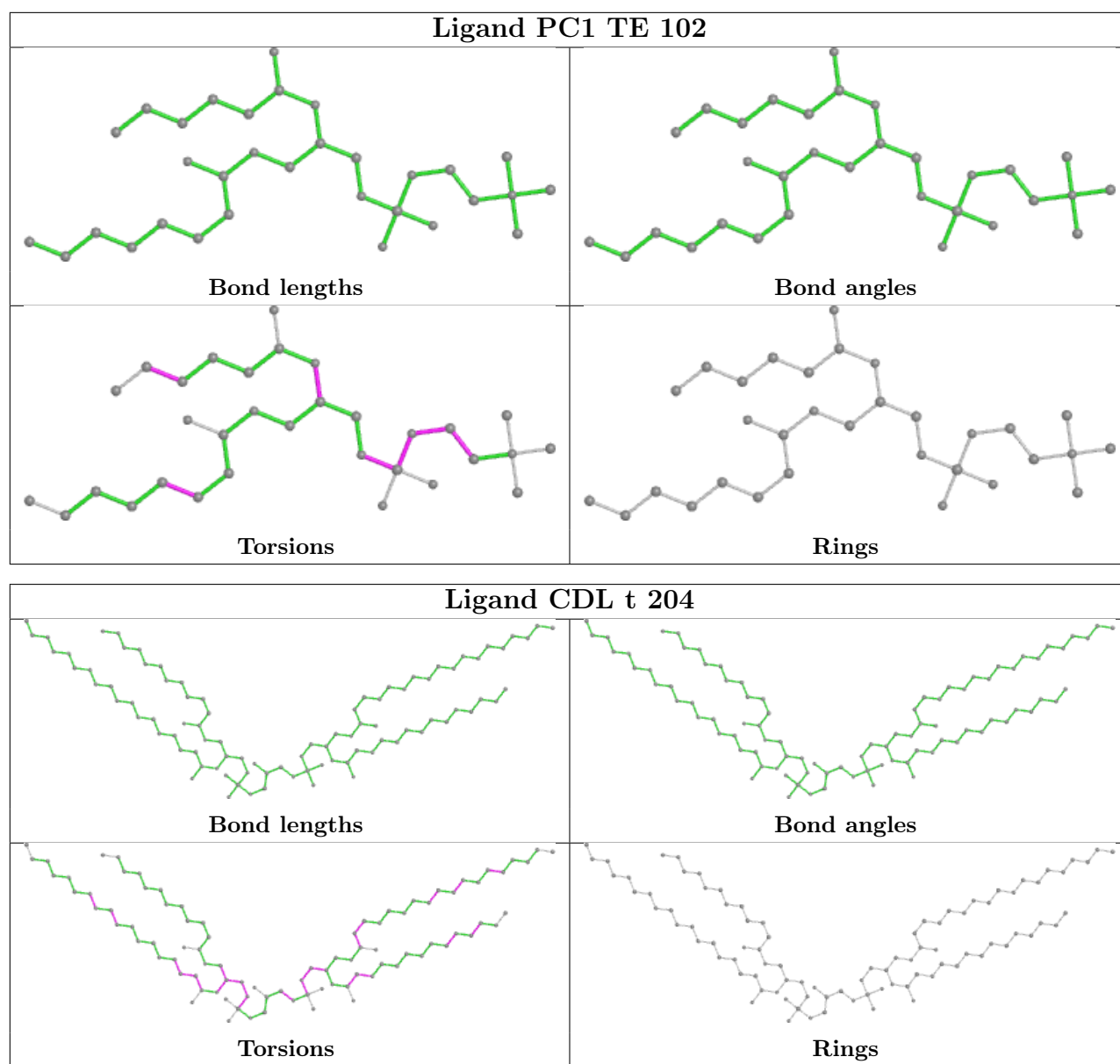




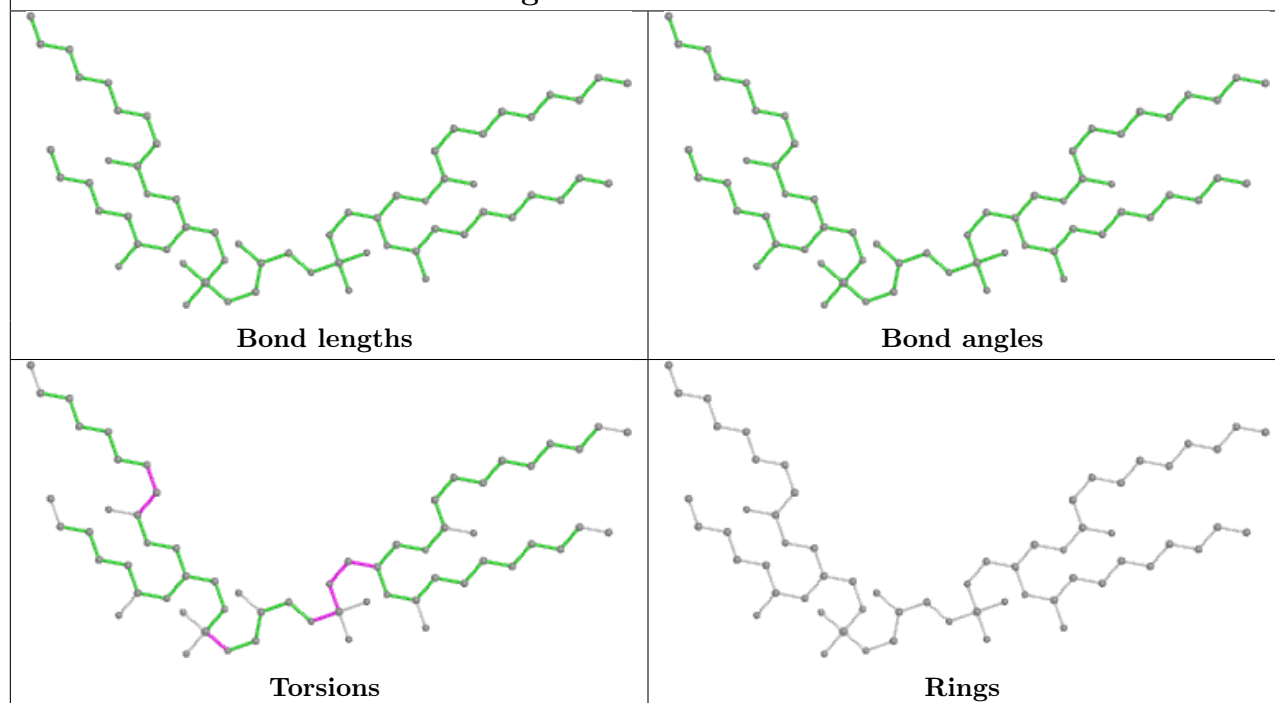




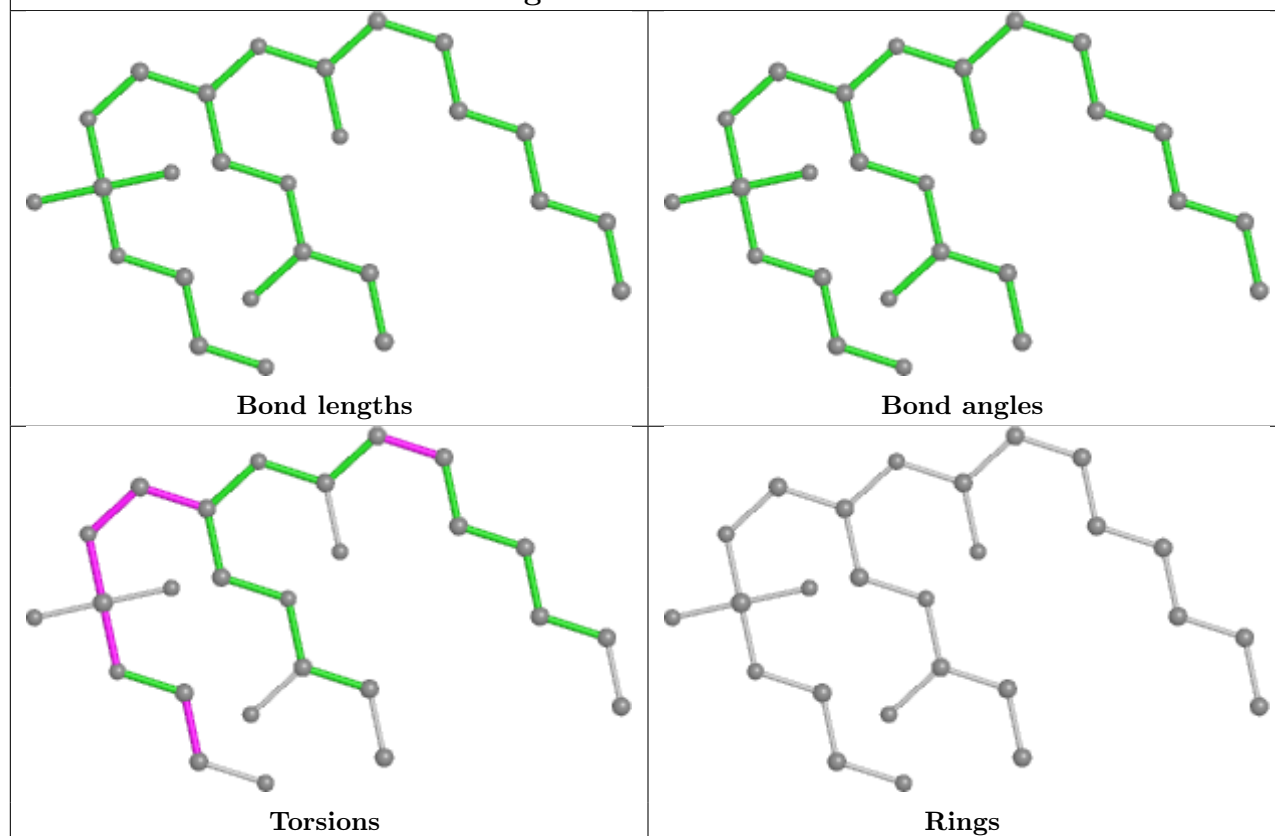


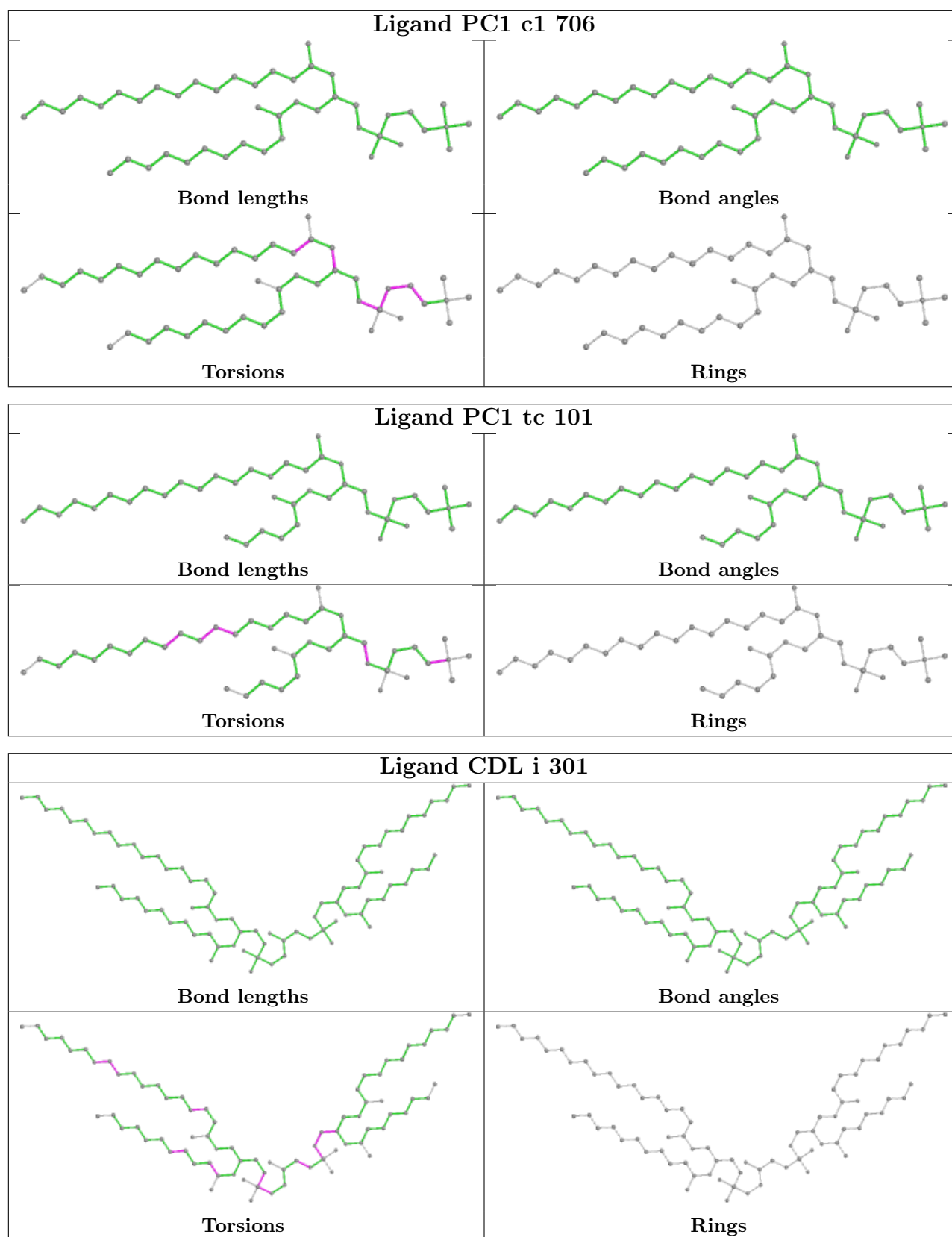


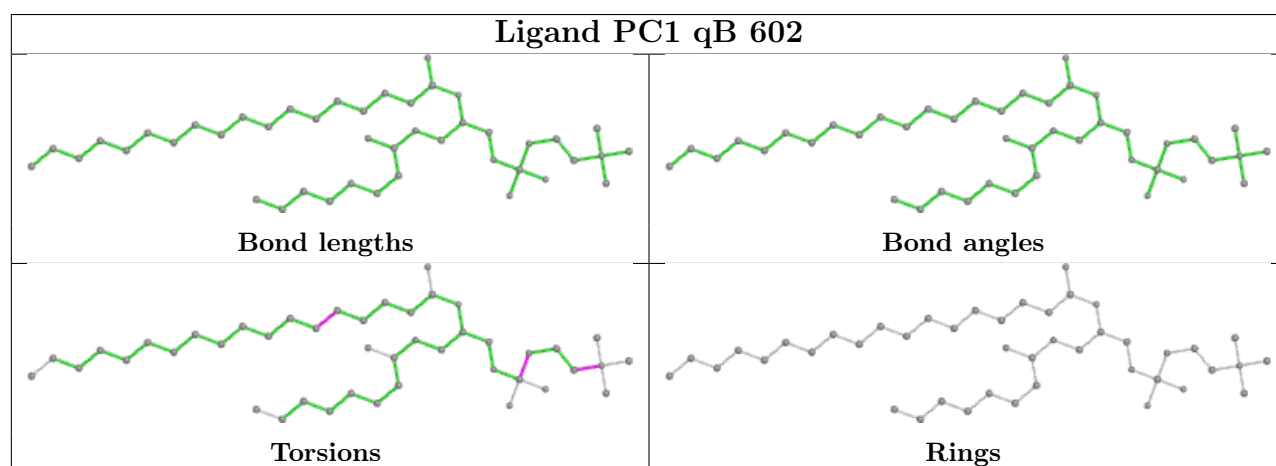
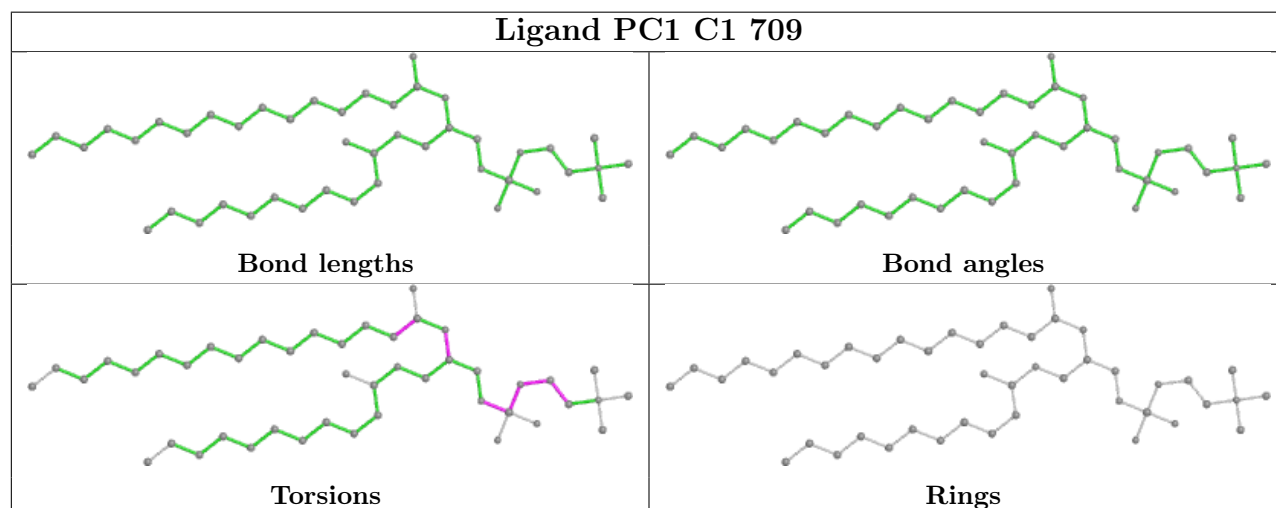
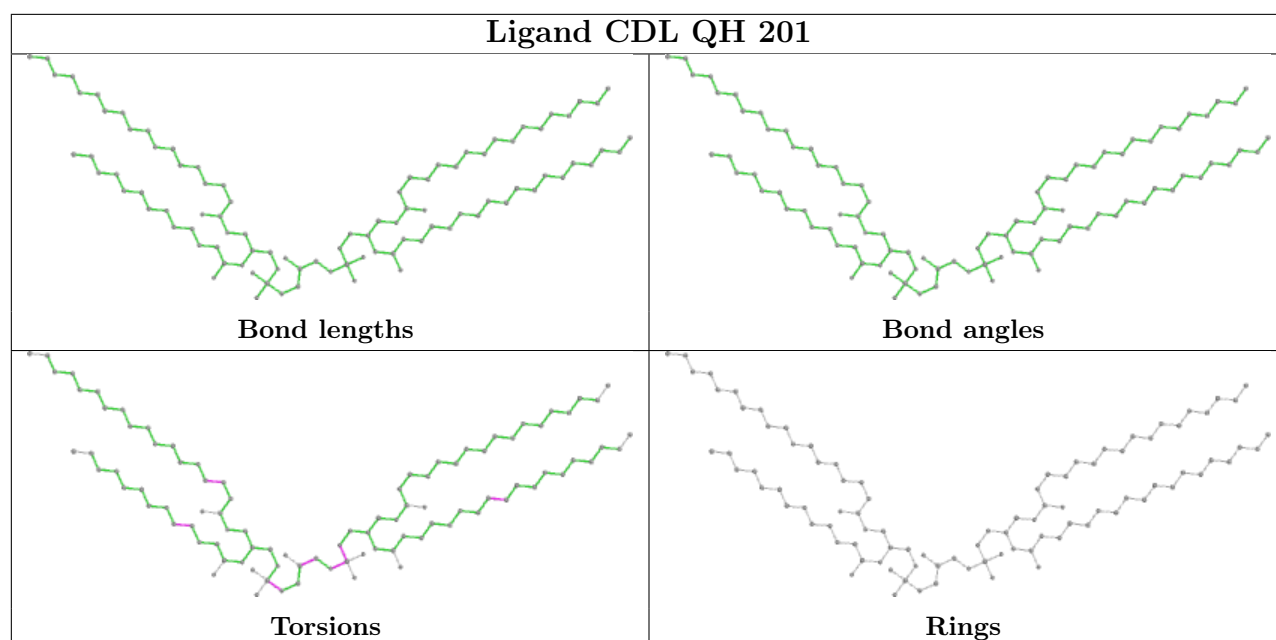
Ligand CDL 7A 203

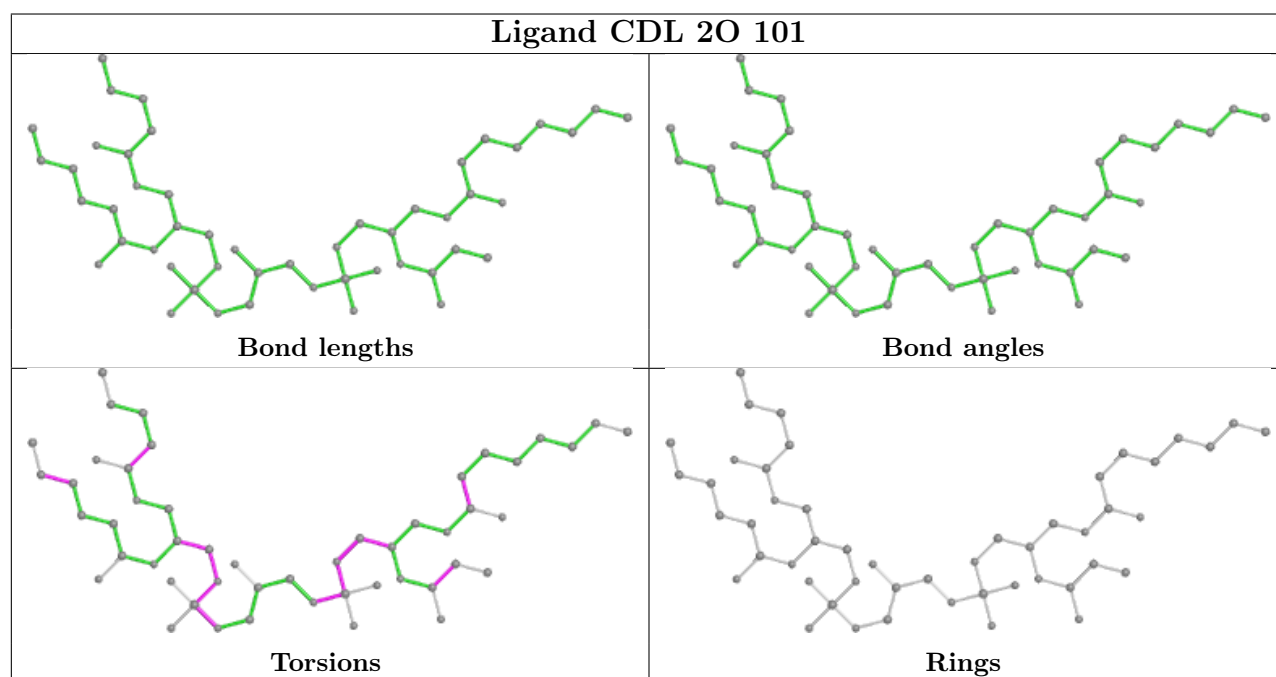
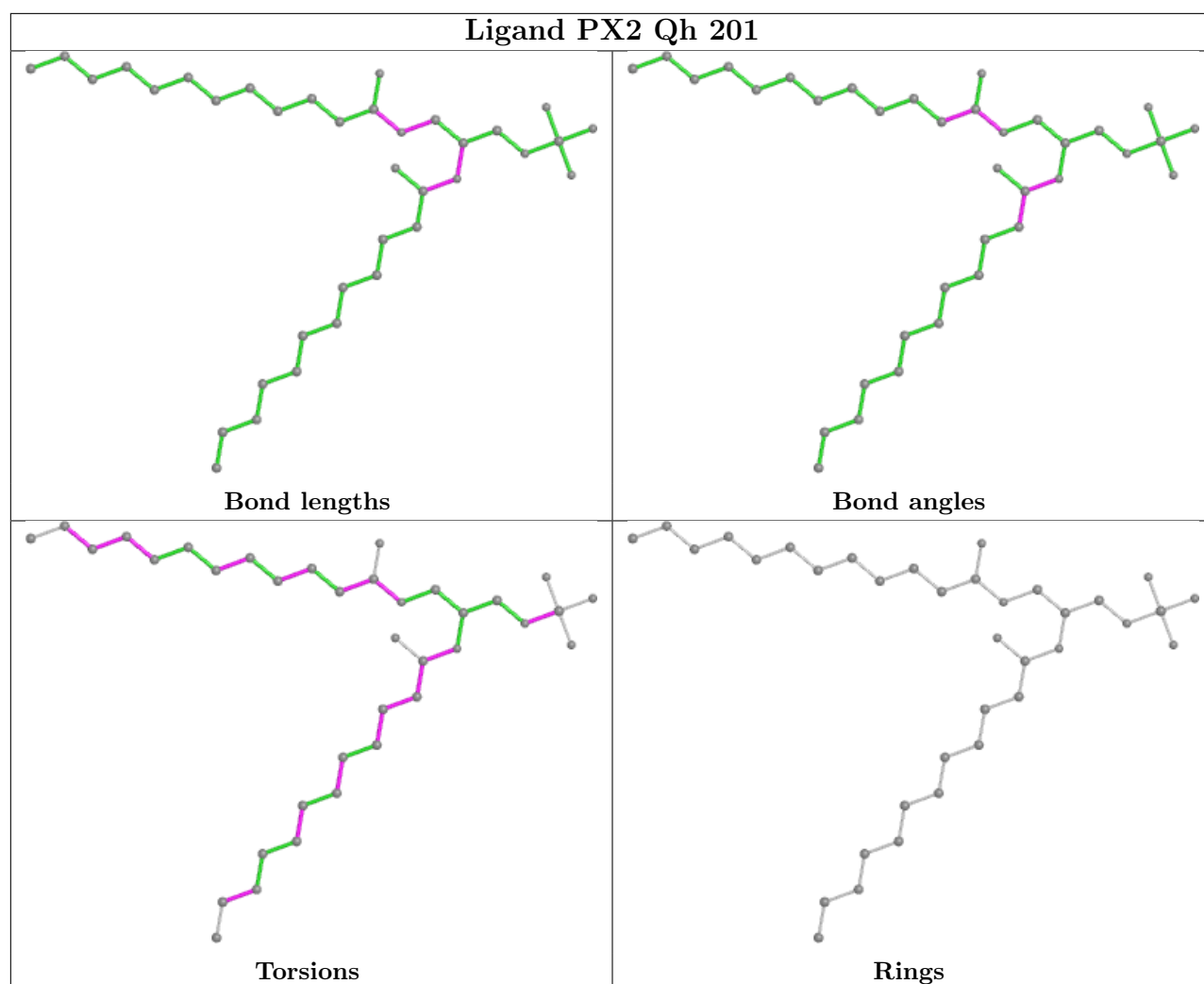


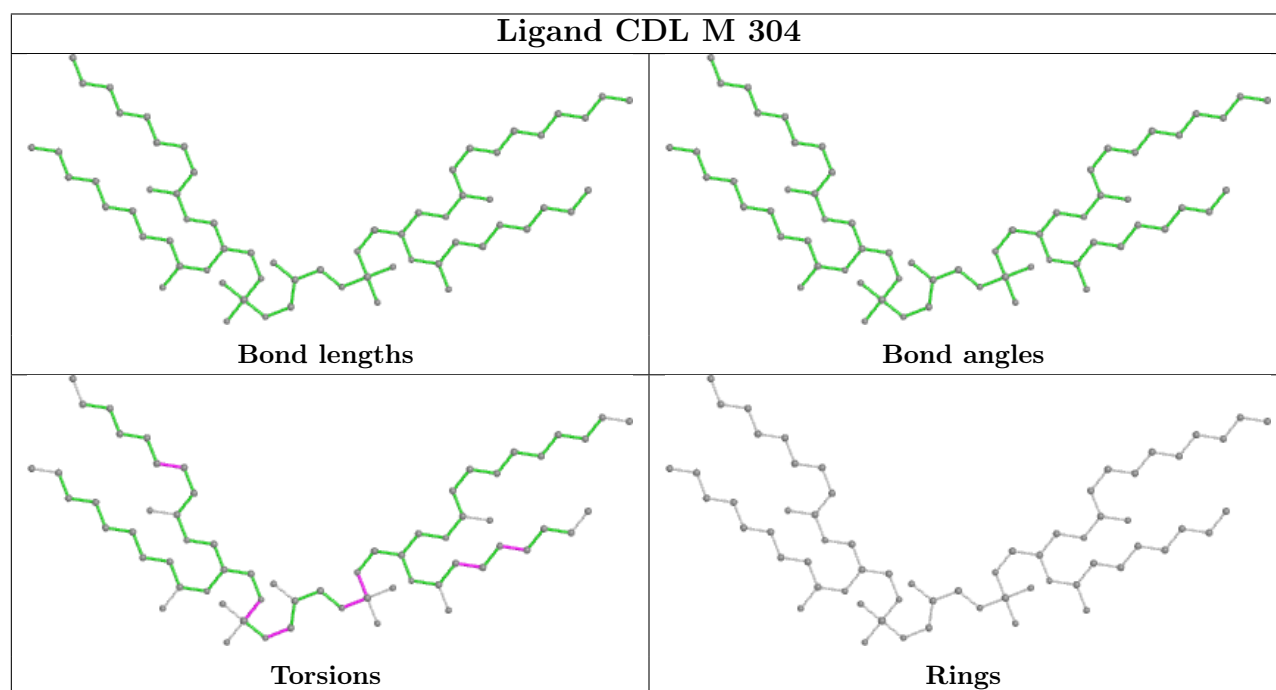
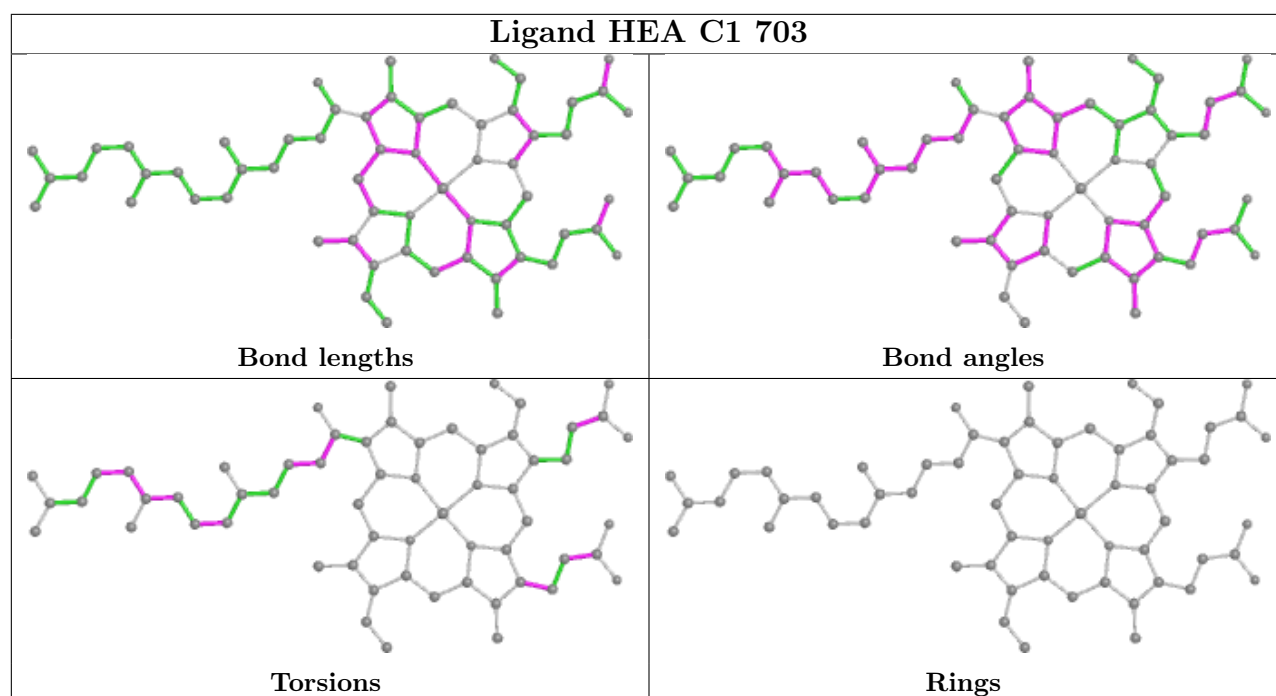
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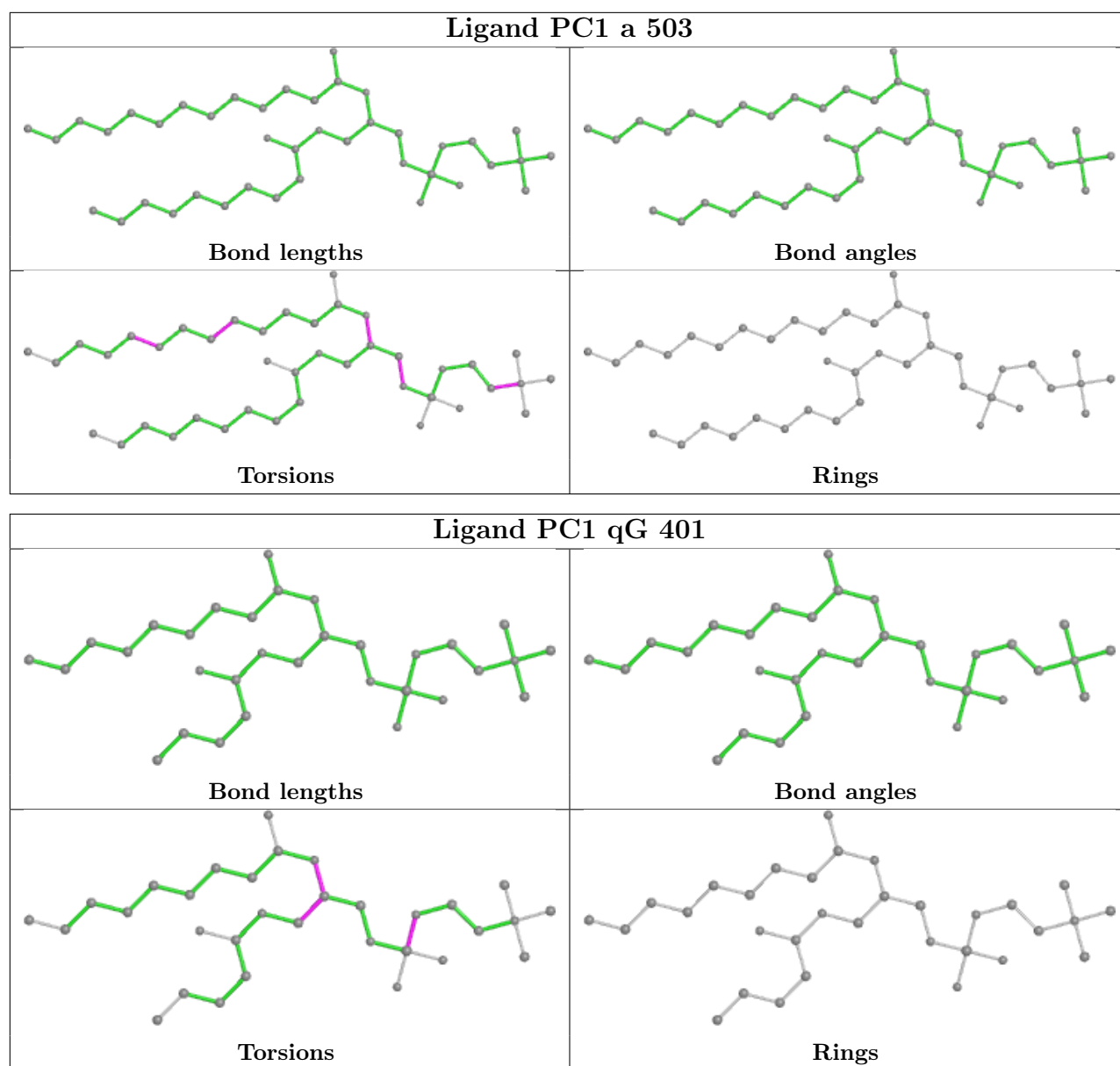


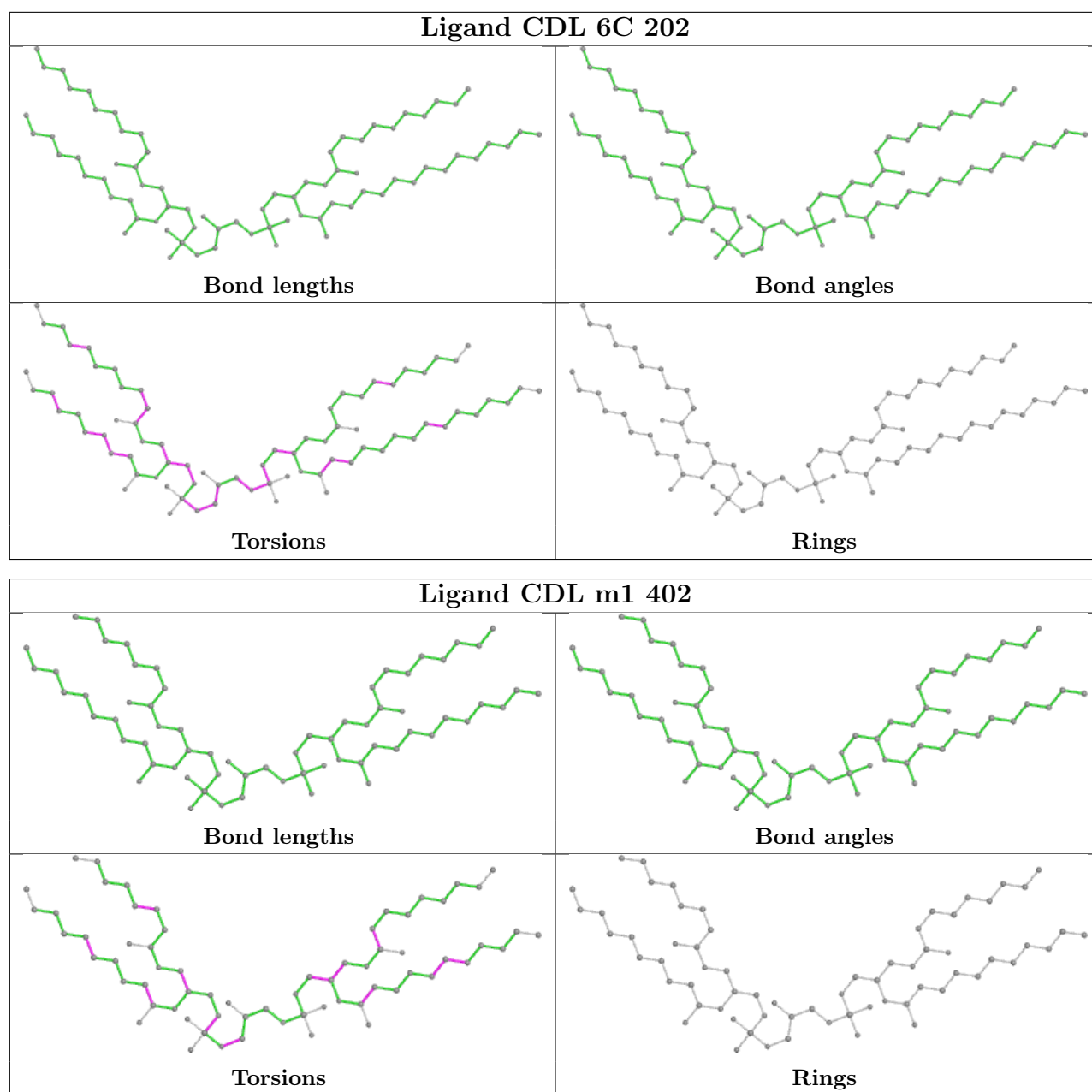


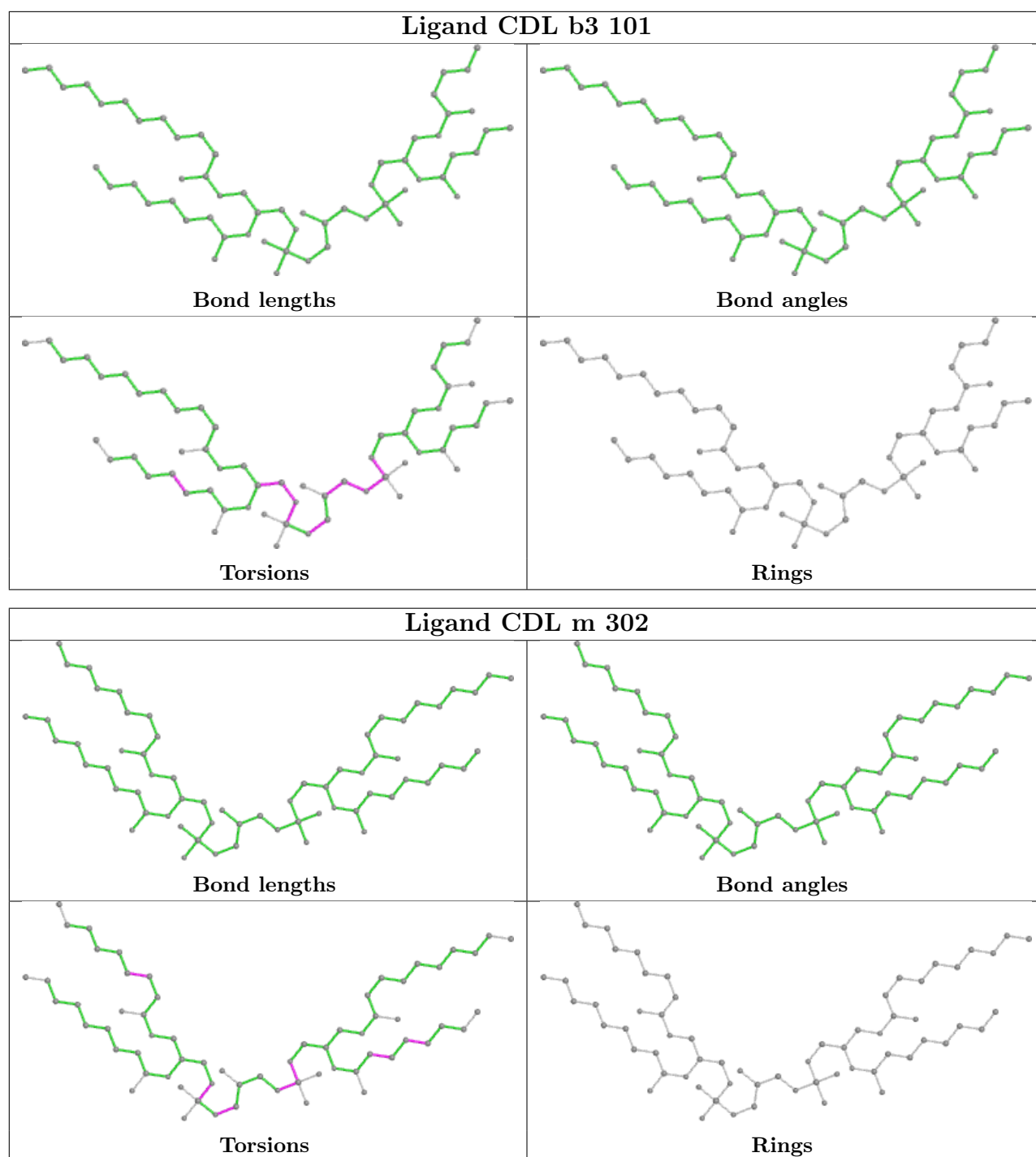


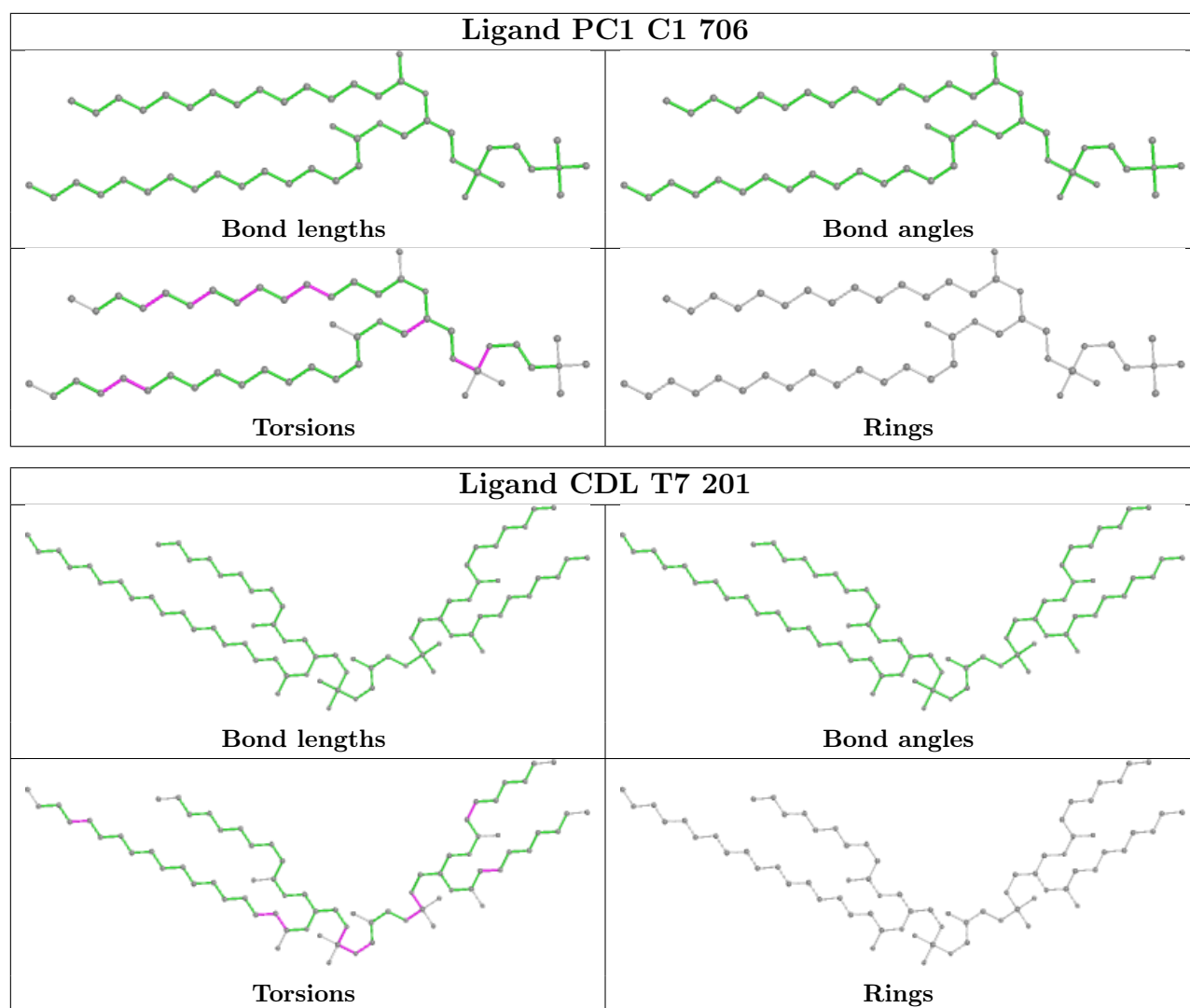




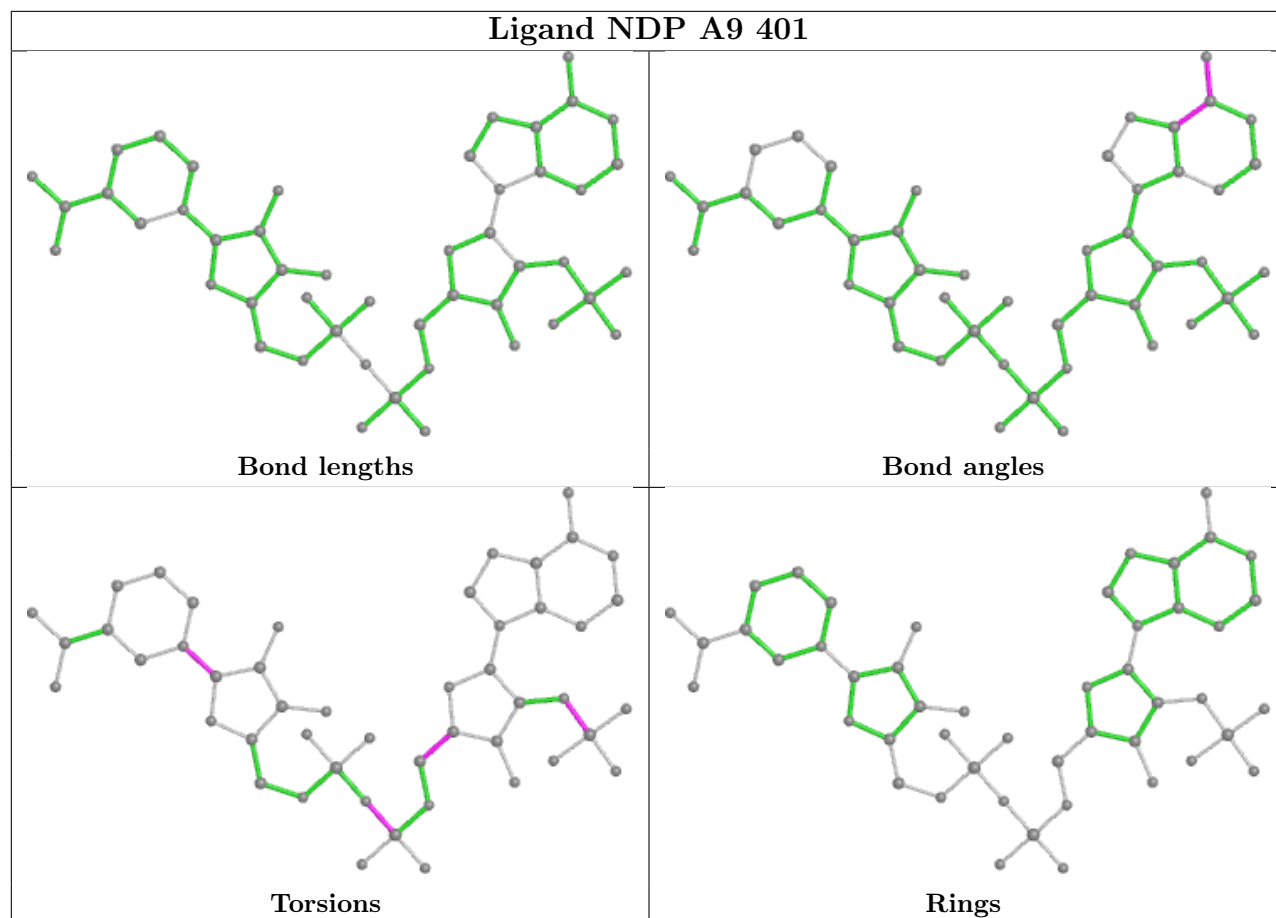




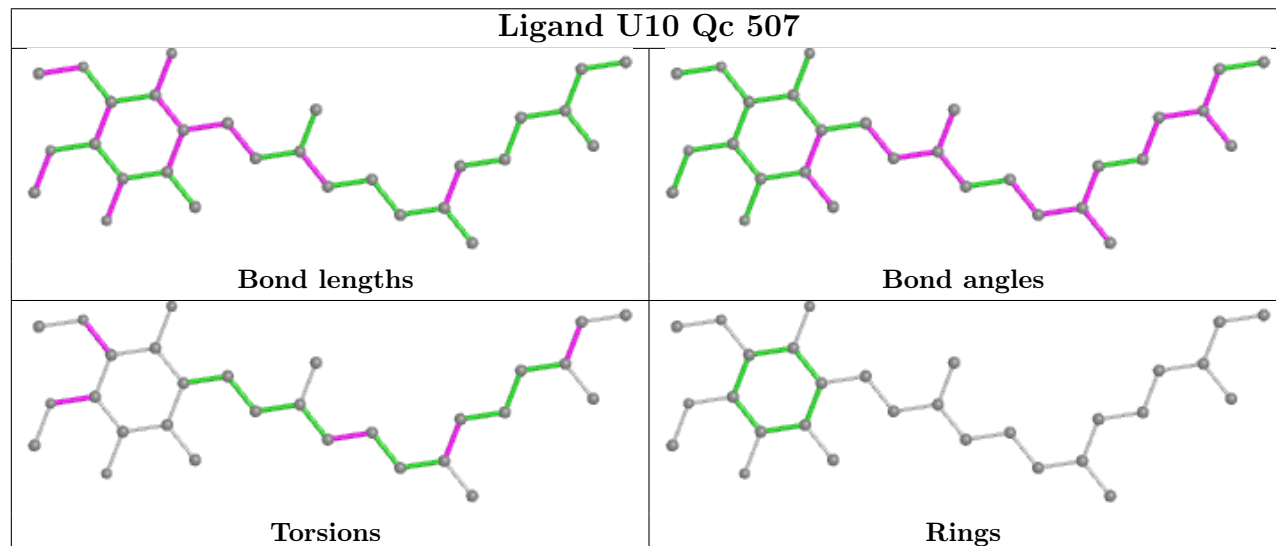


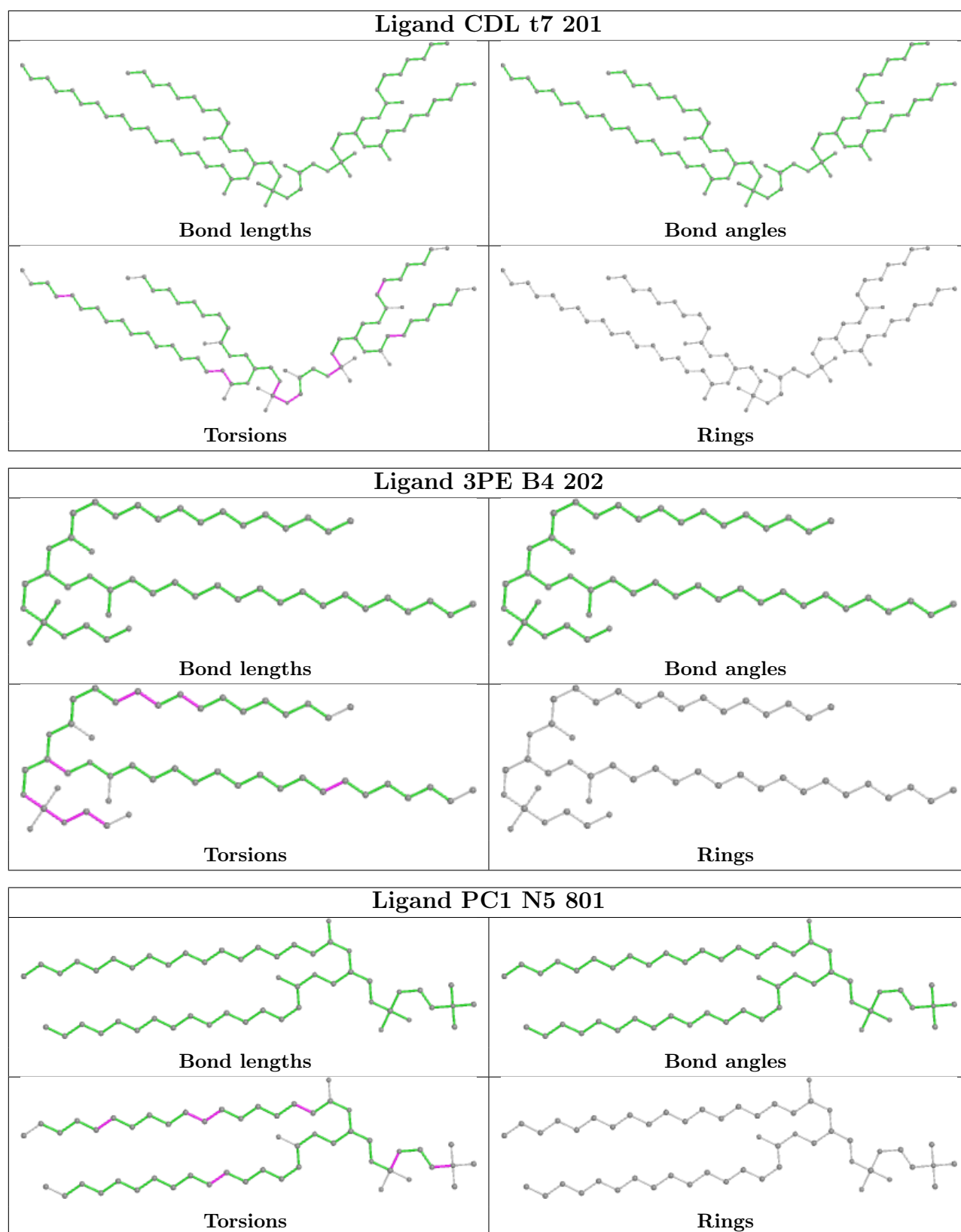


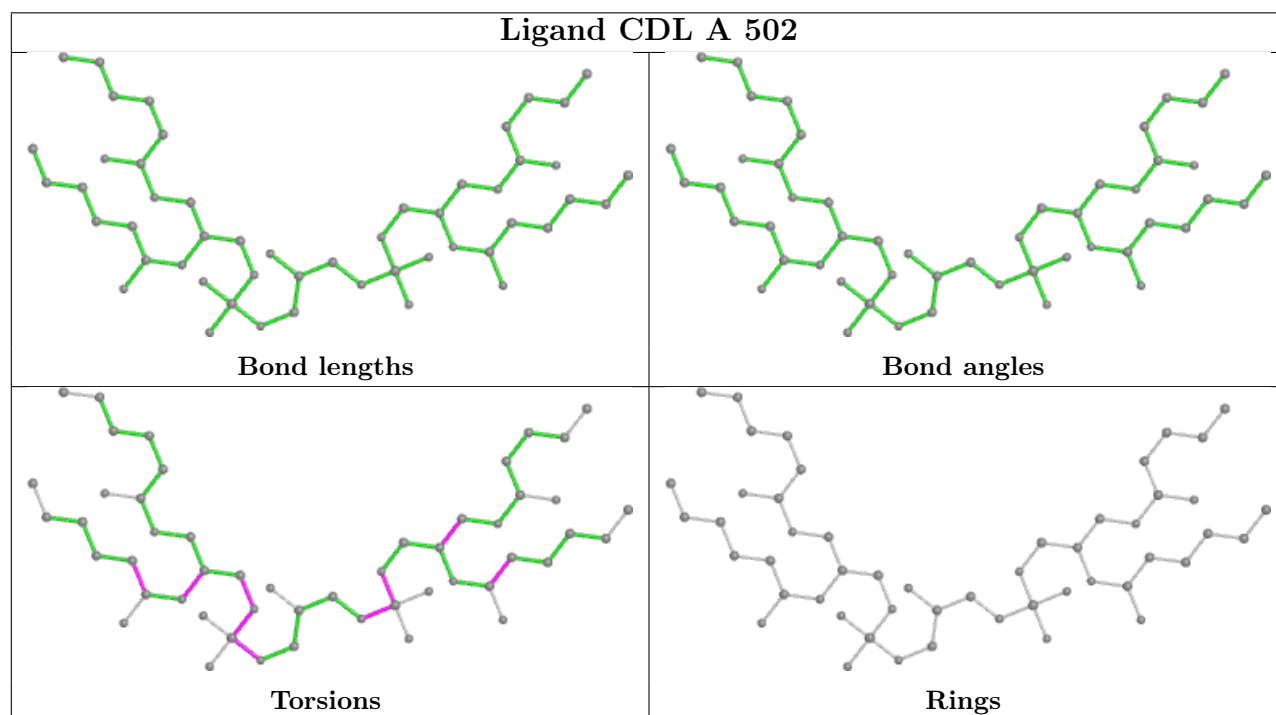
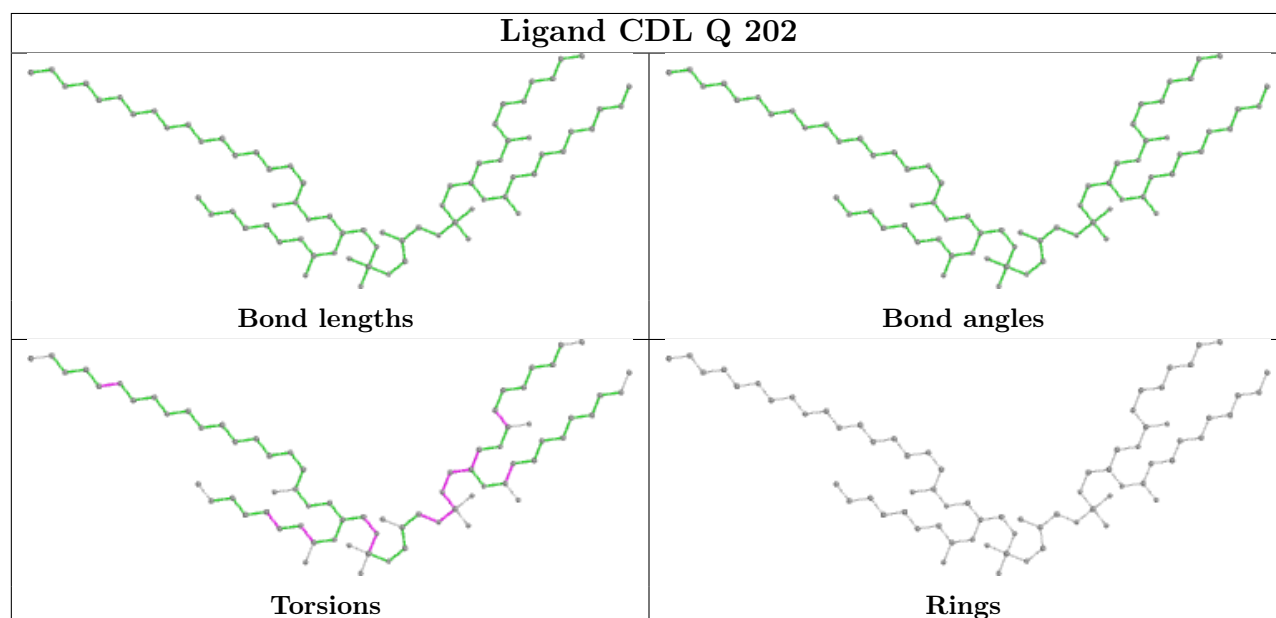
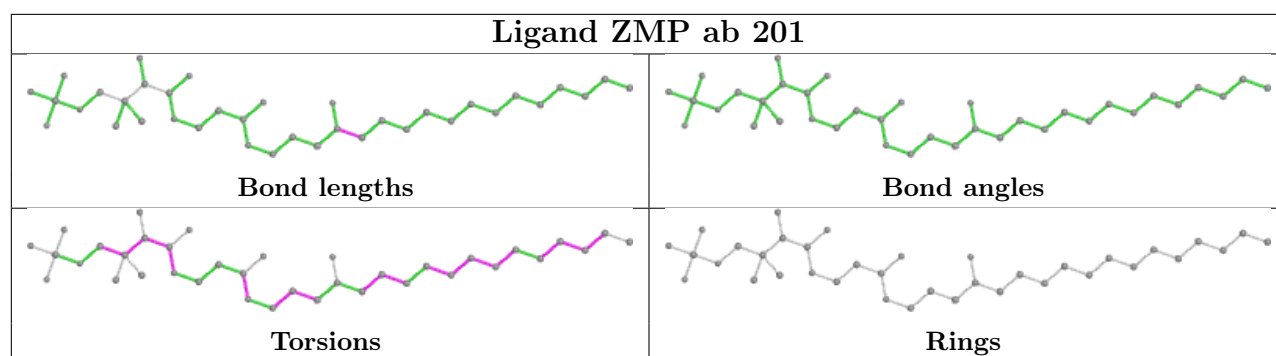
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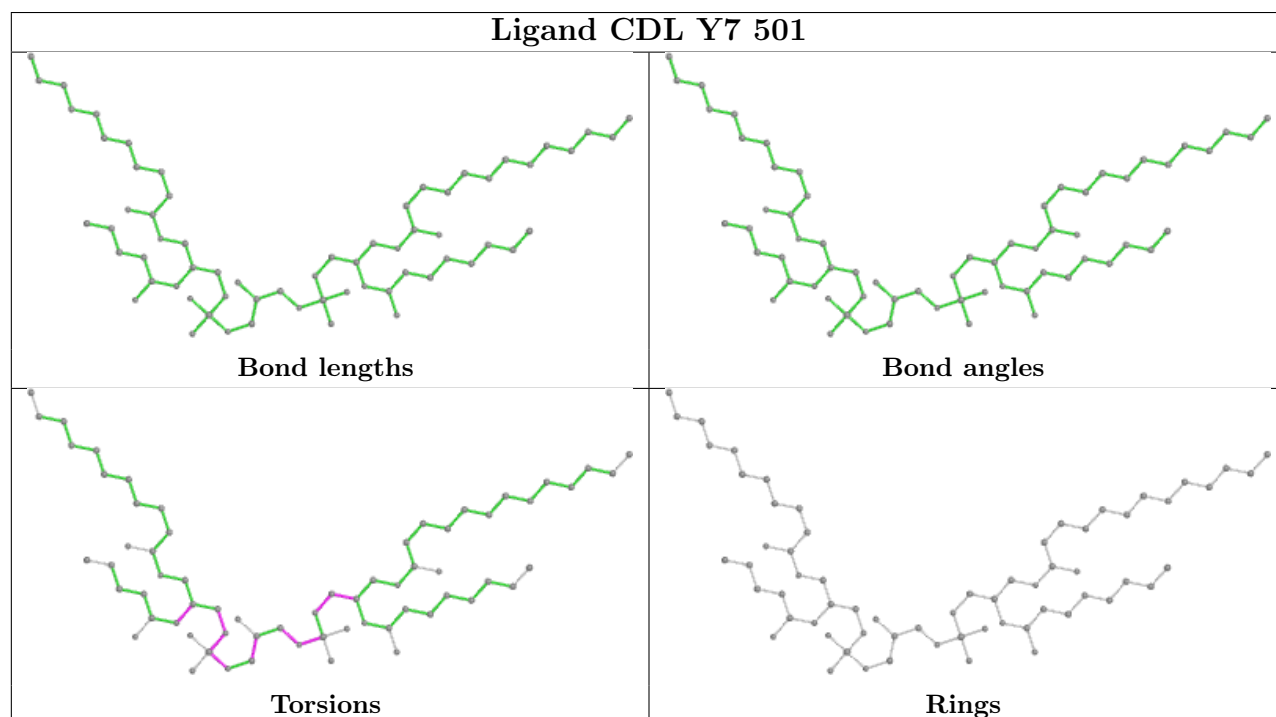
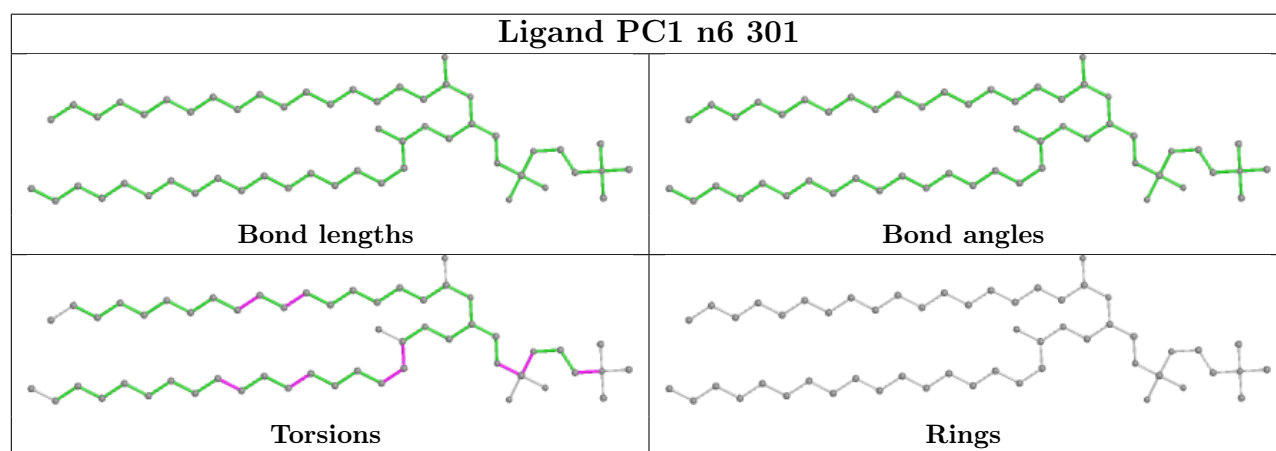
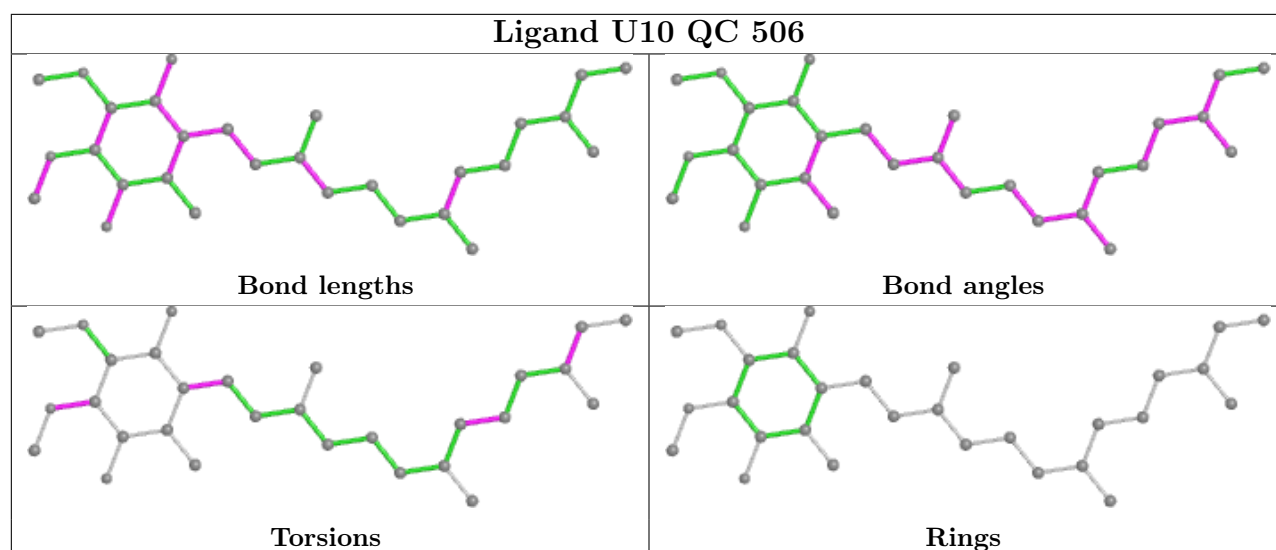


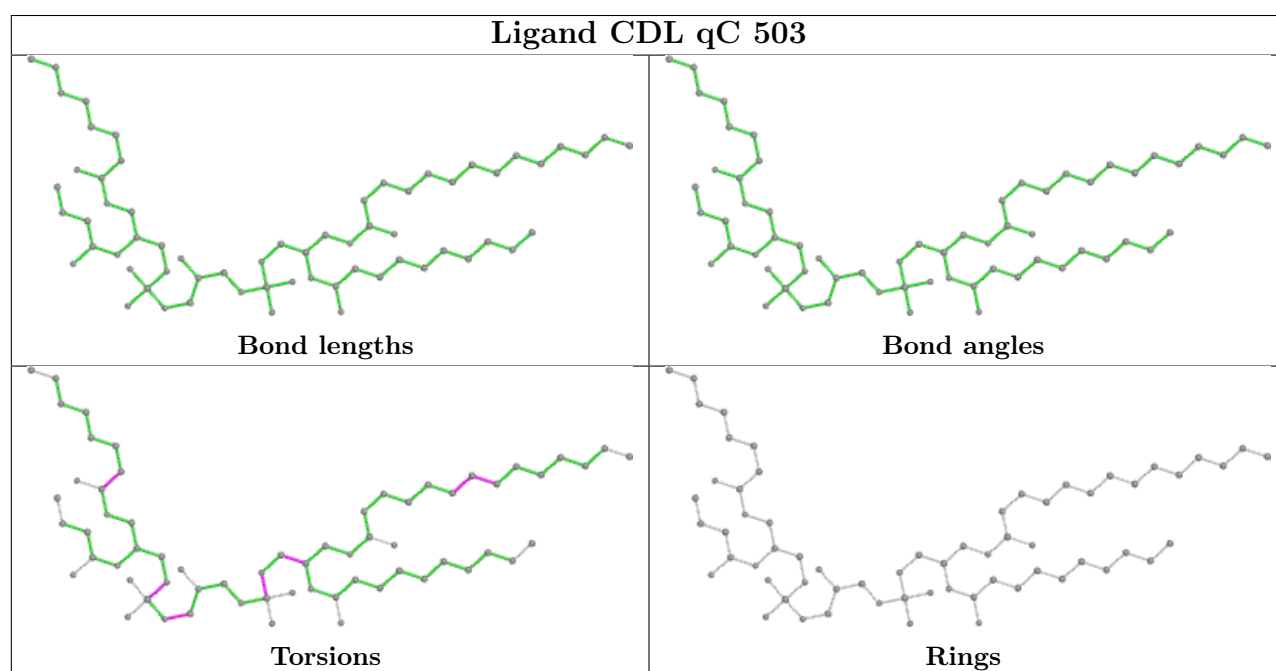
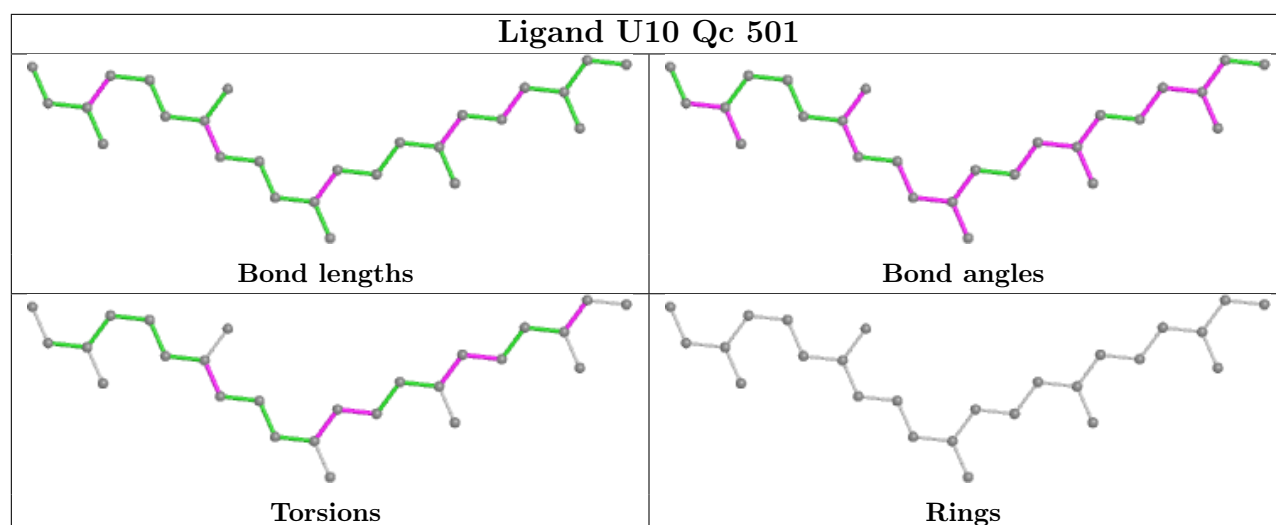
Ligand U10 Qc 507



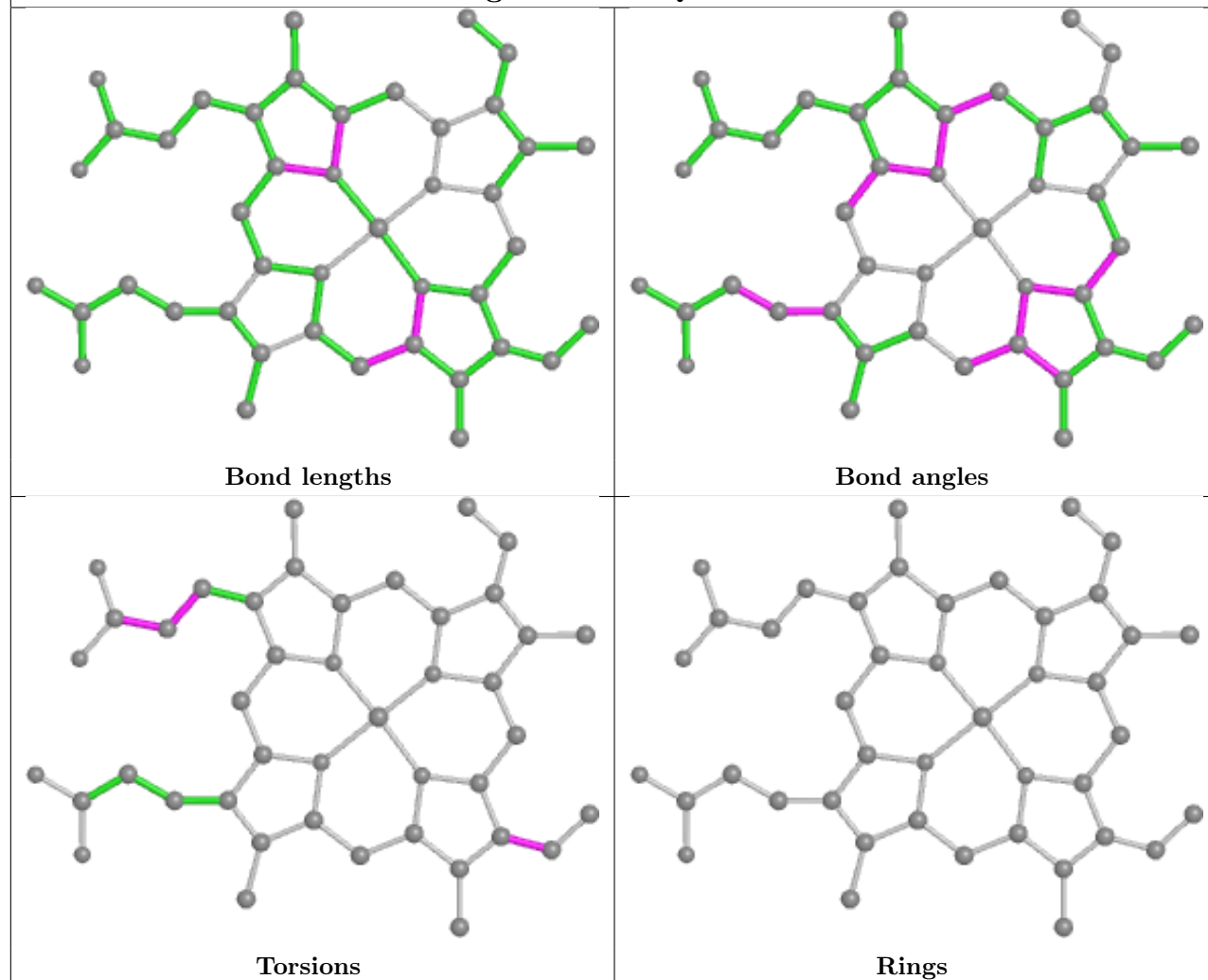




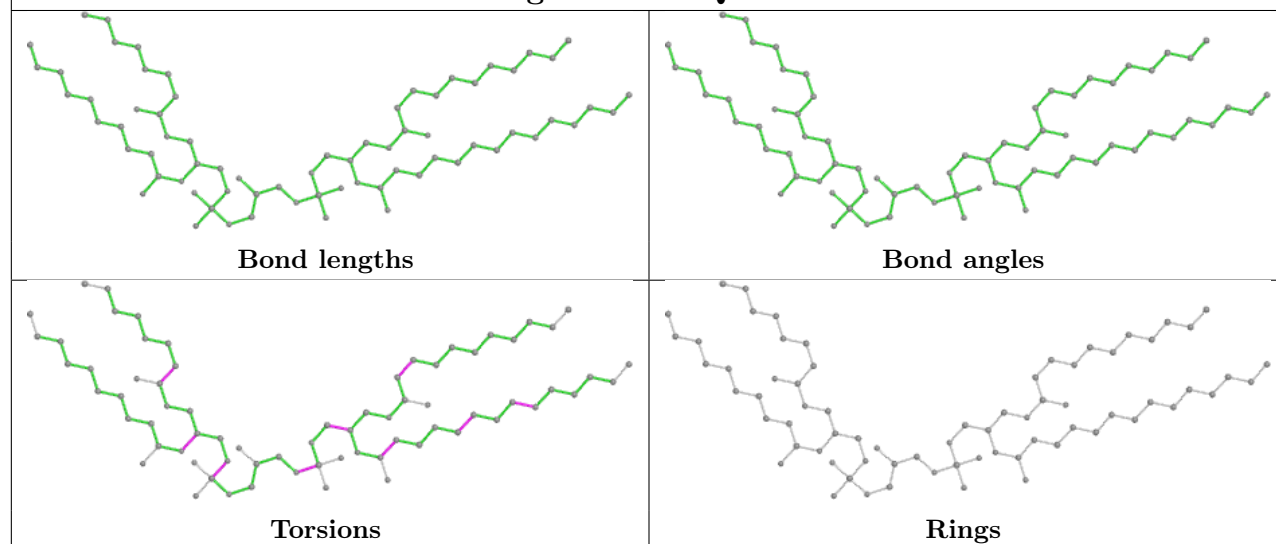


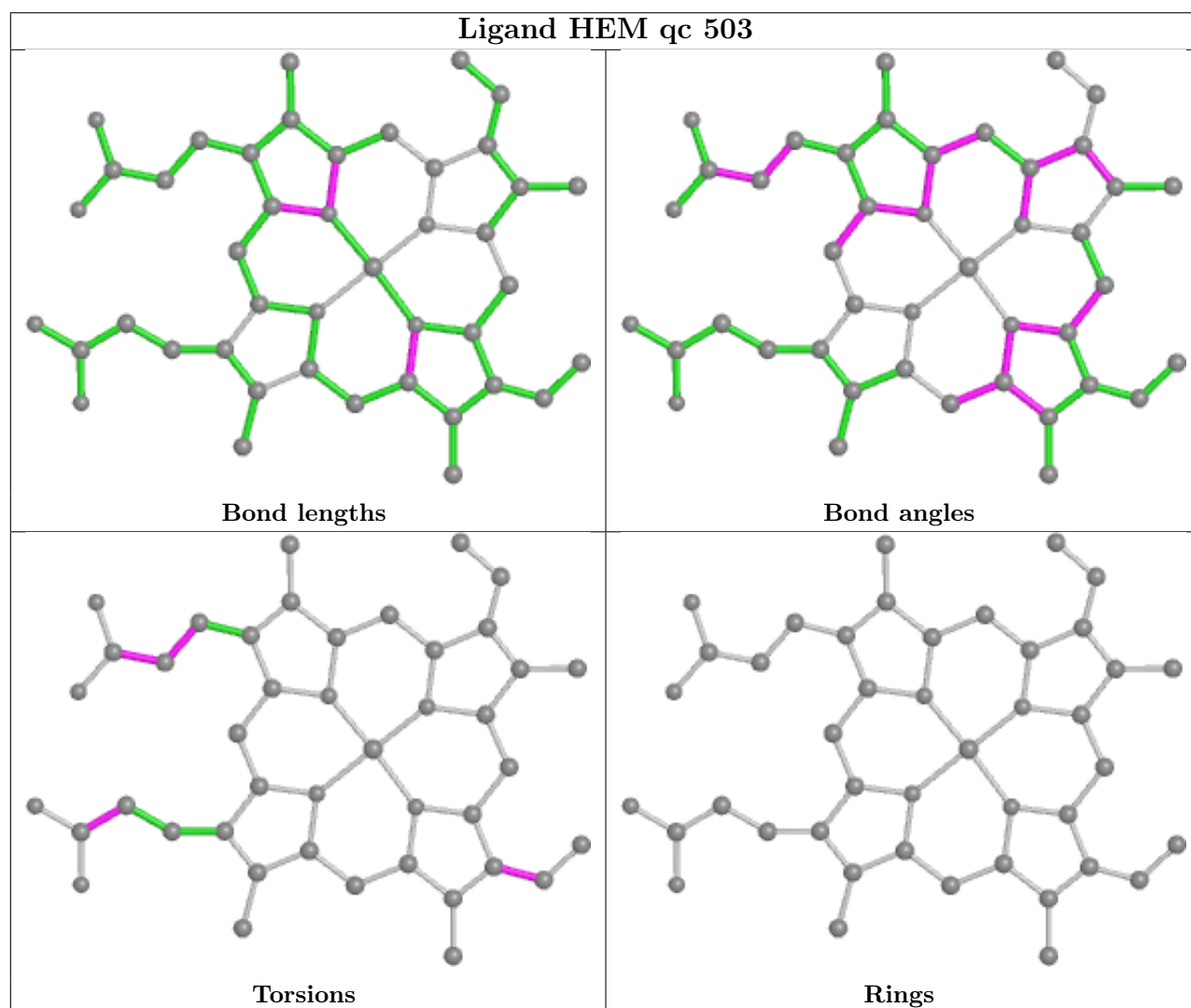
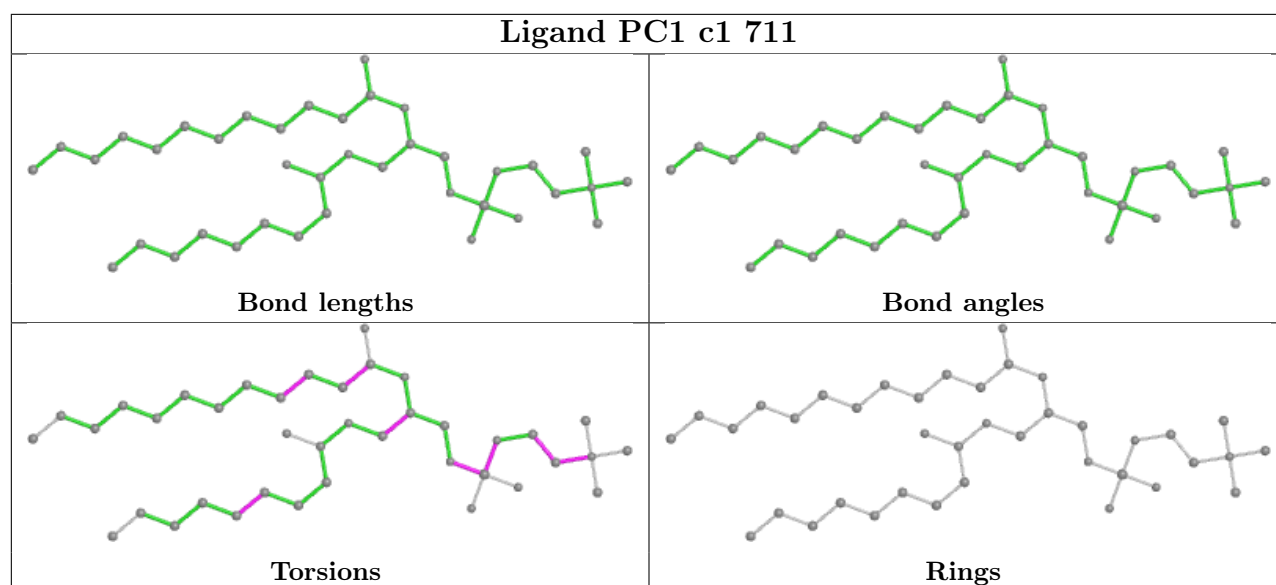


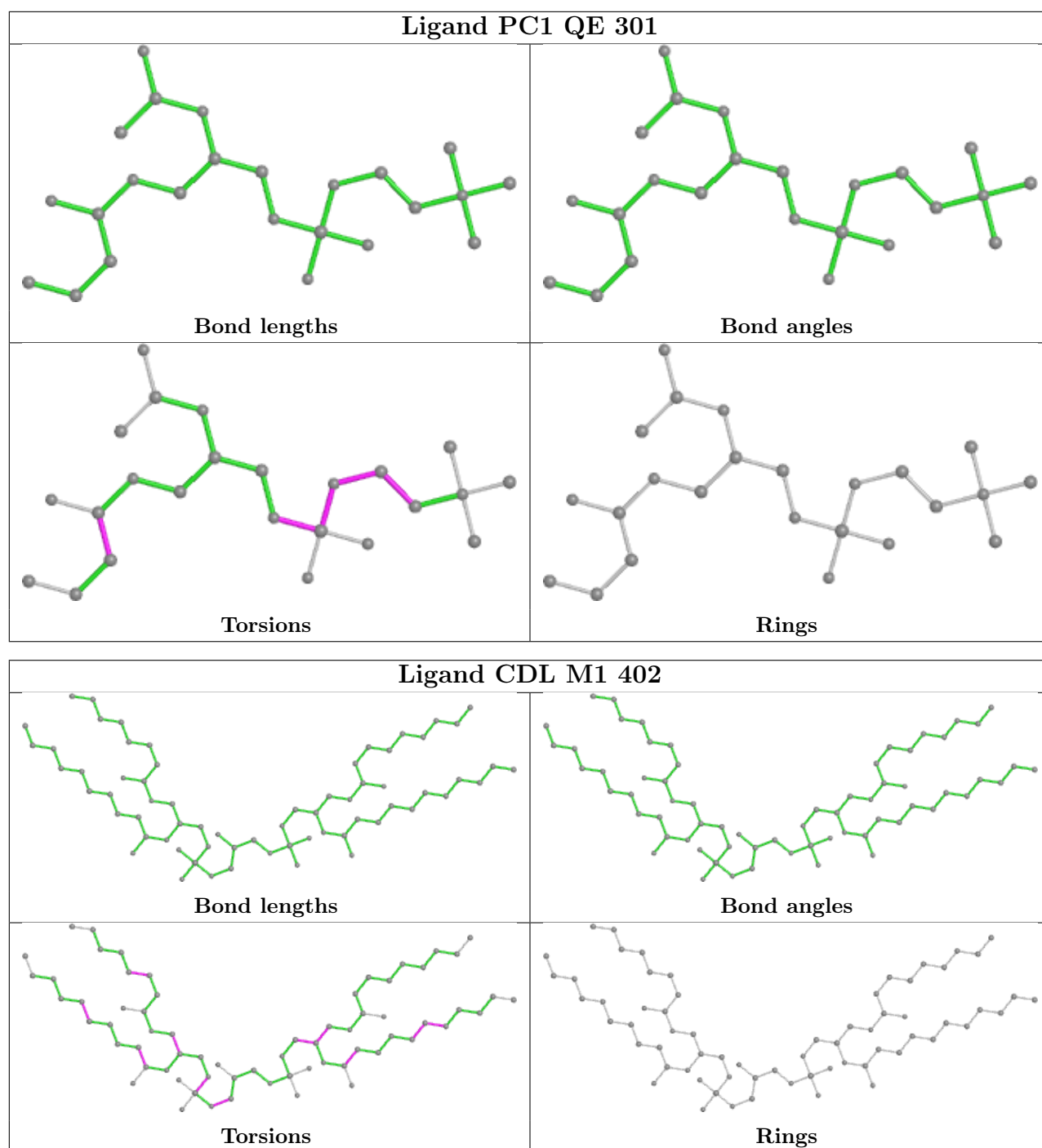
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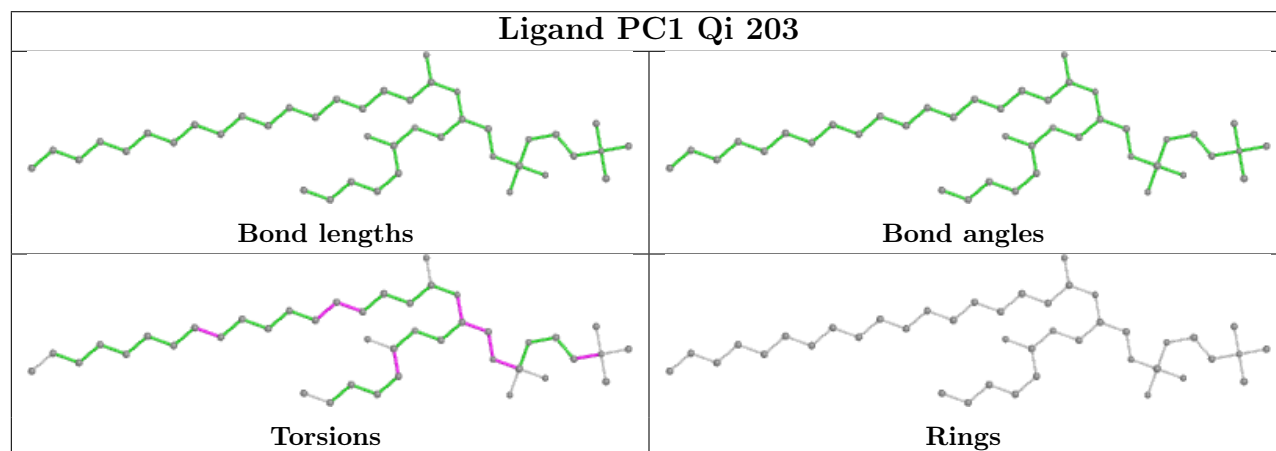
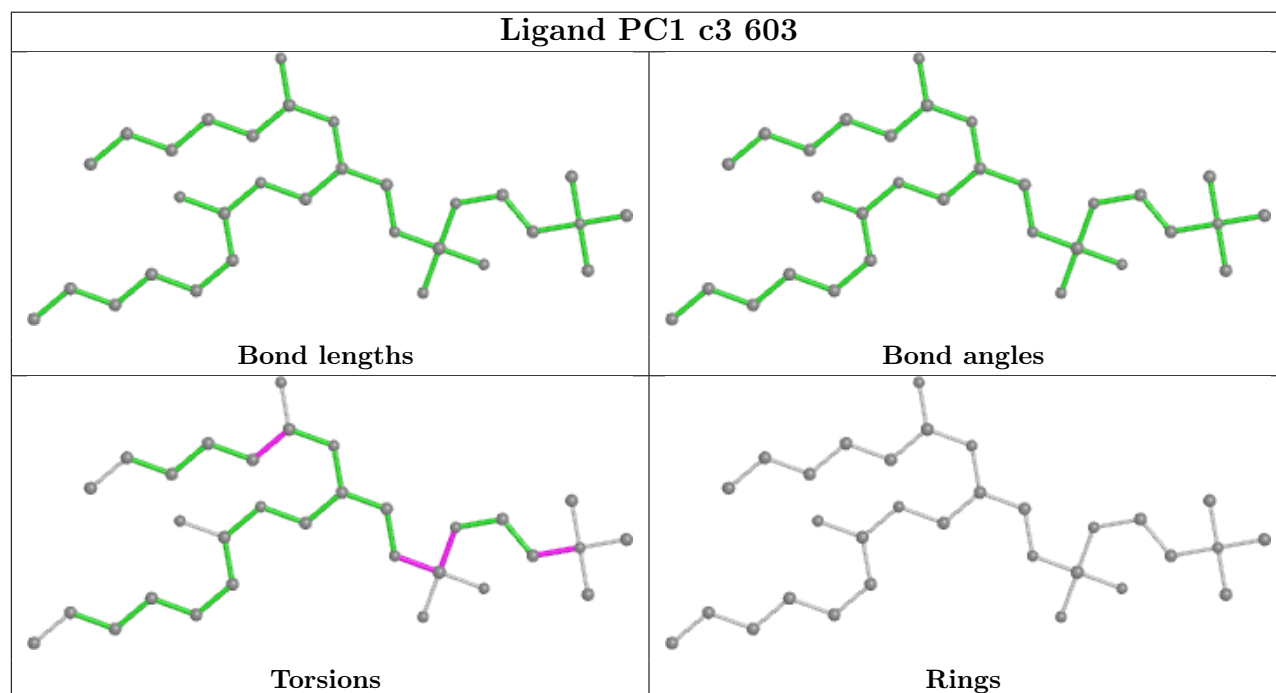
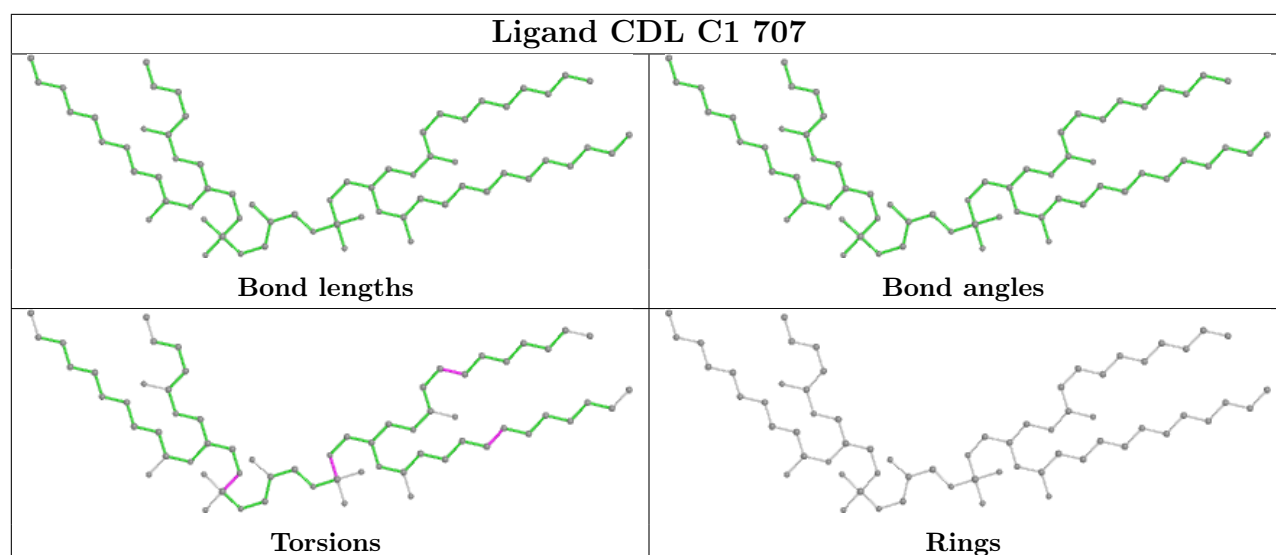


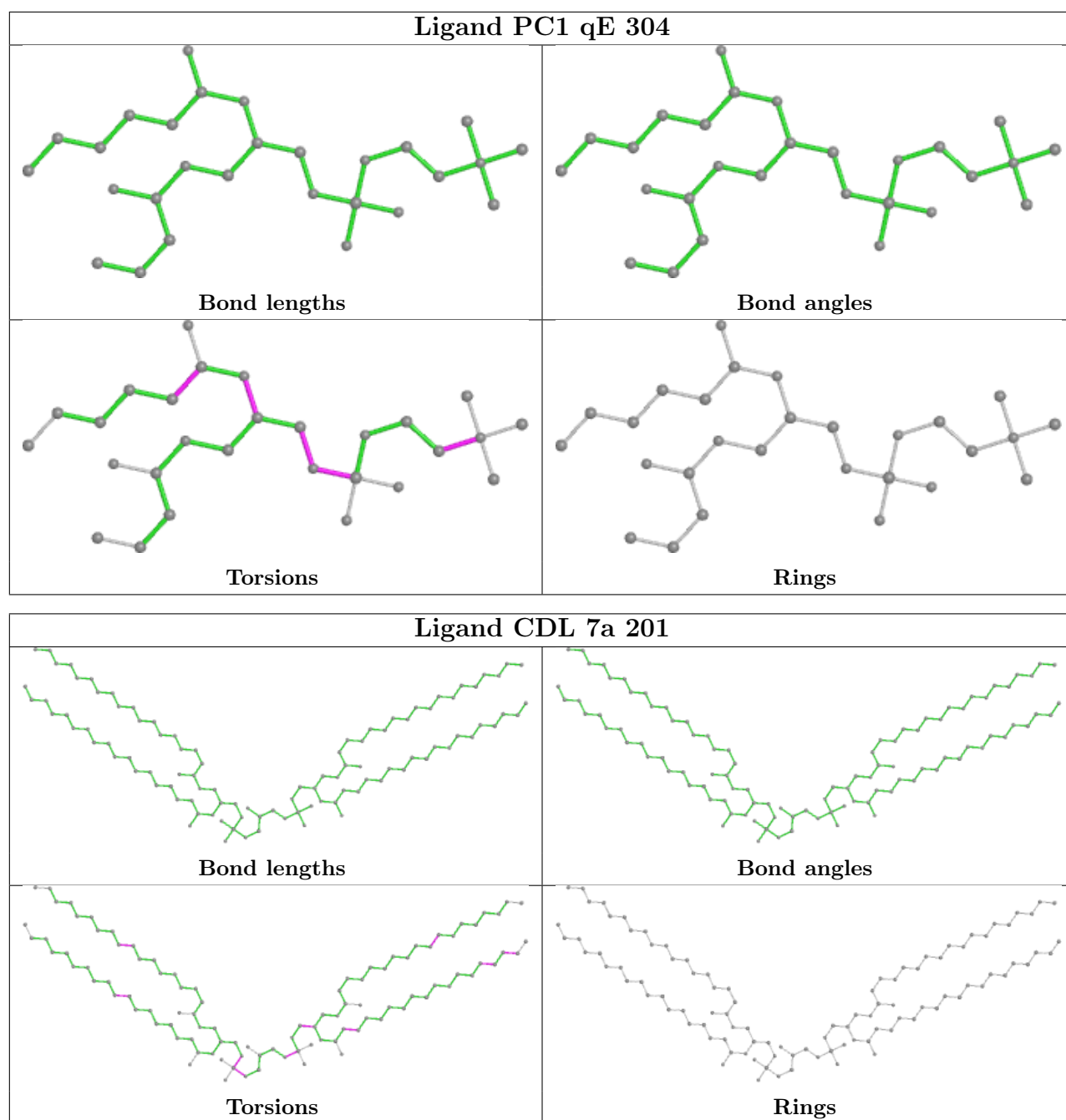
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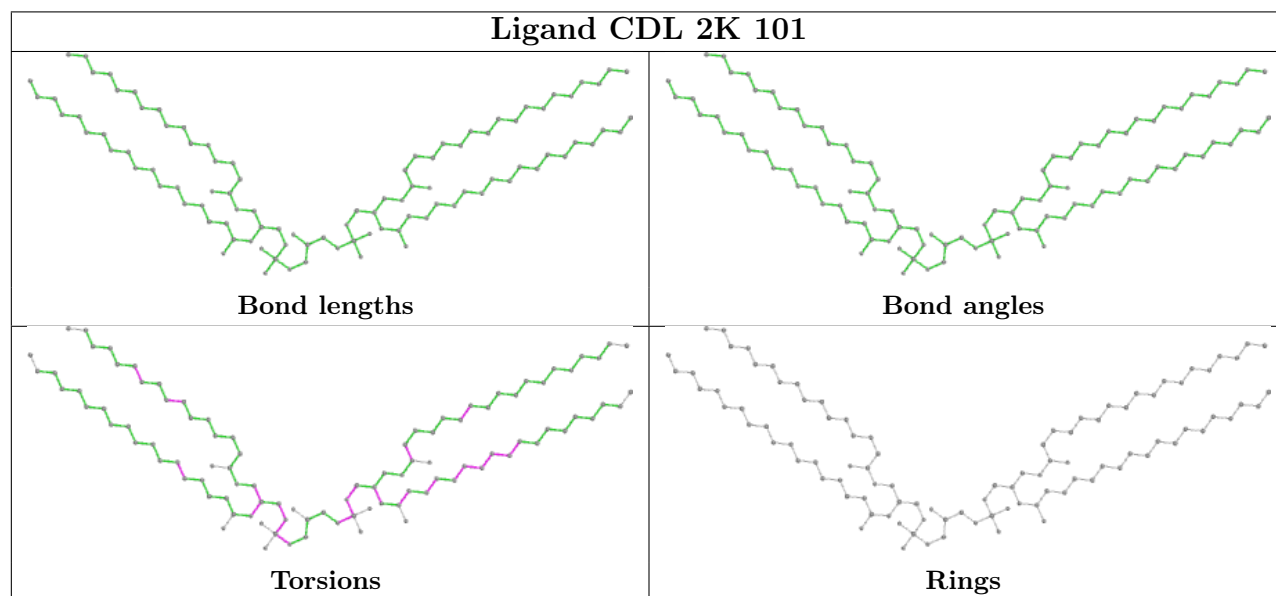
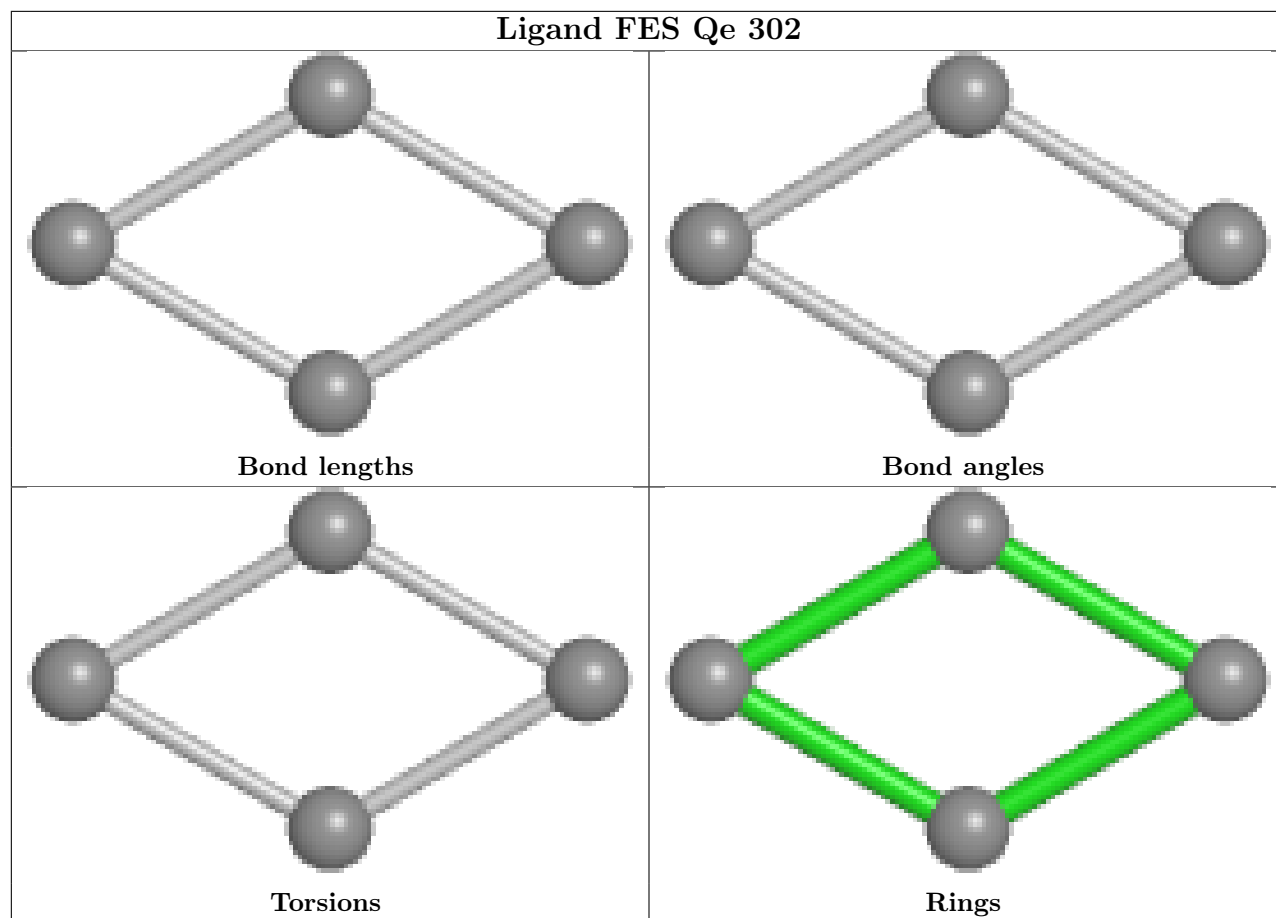


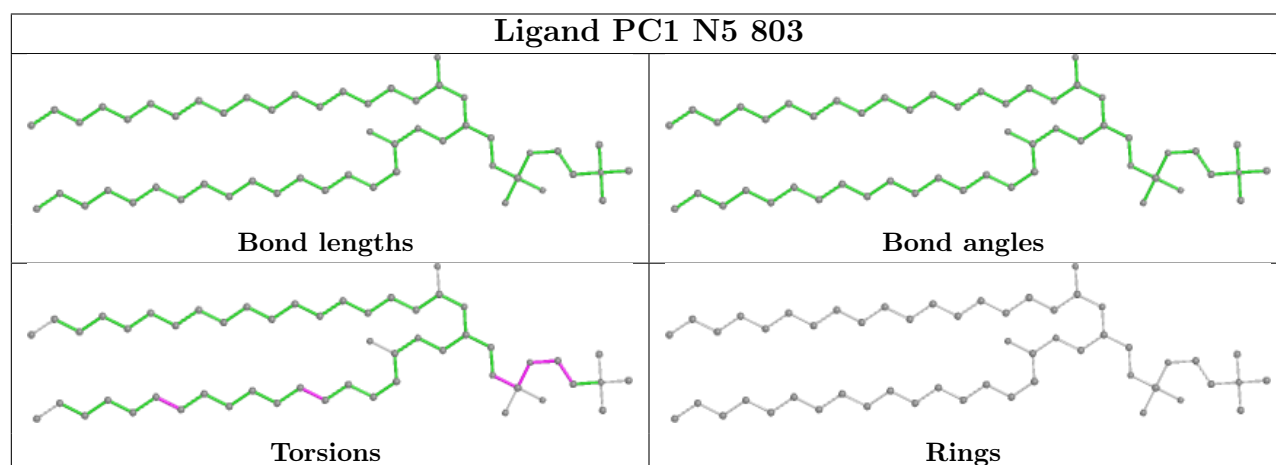
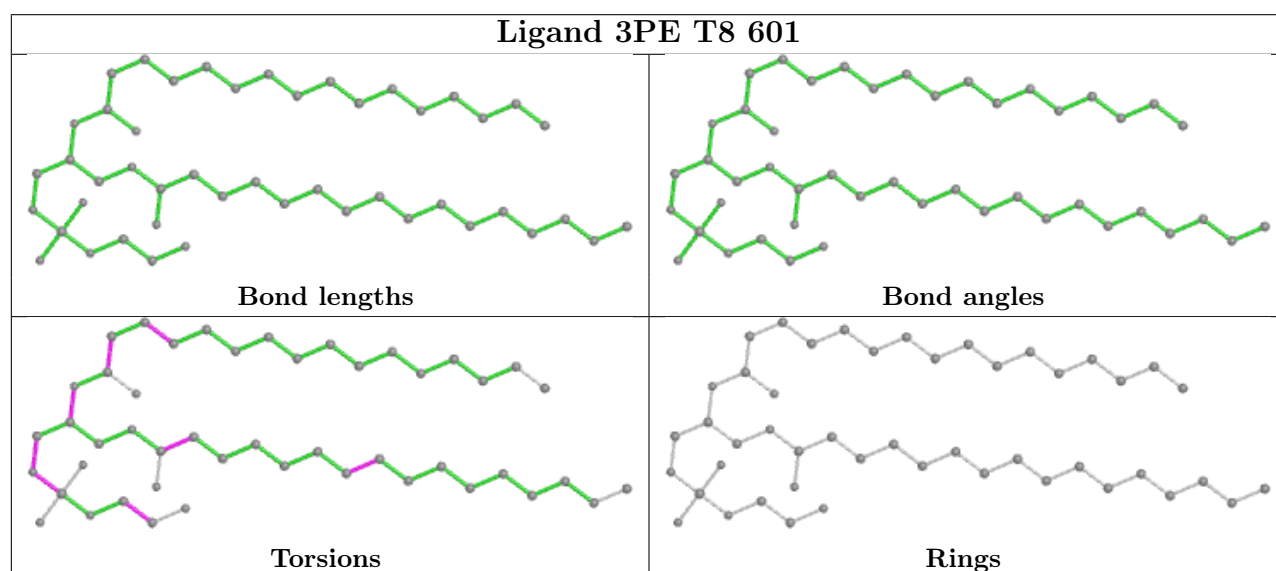
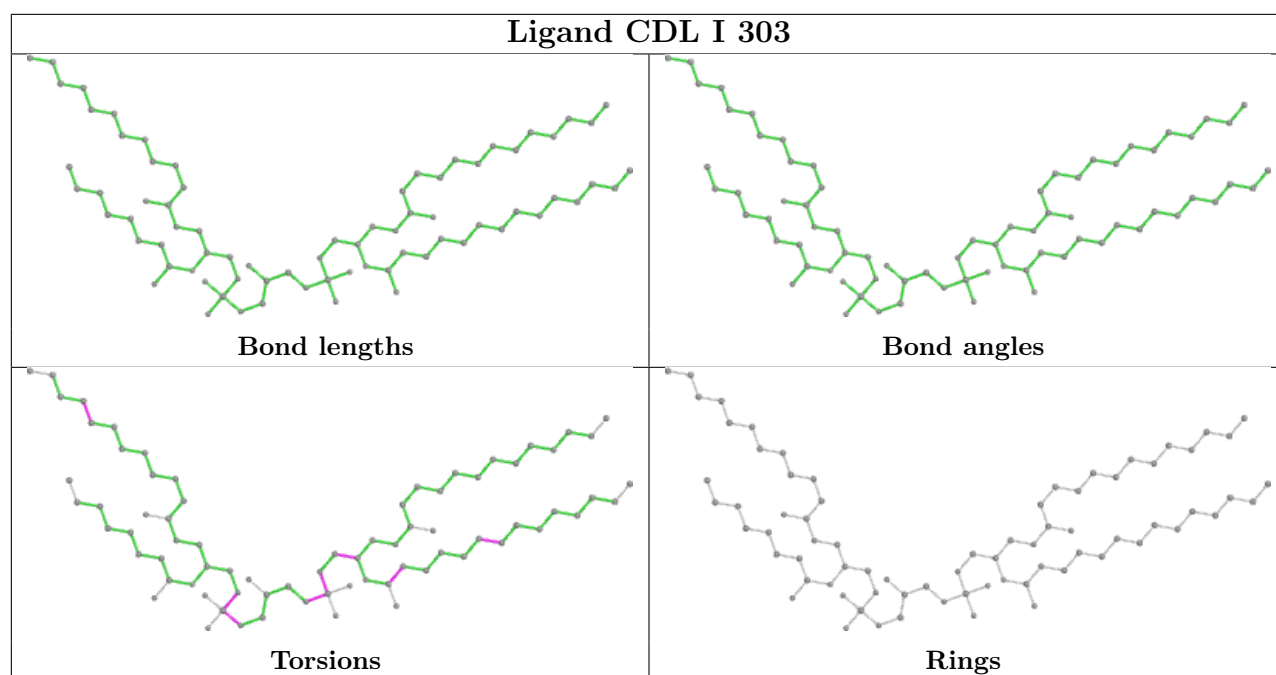


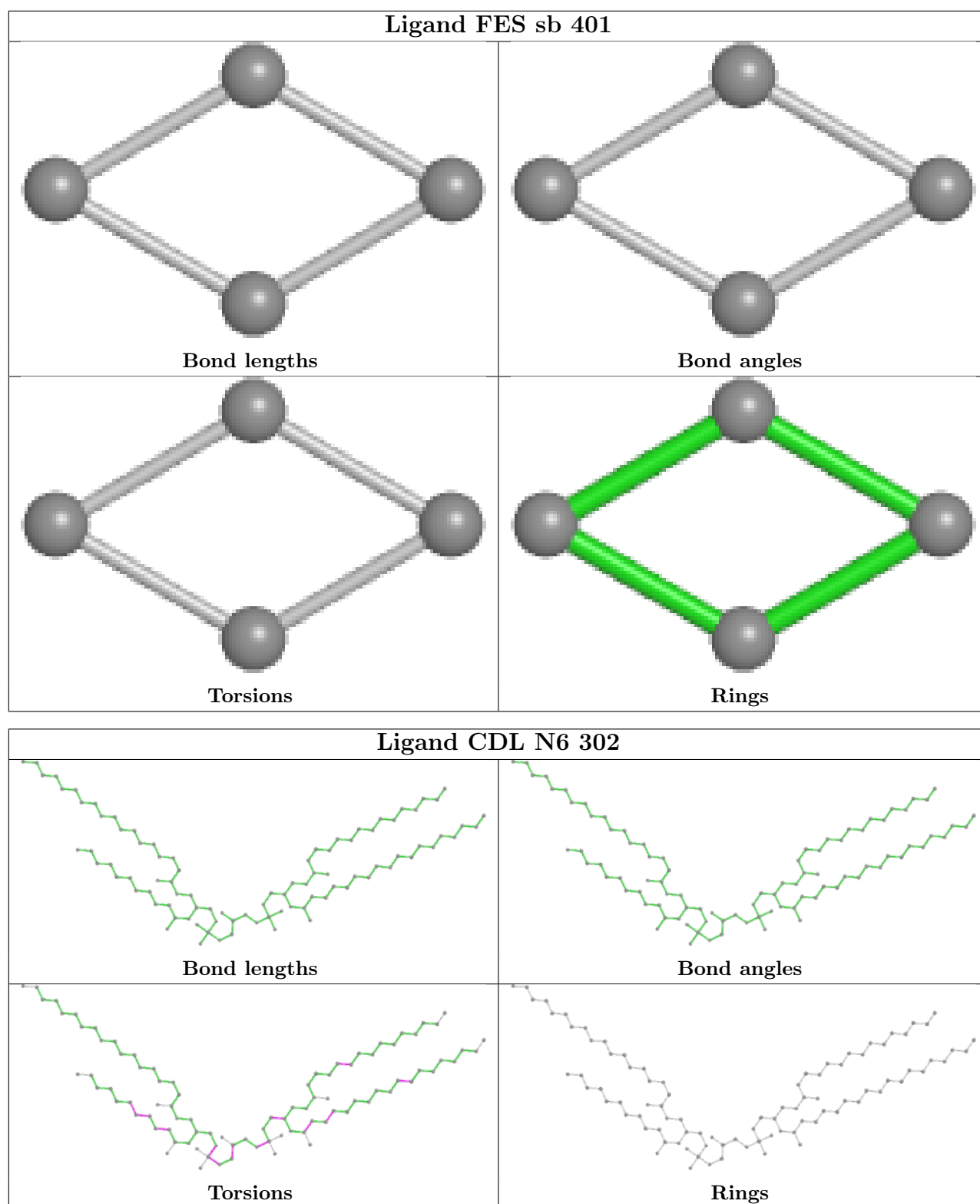


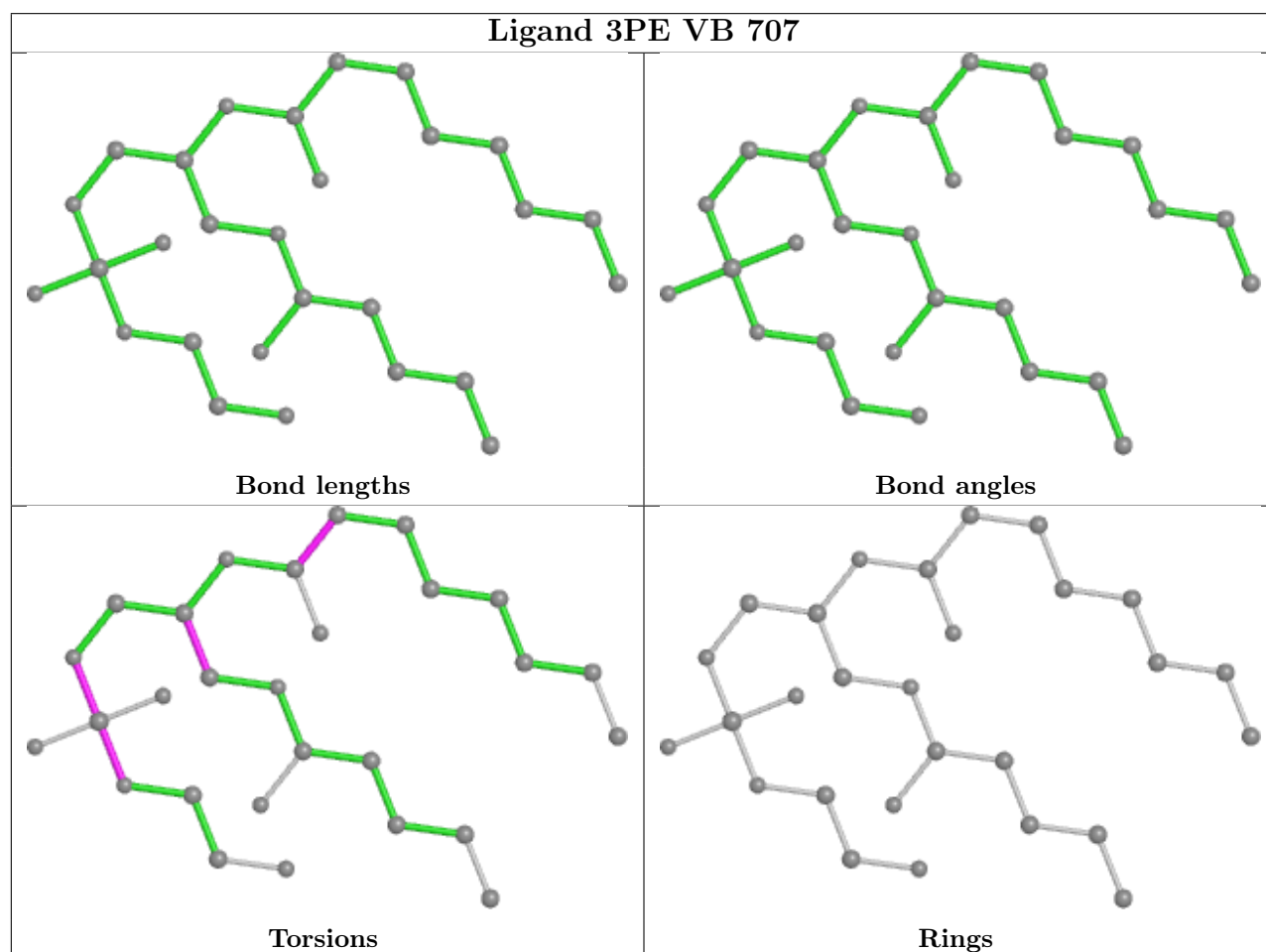
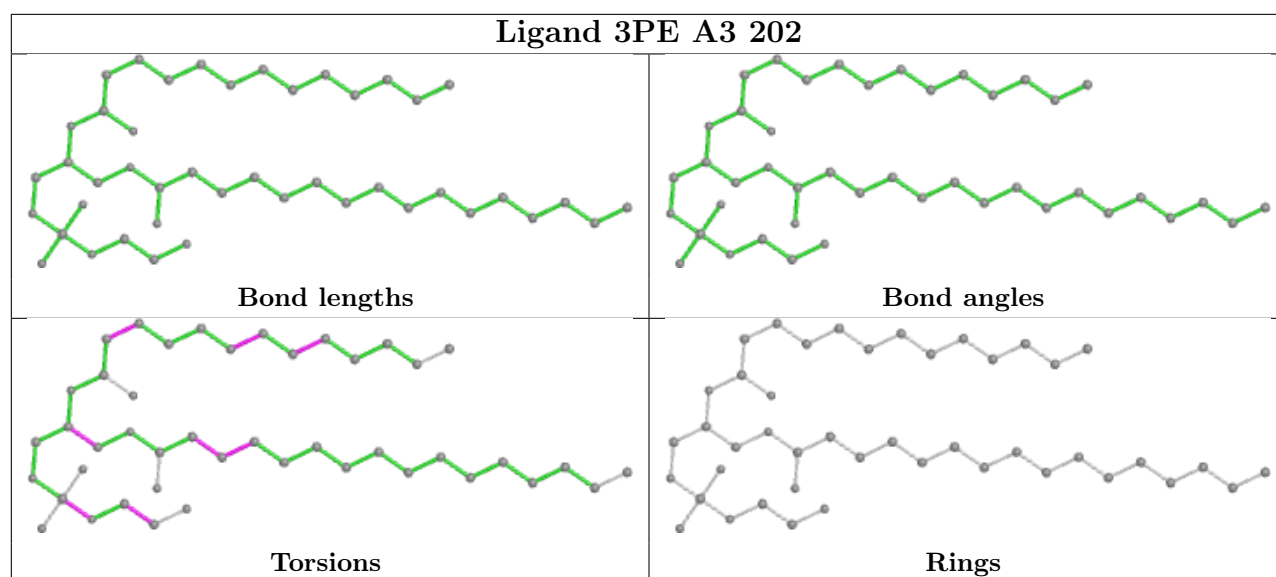


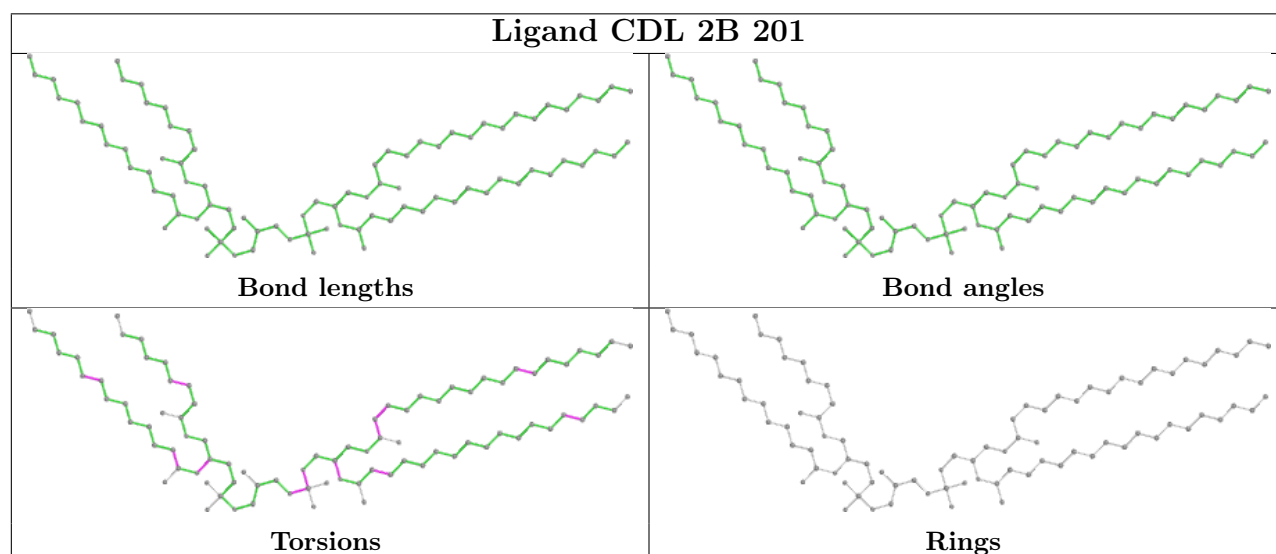
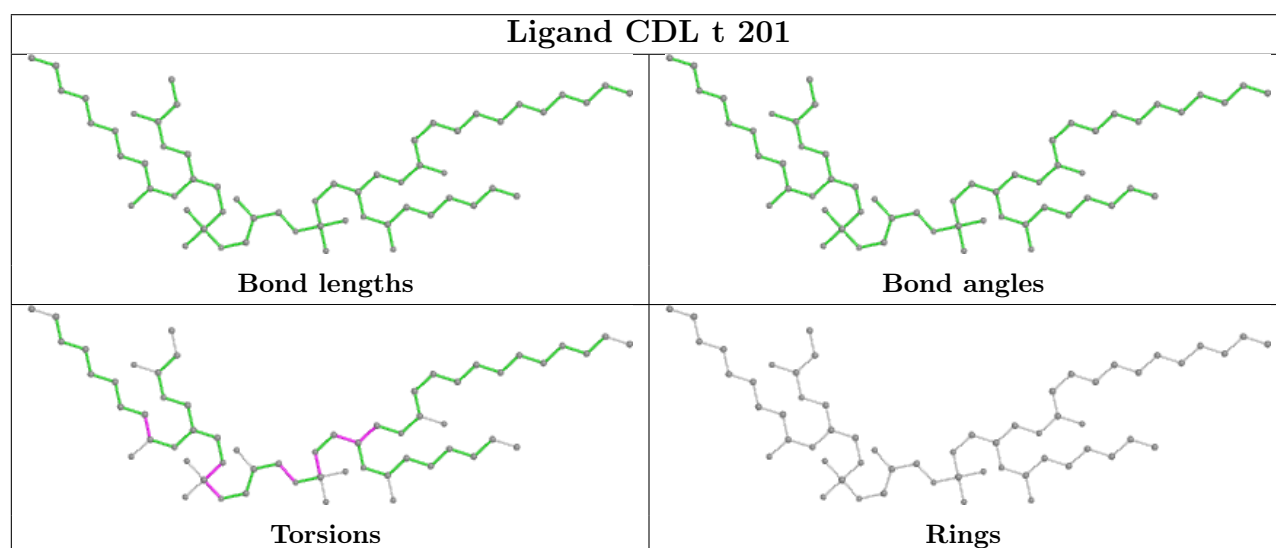
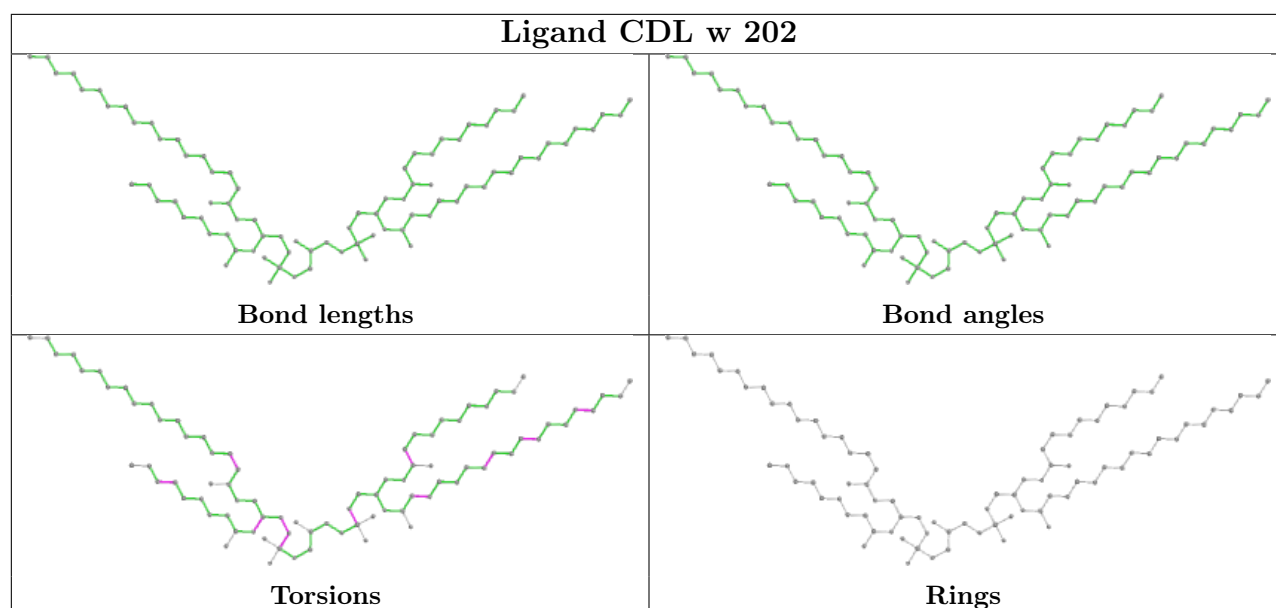


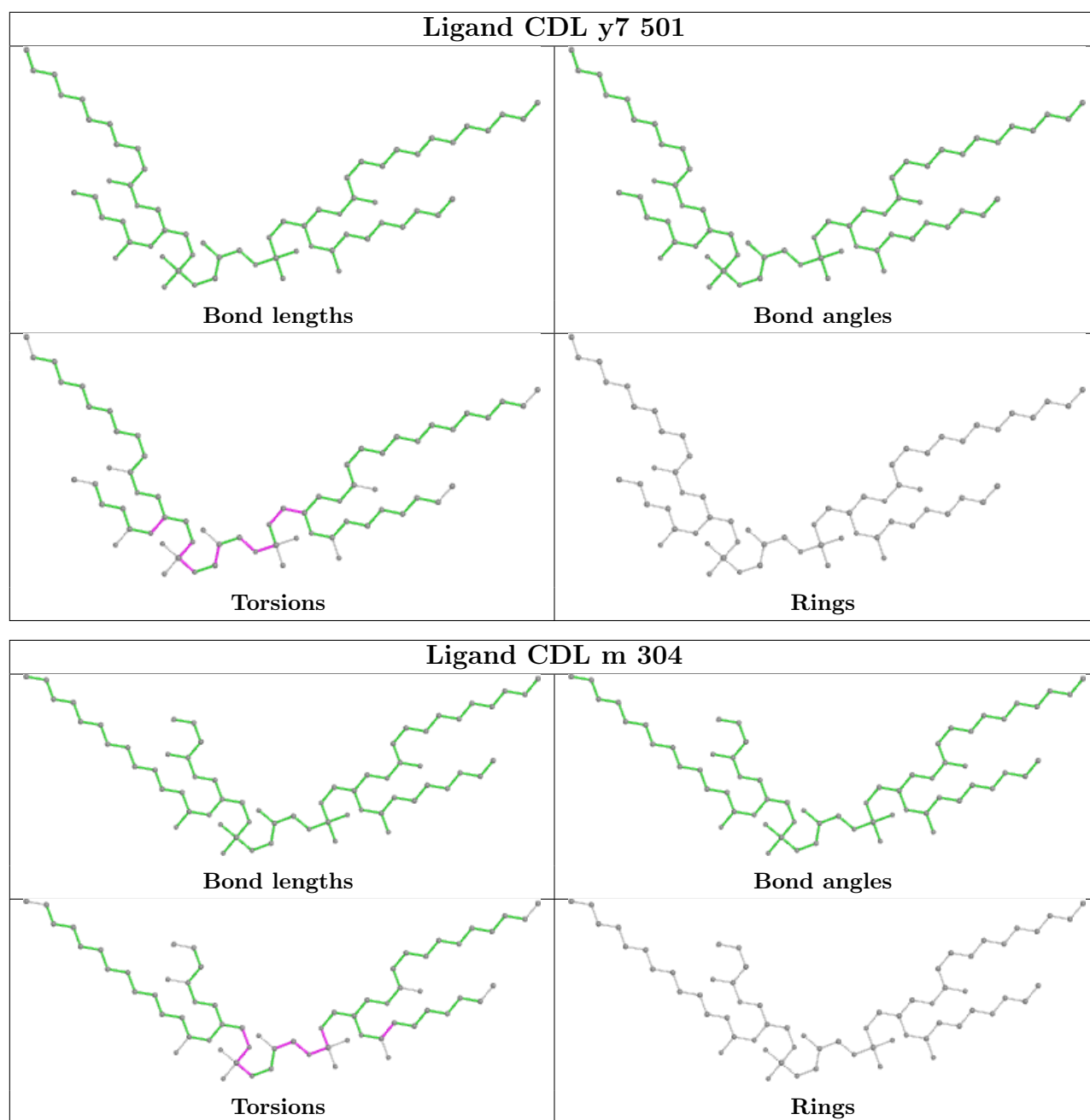


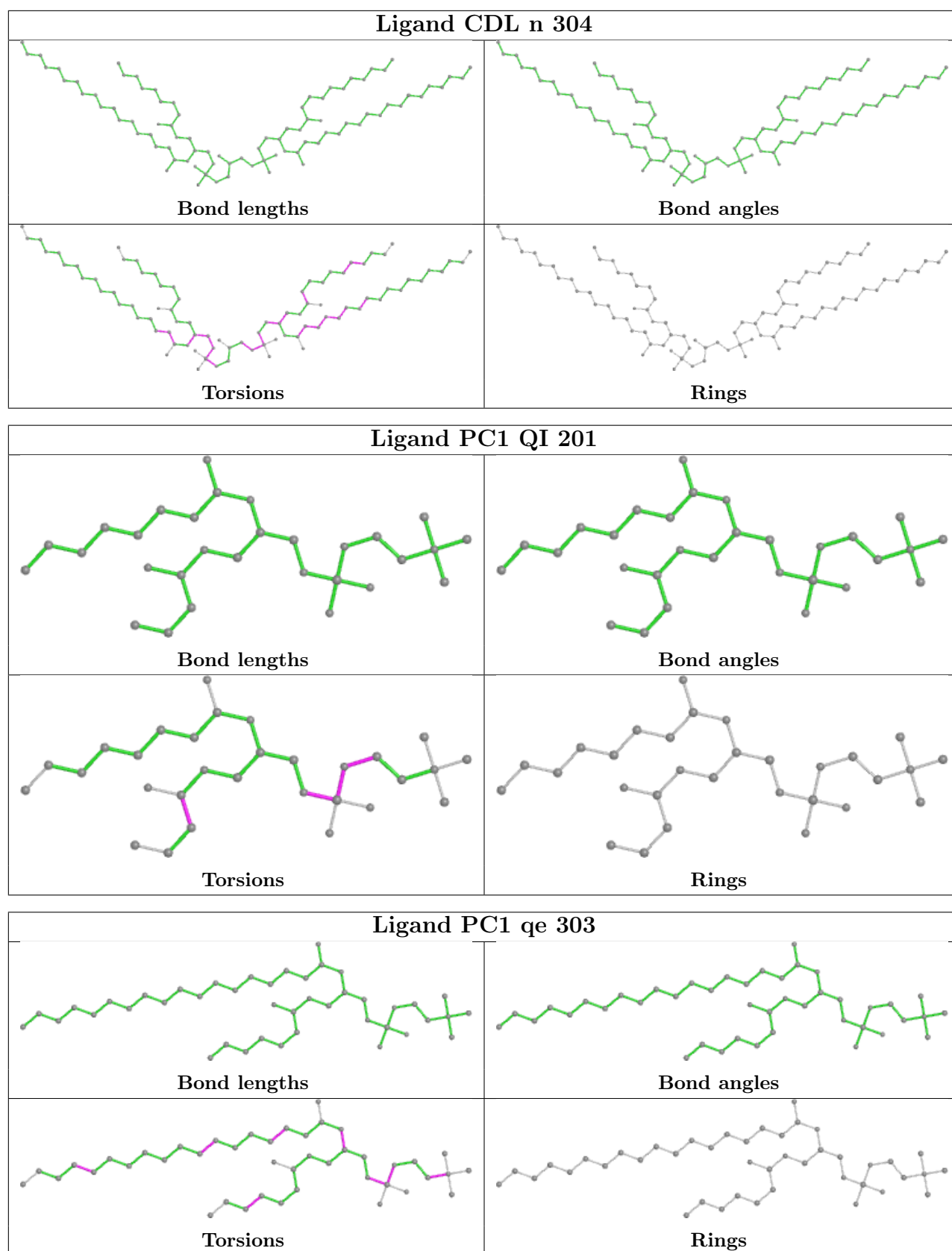


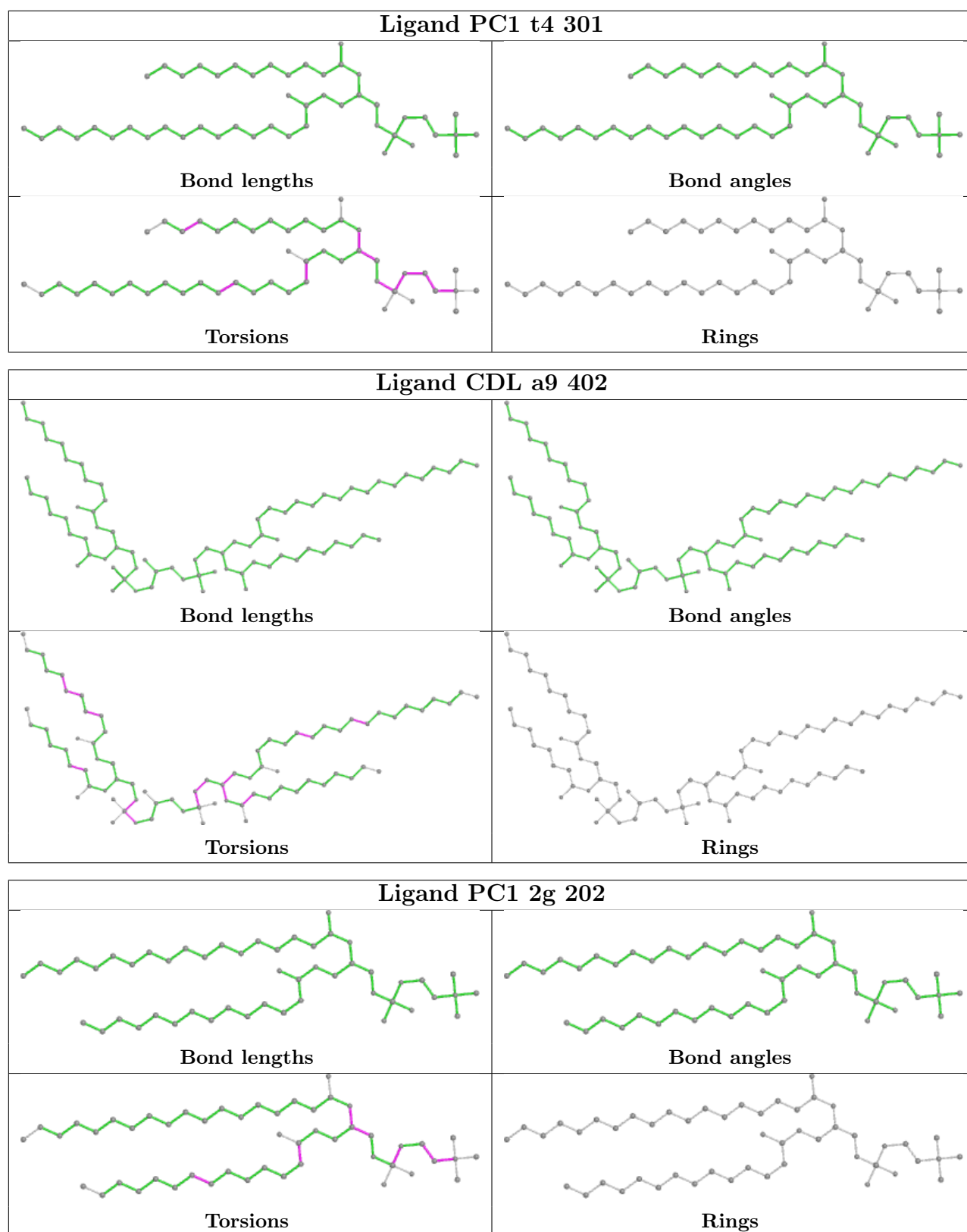


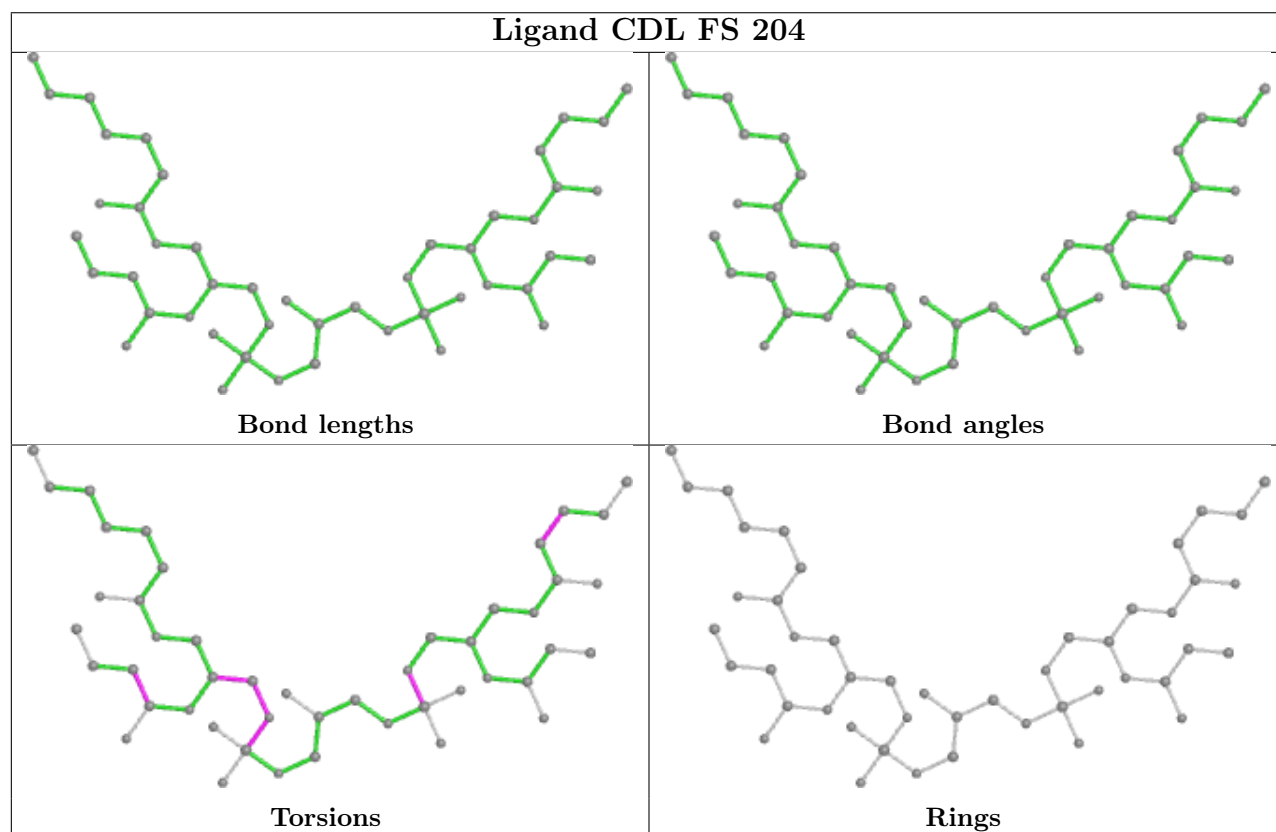
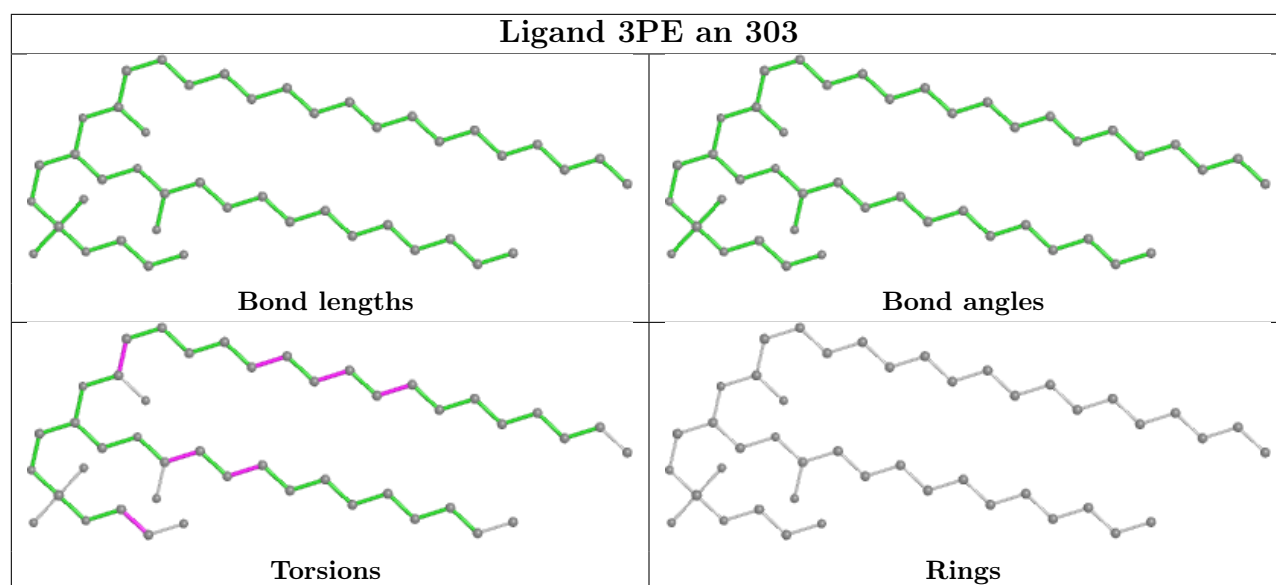


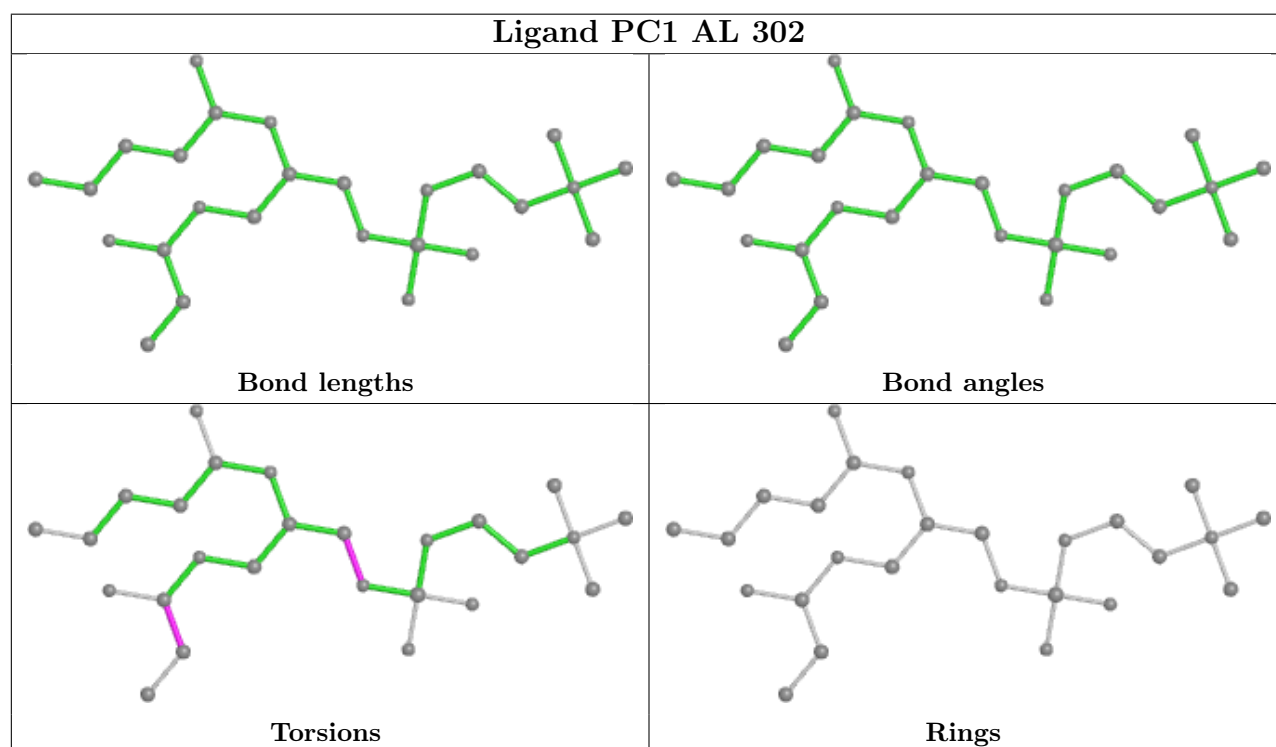
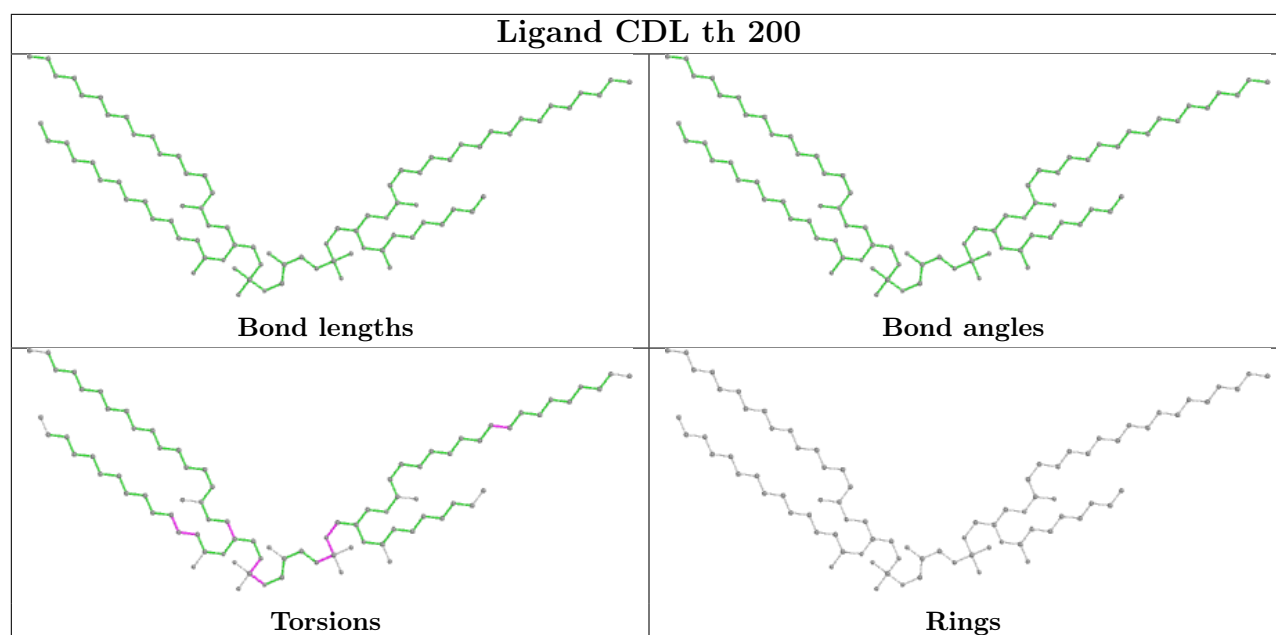


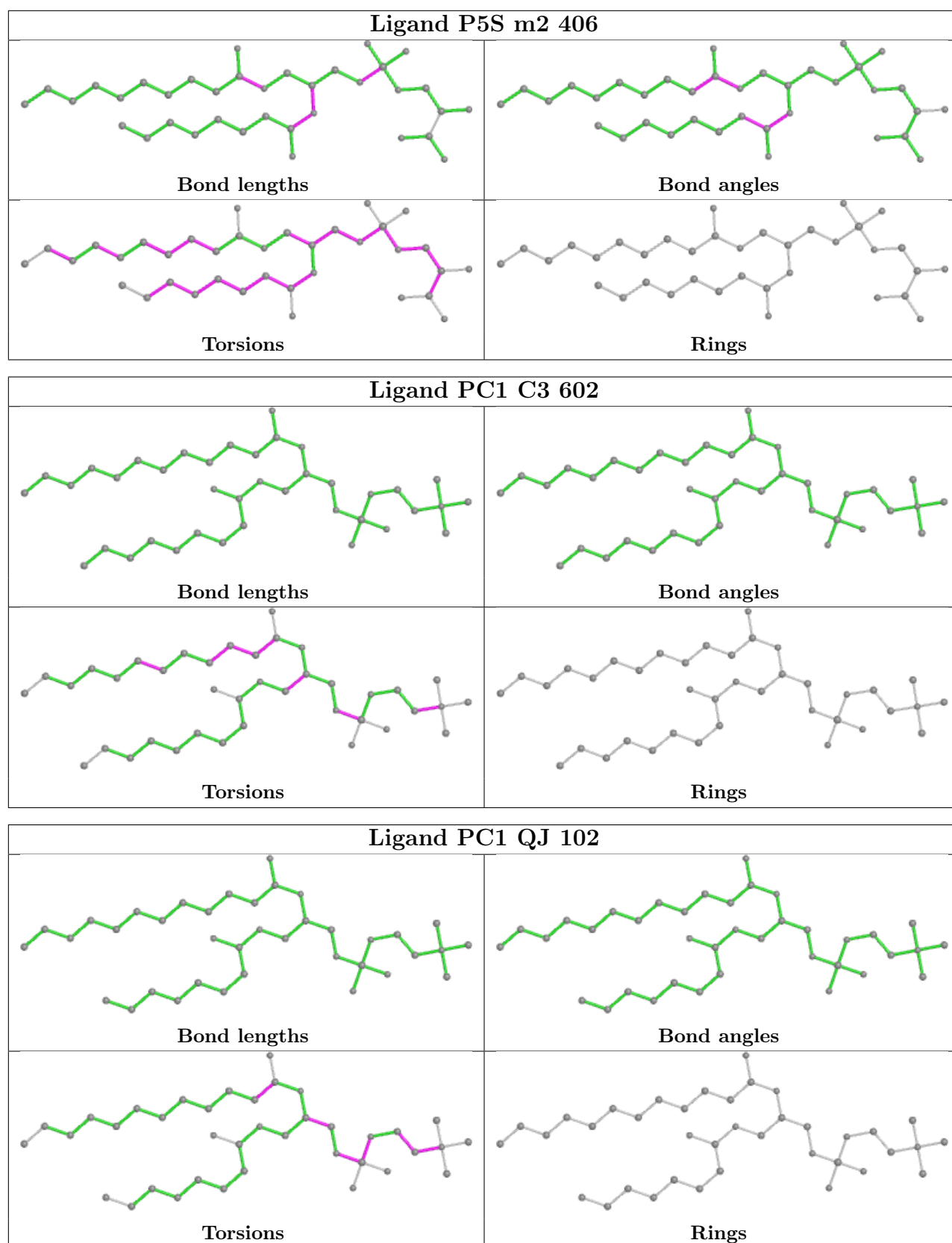


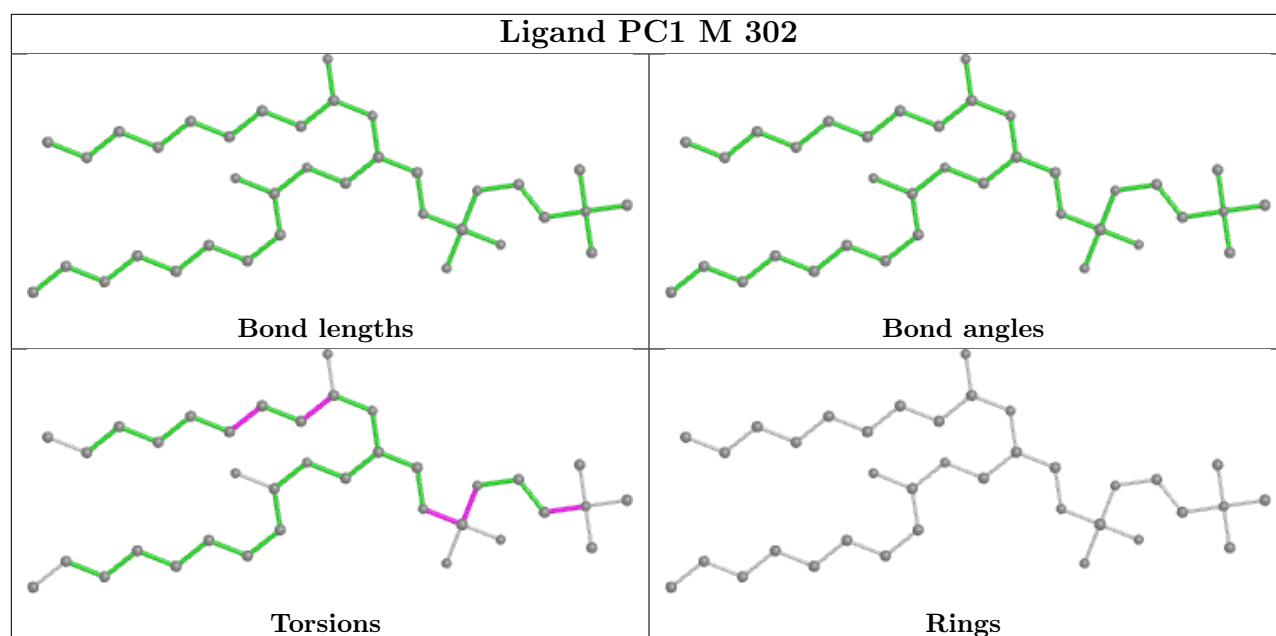
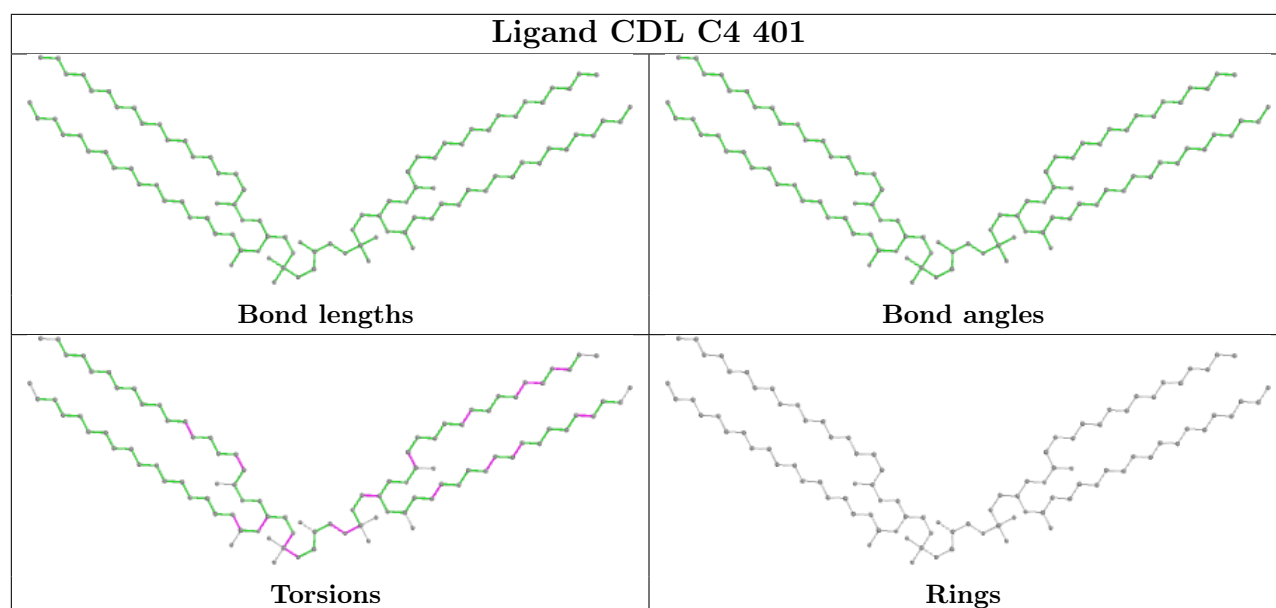


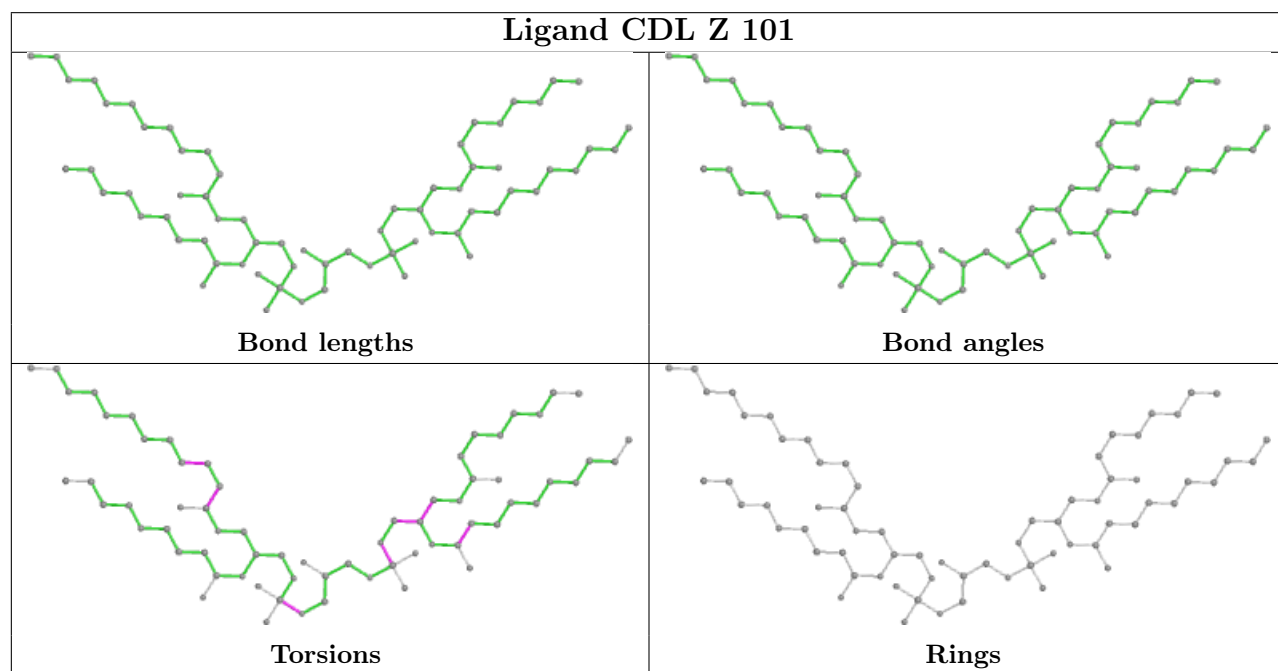
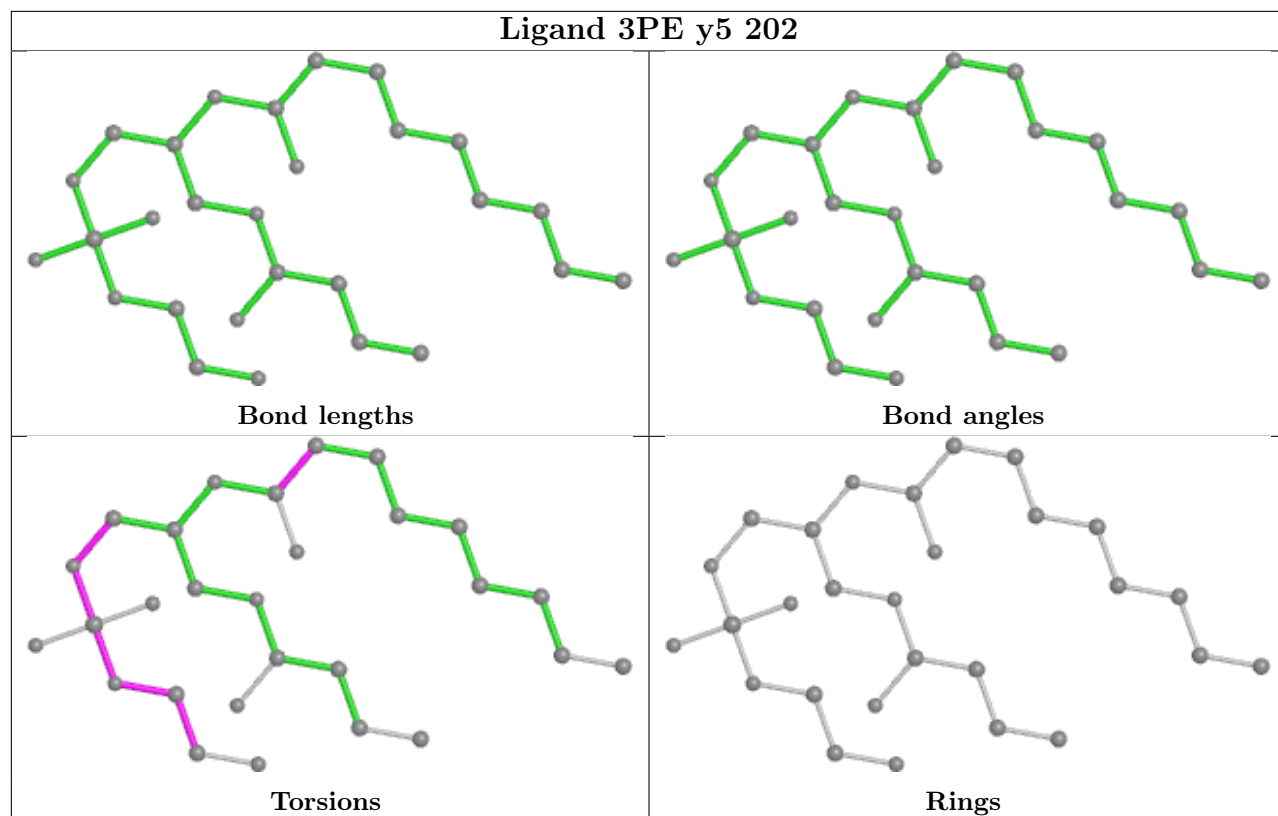


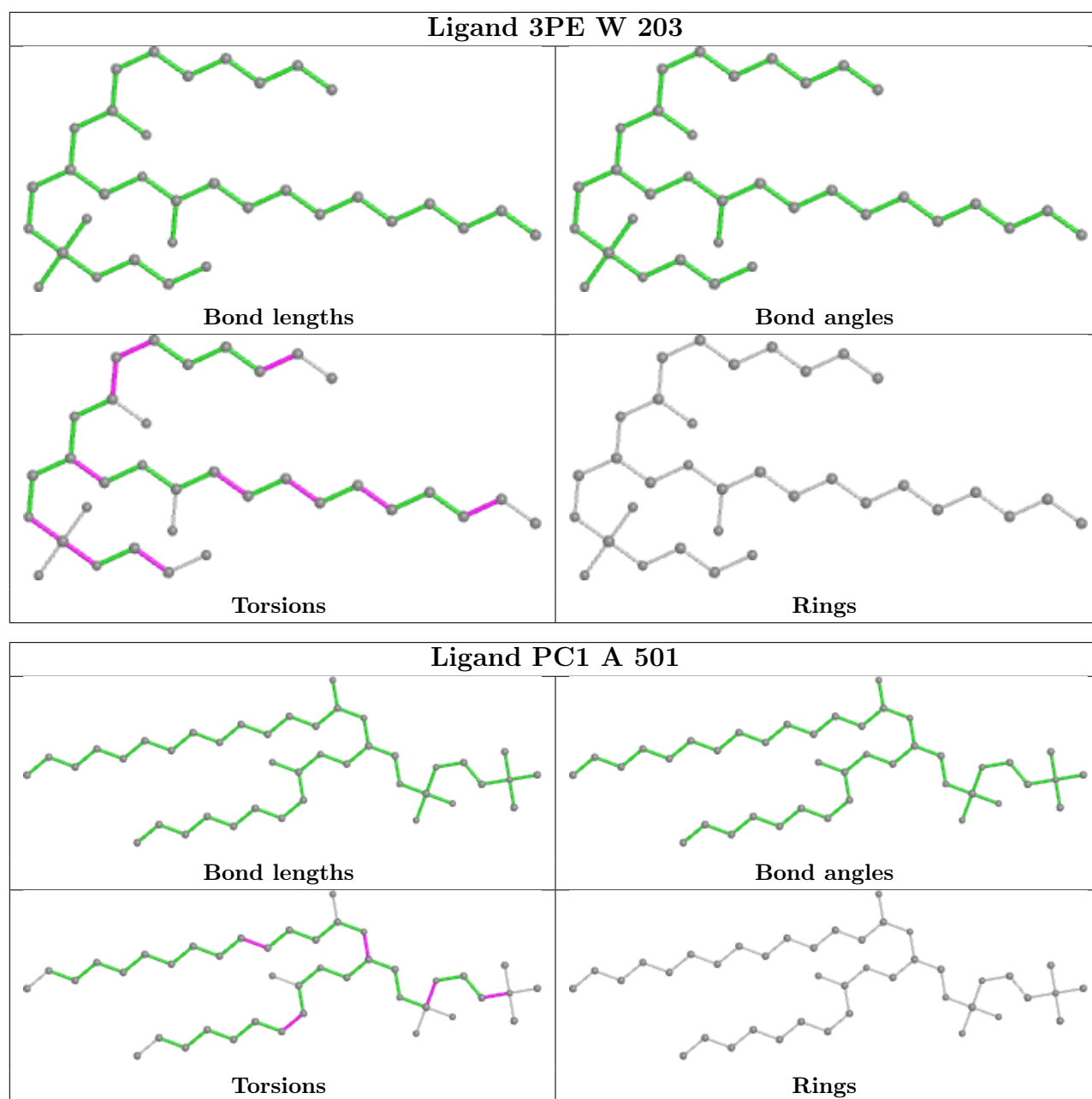


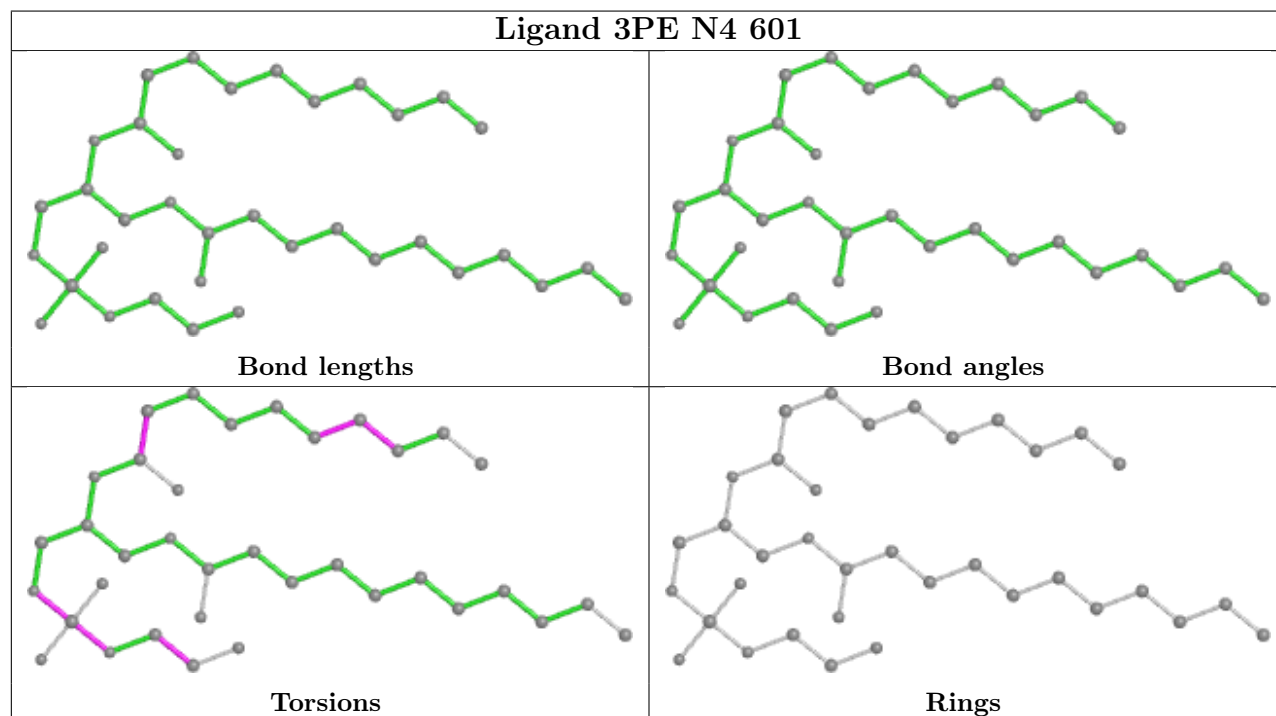
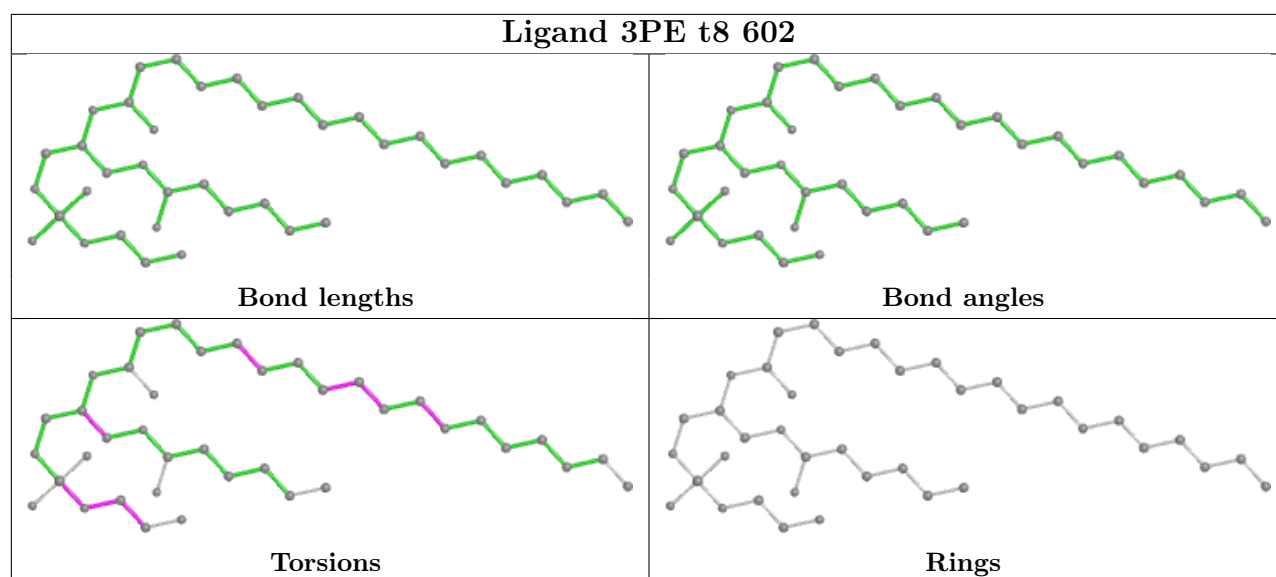


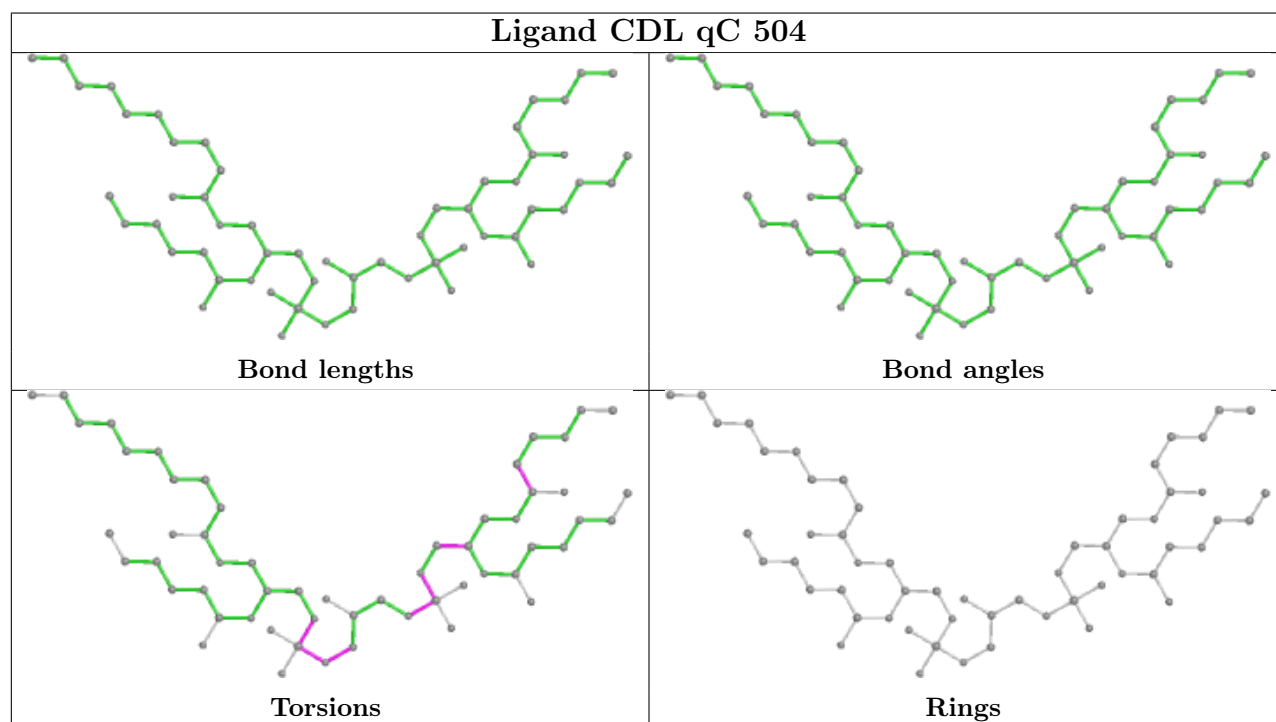
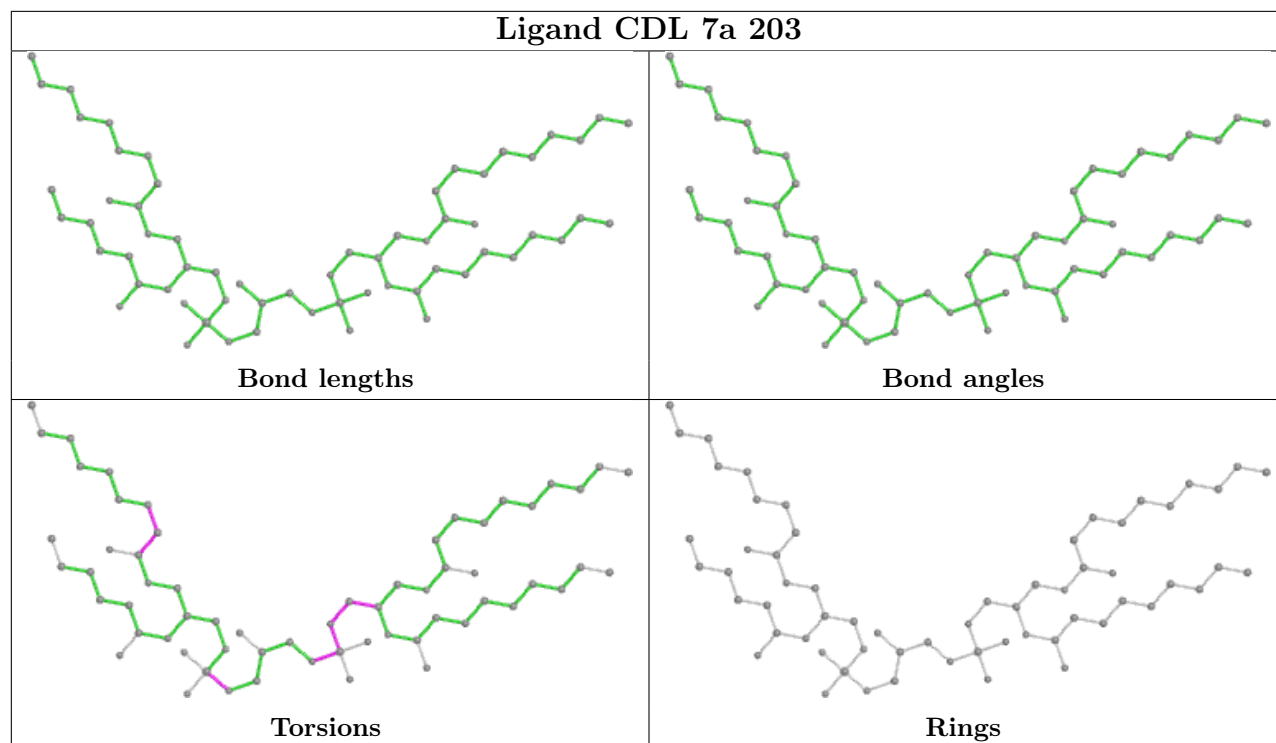


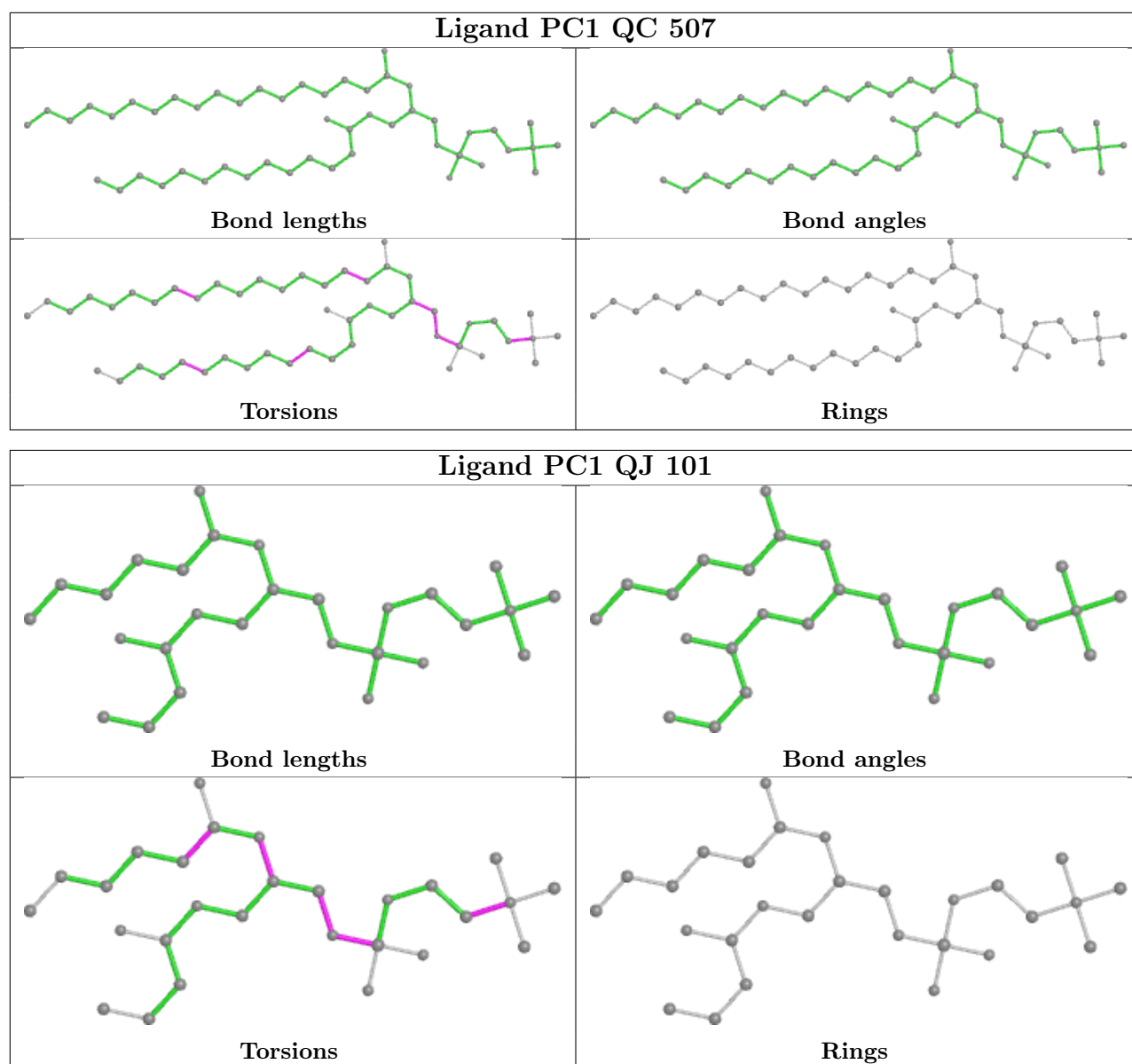




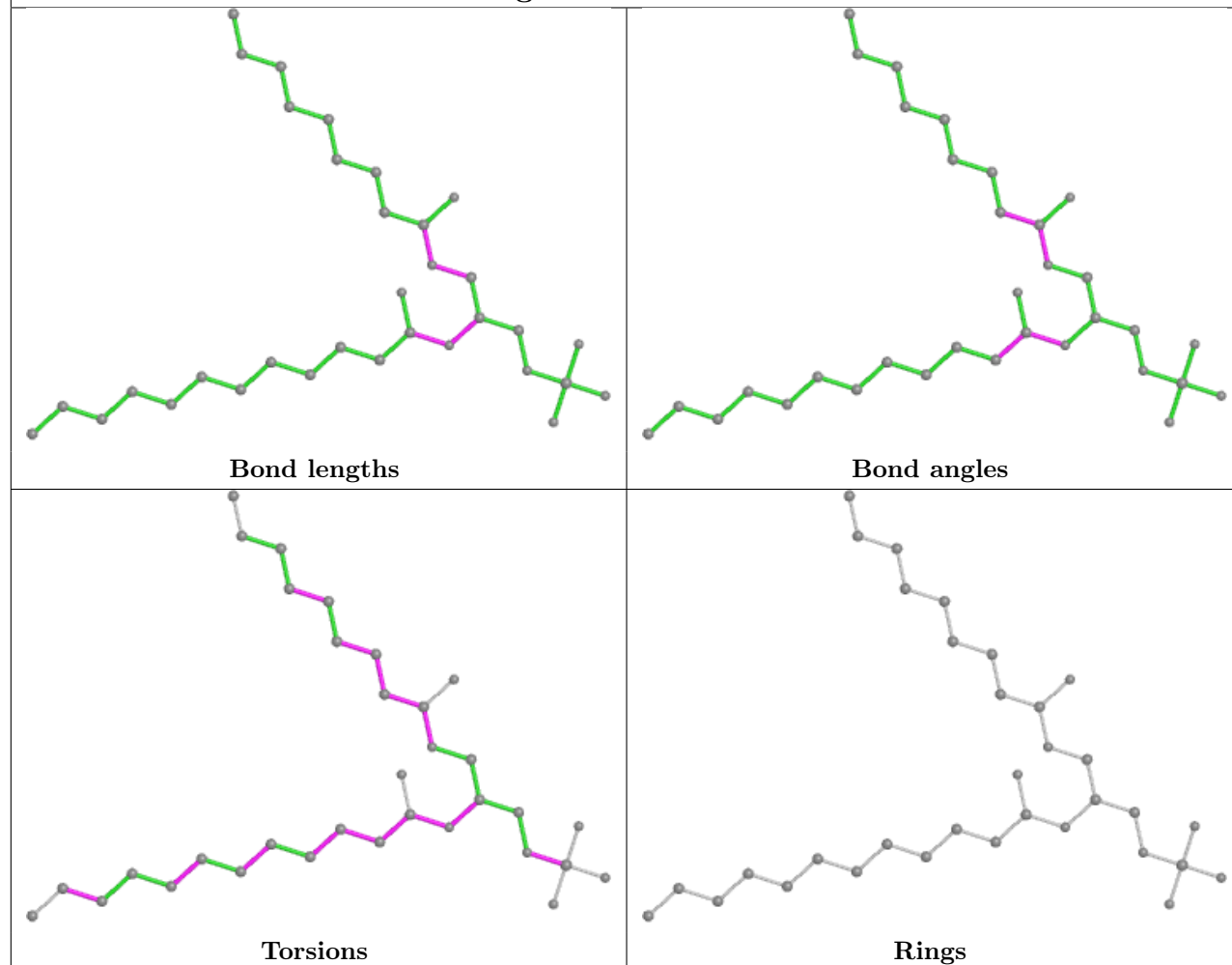




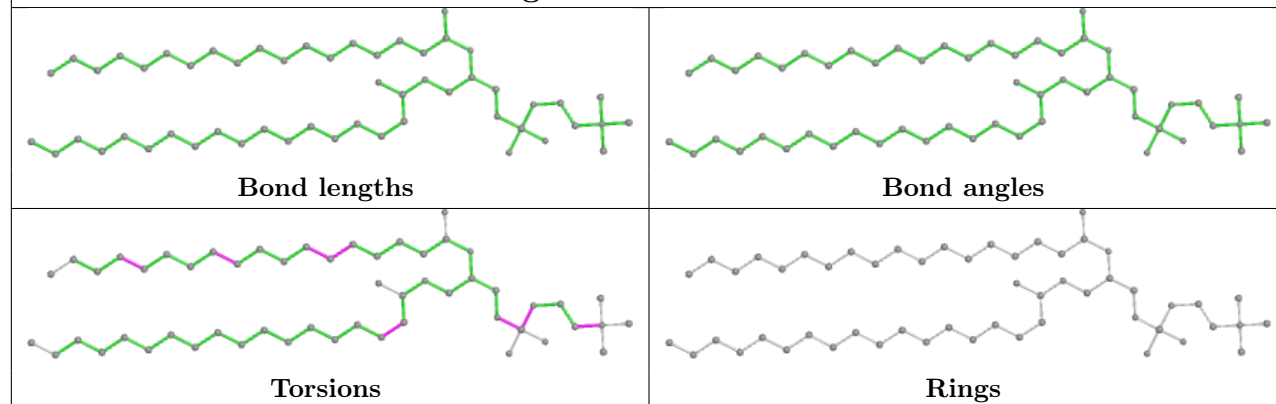




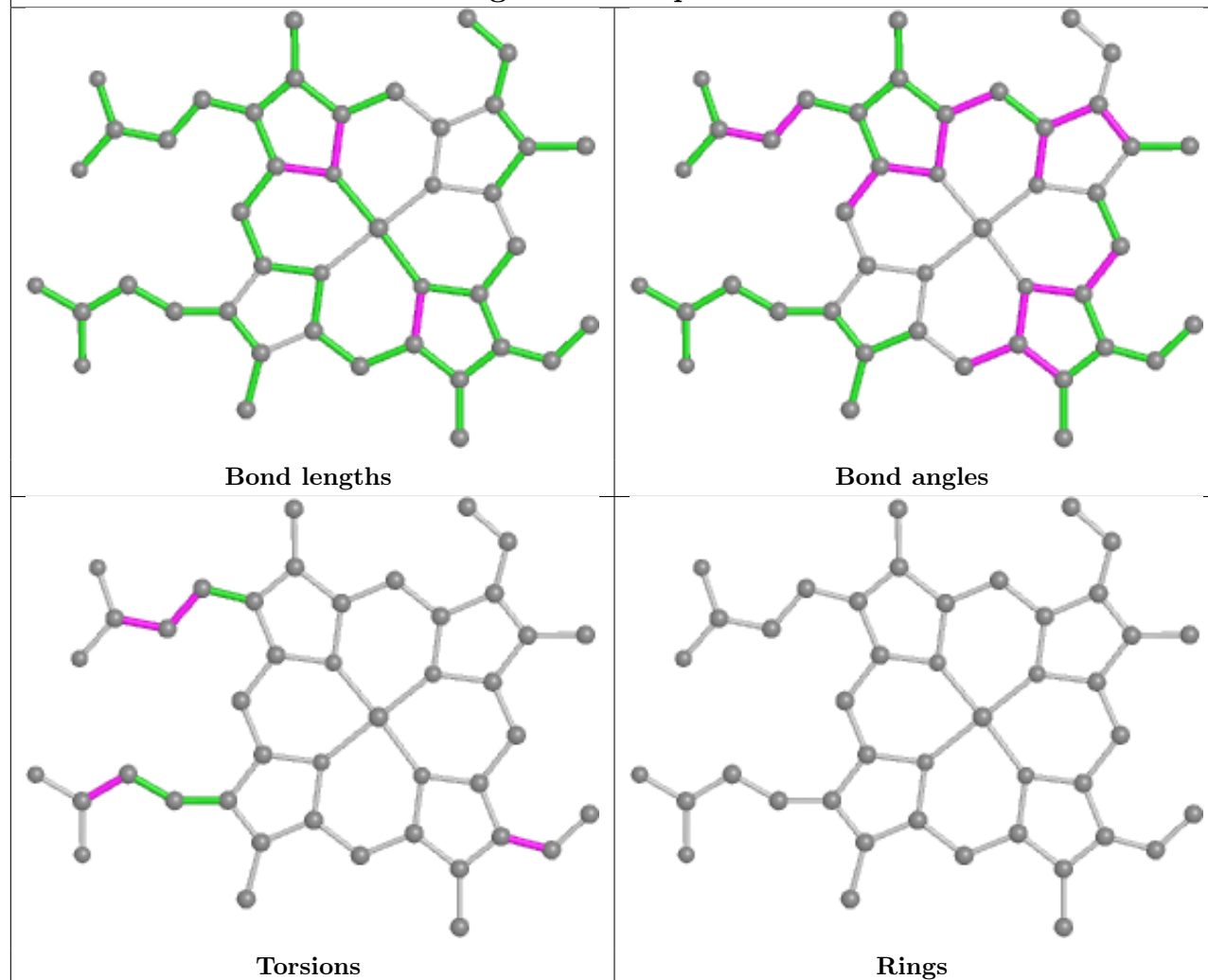
Ligand PX2 R 202



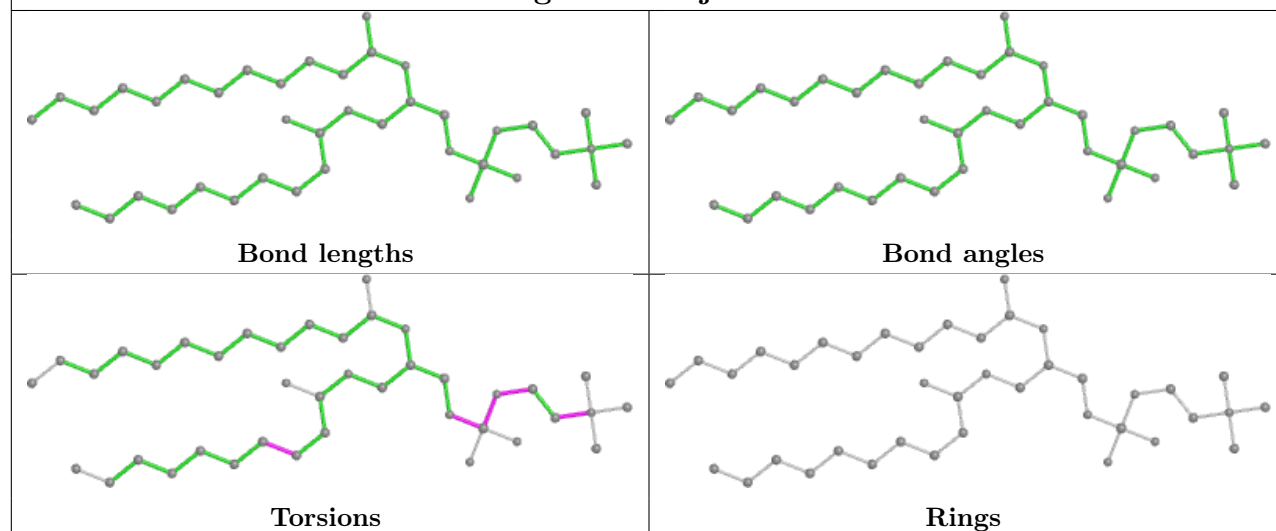
Ligand PC1 M1 401

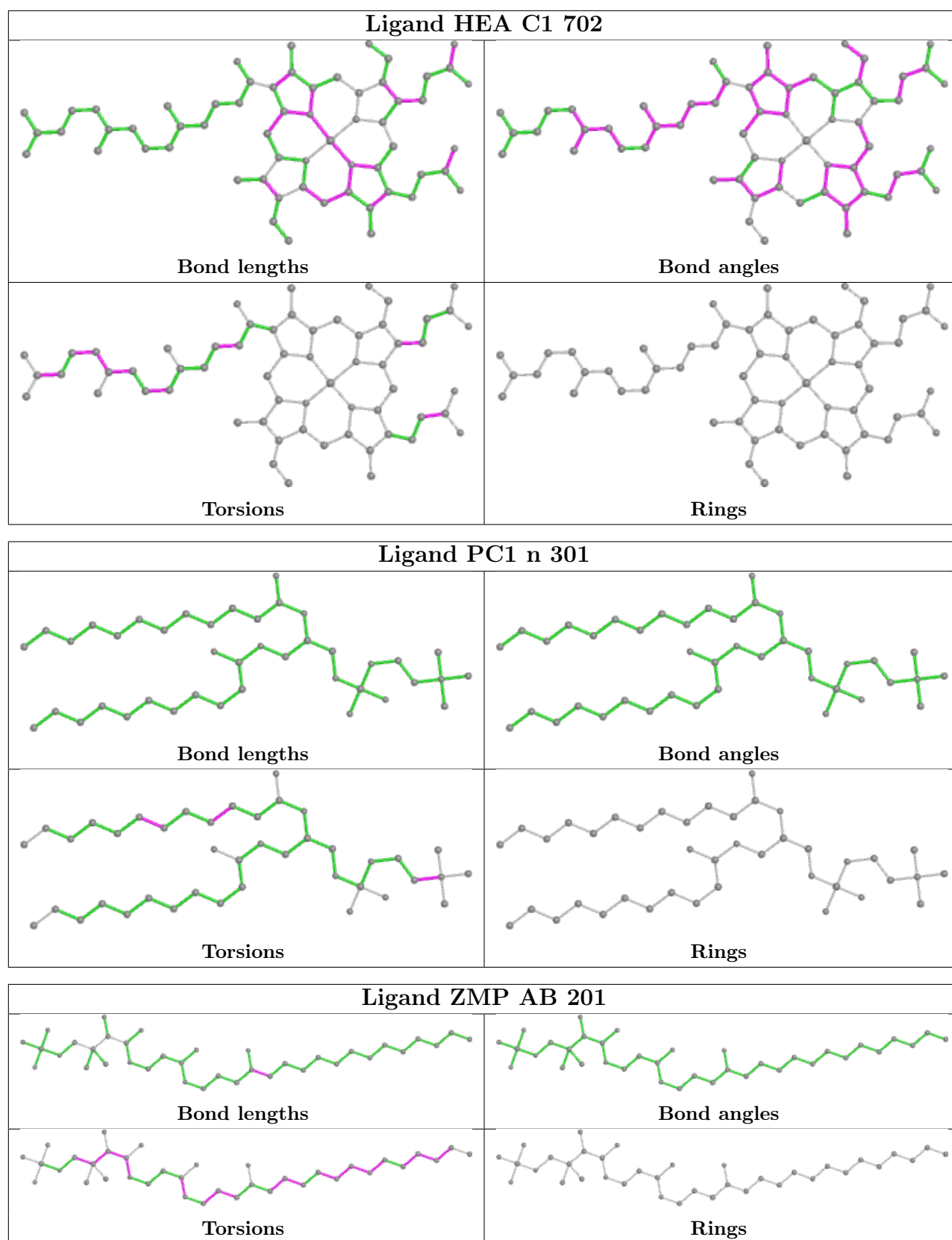


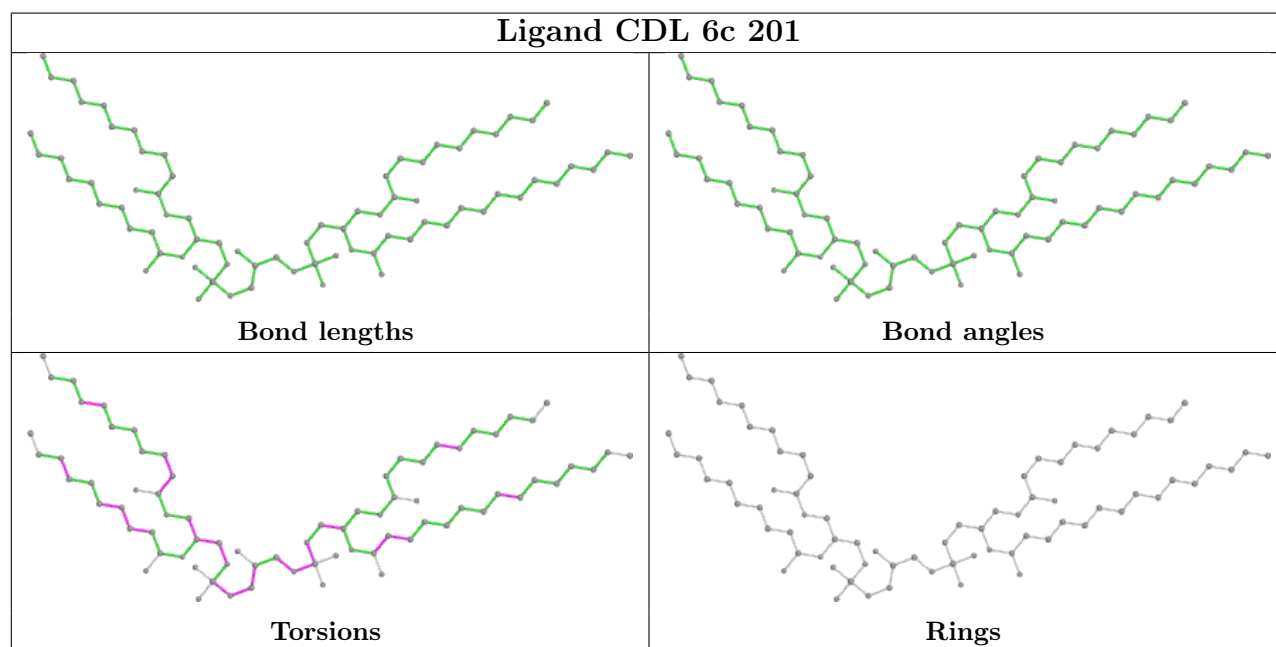
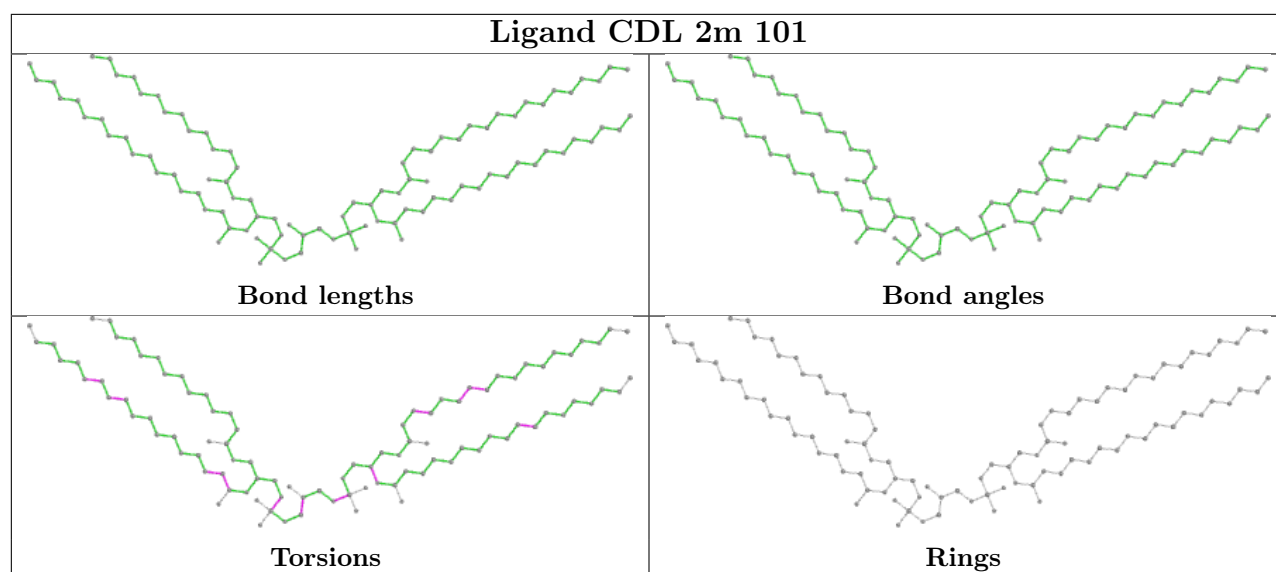
Ligand HEM qC 502

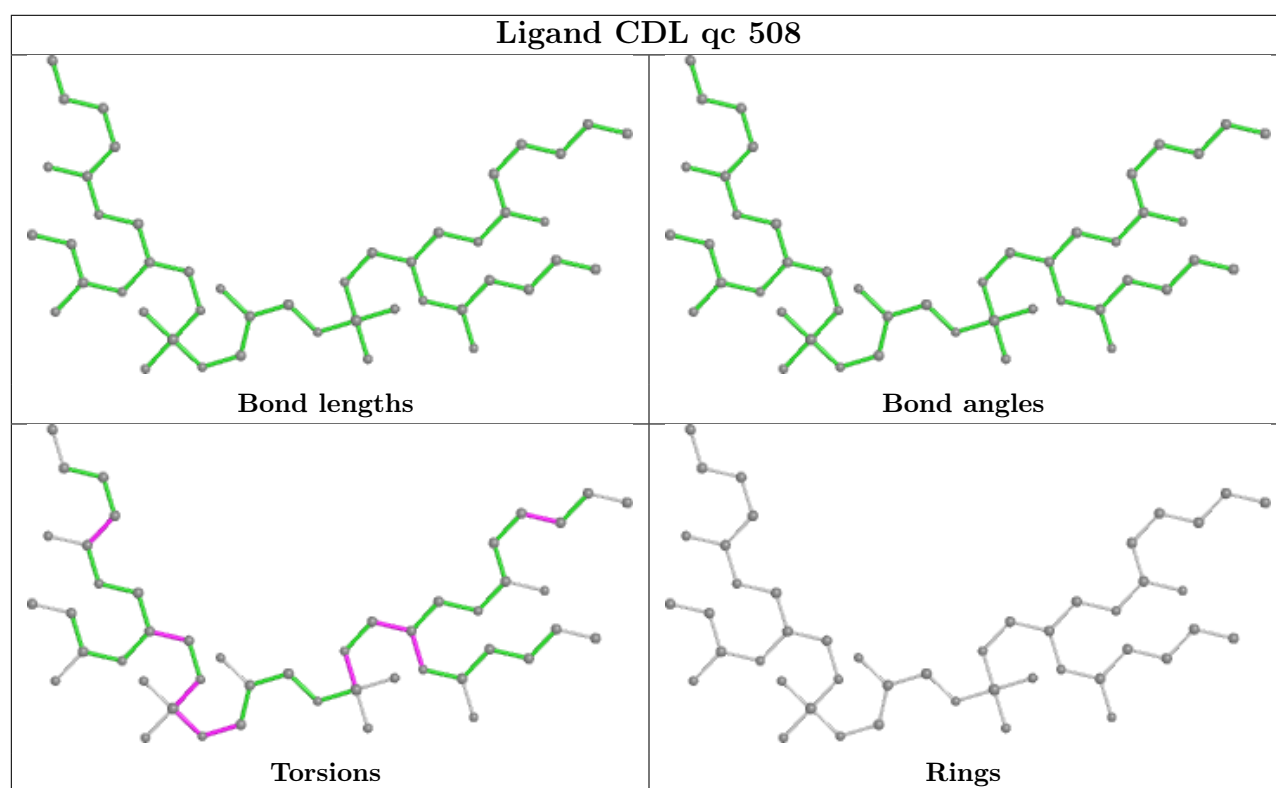
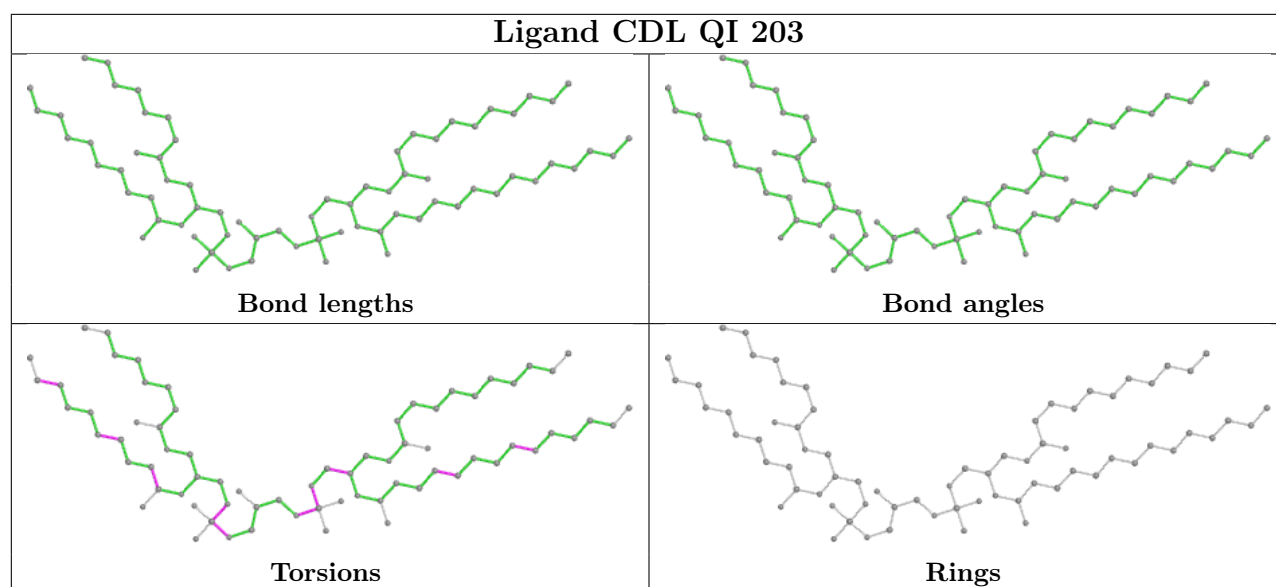


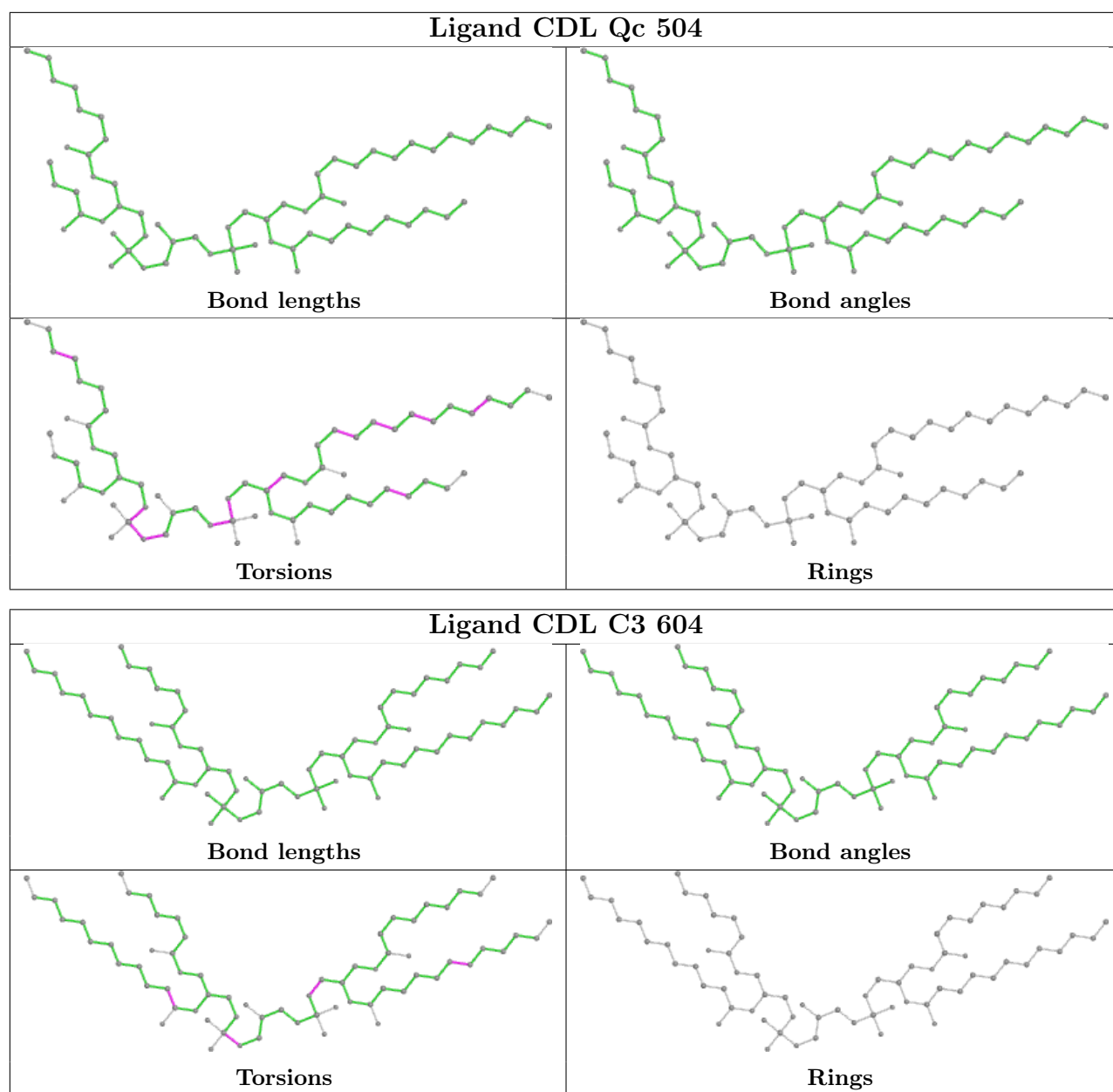
Ligand PC1 j1 400

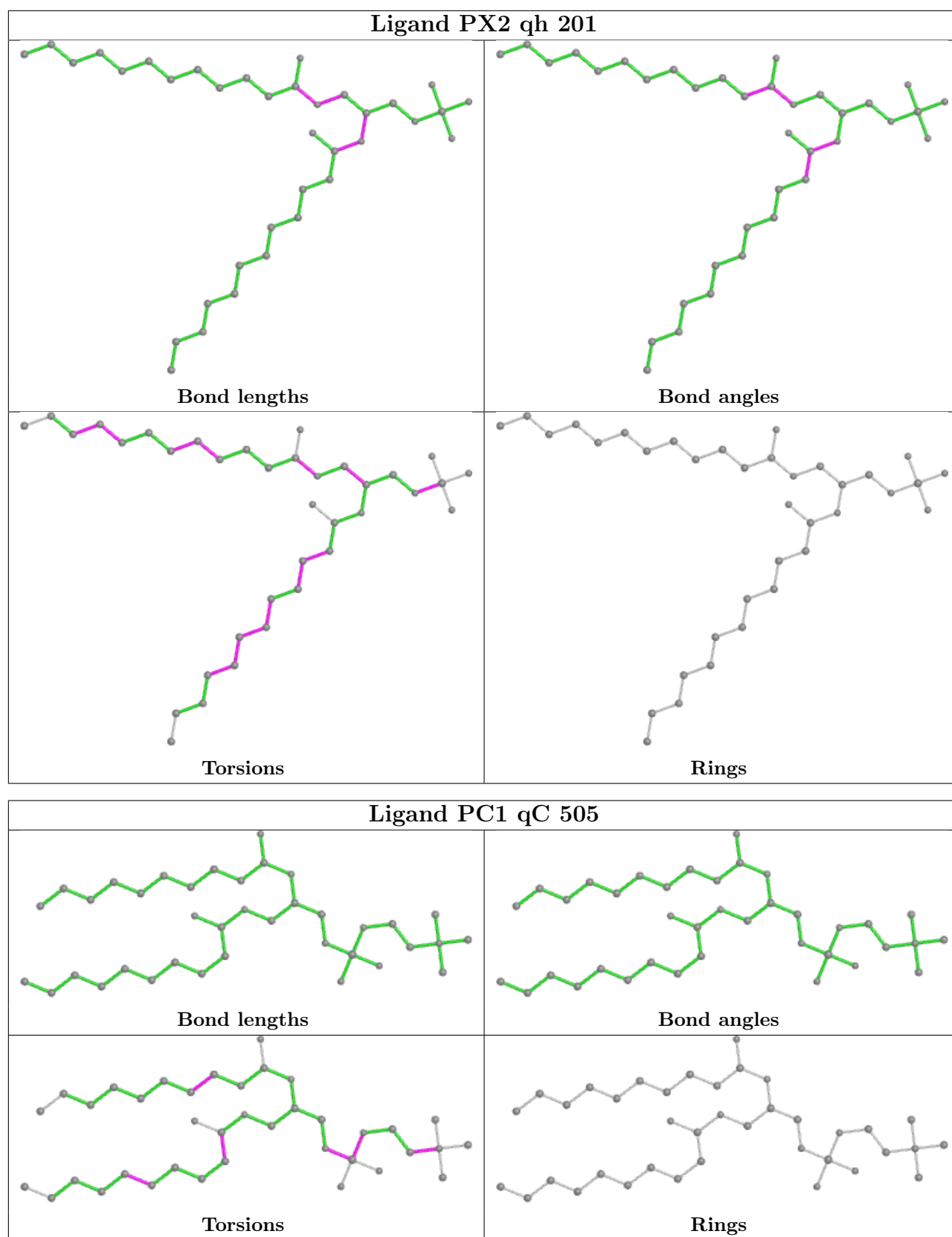


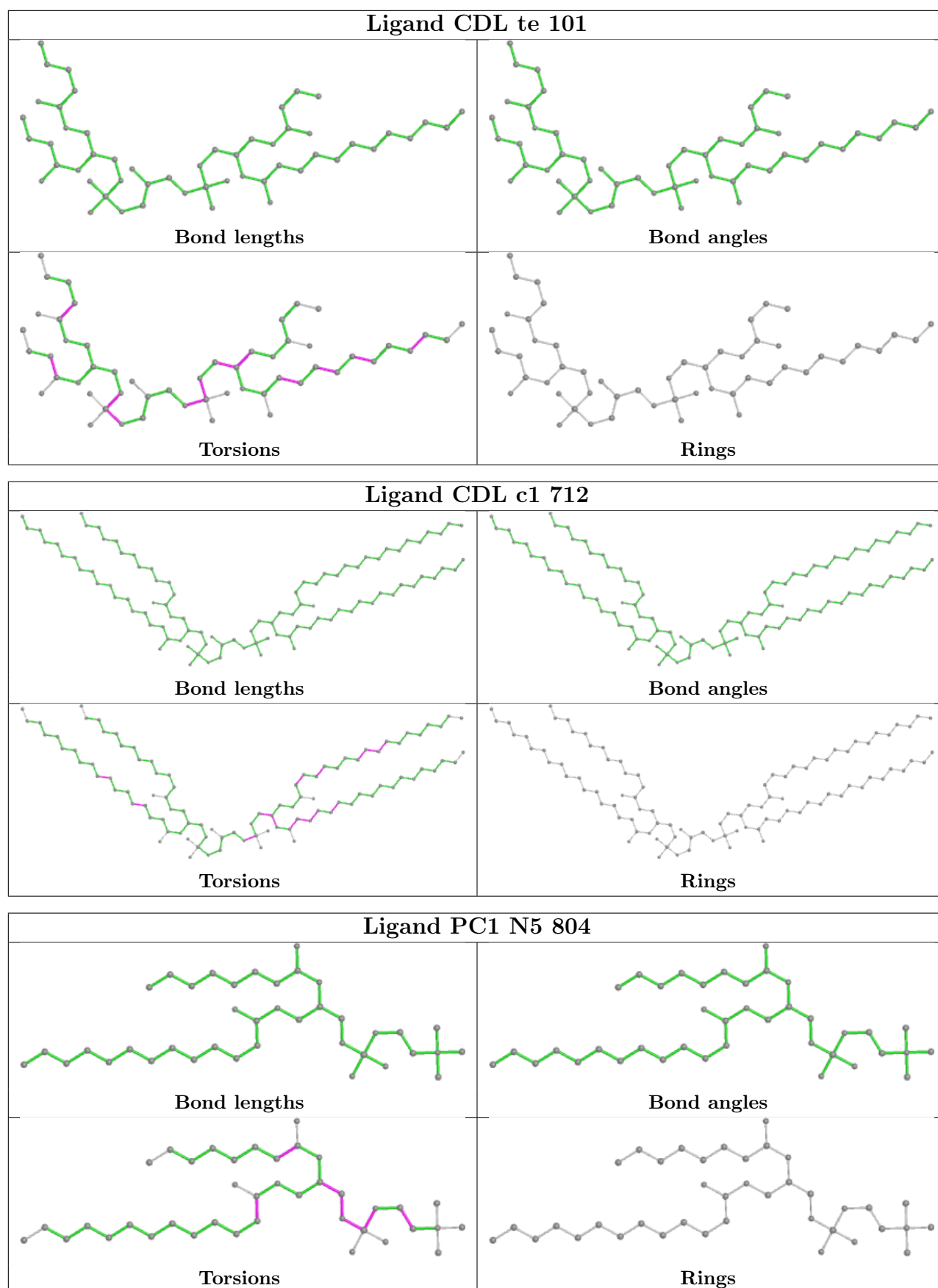


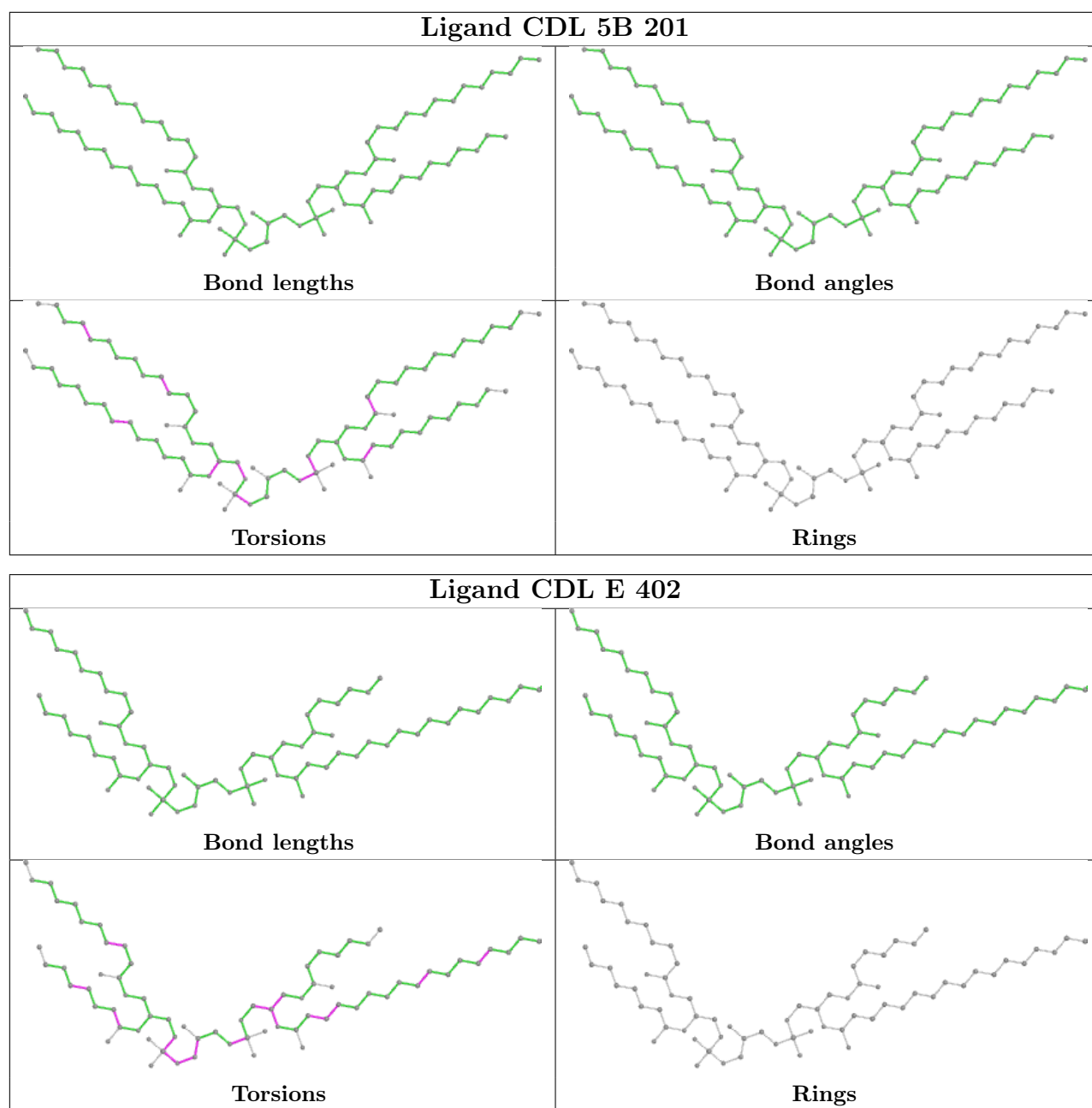


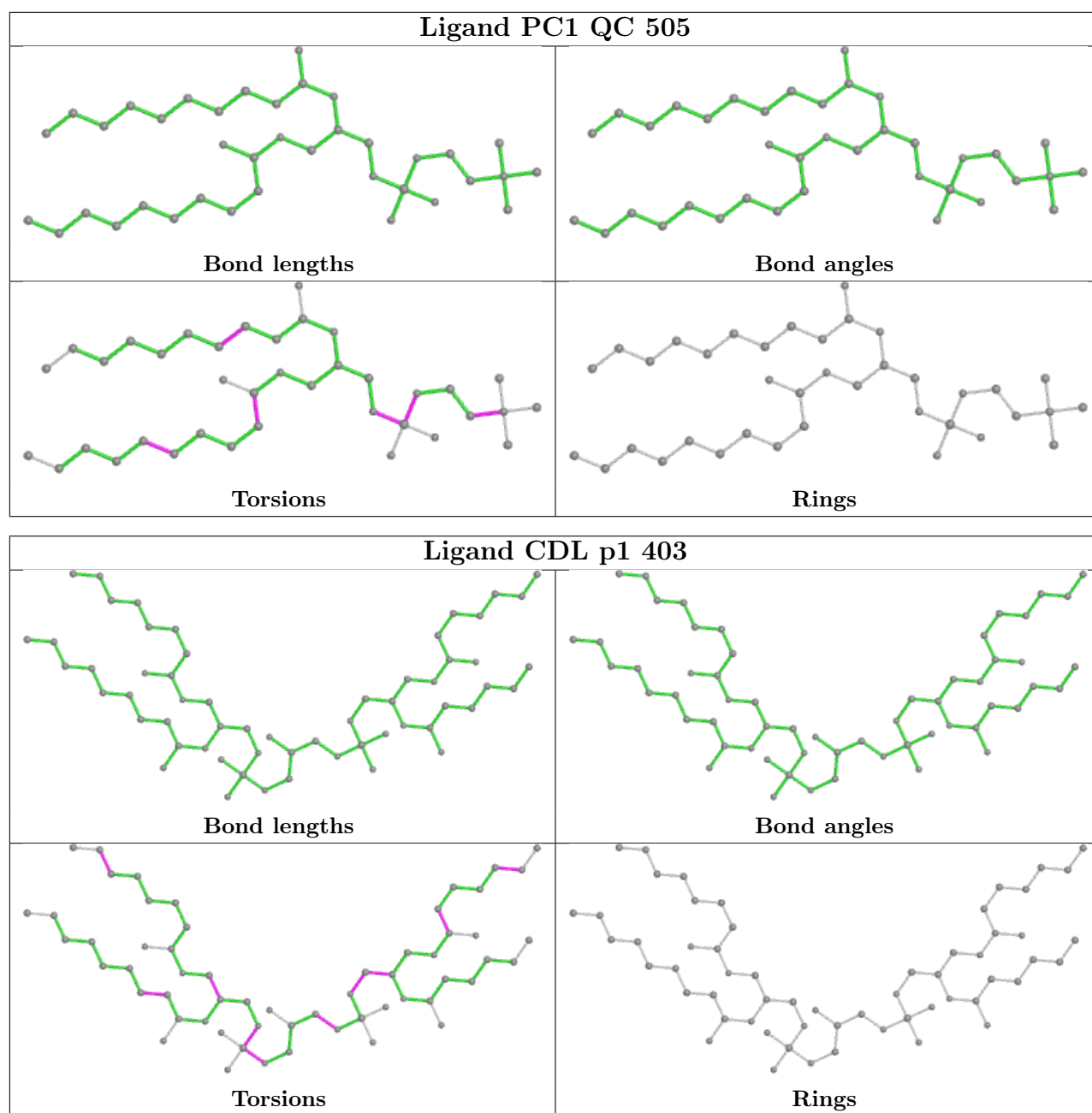


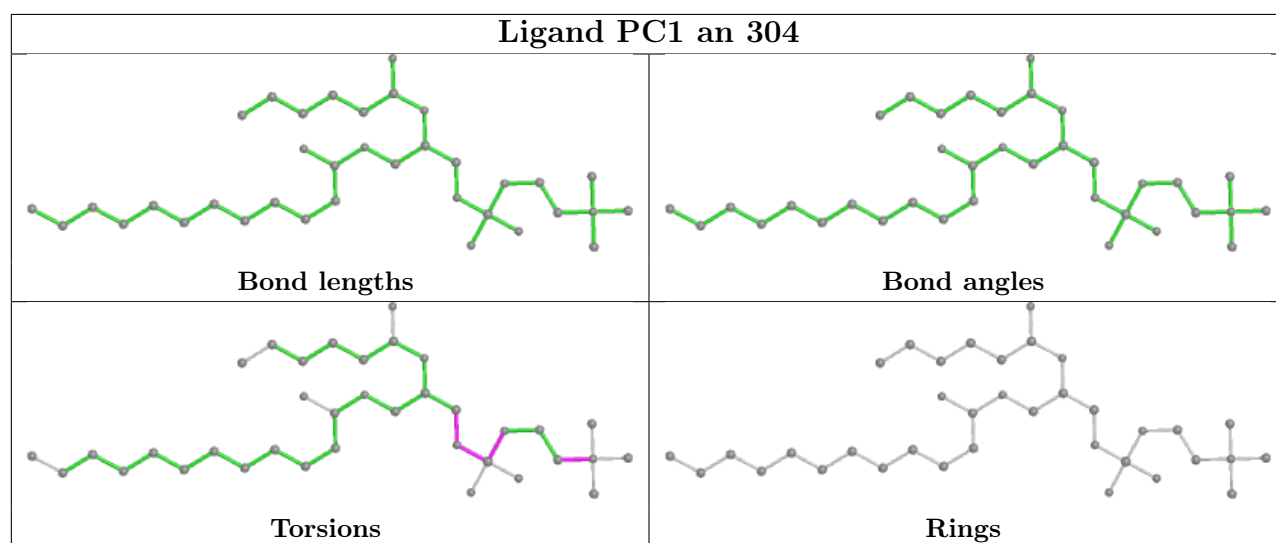
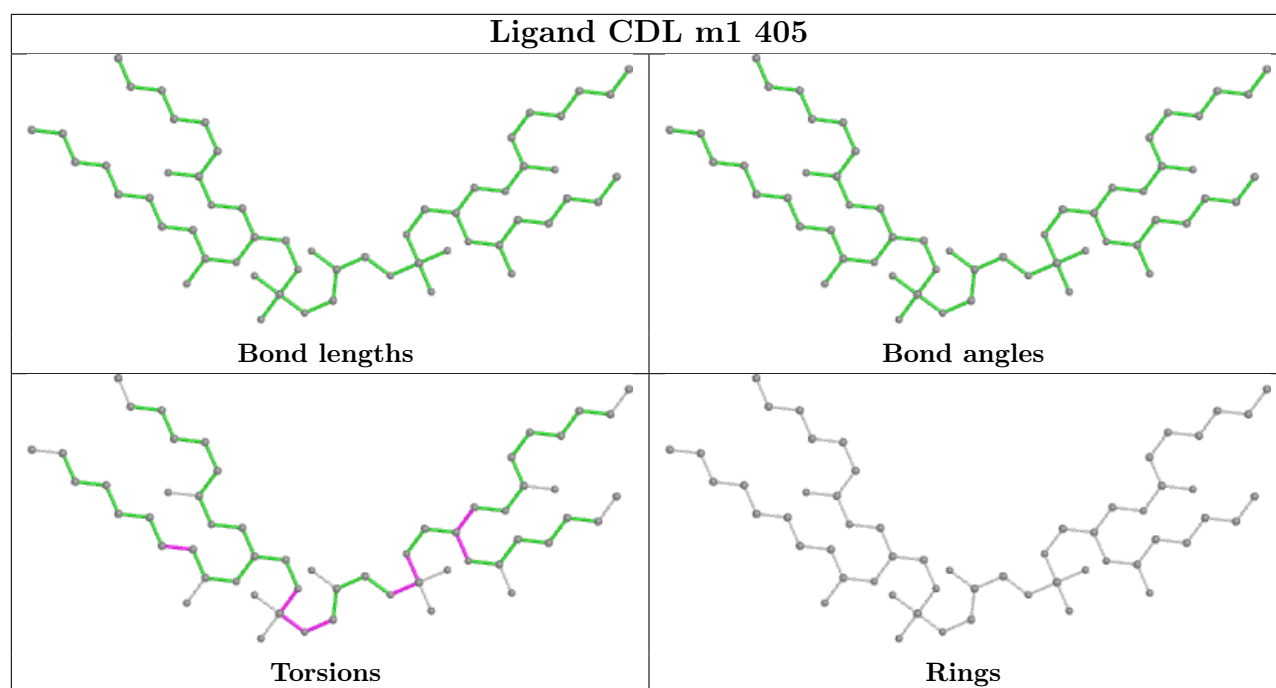


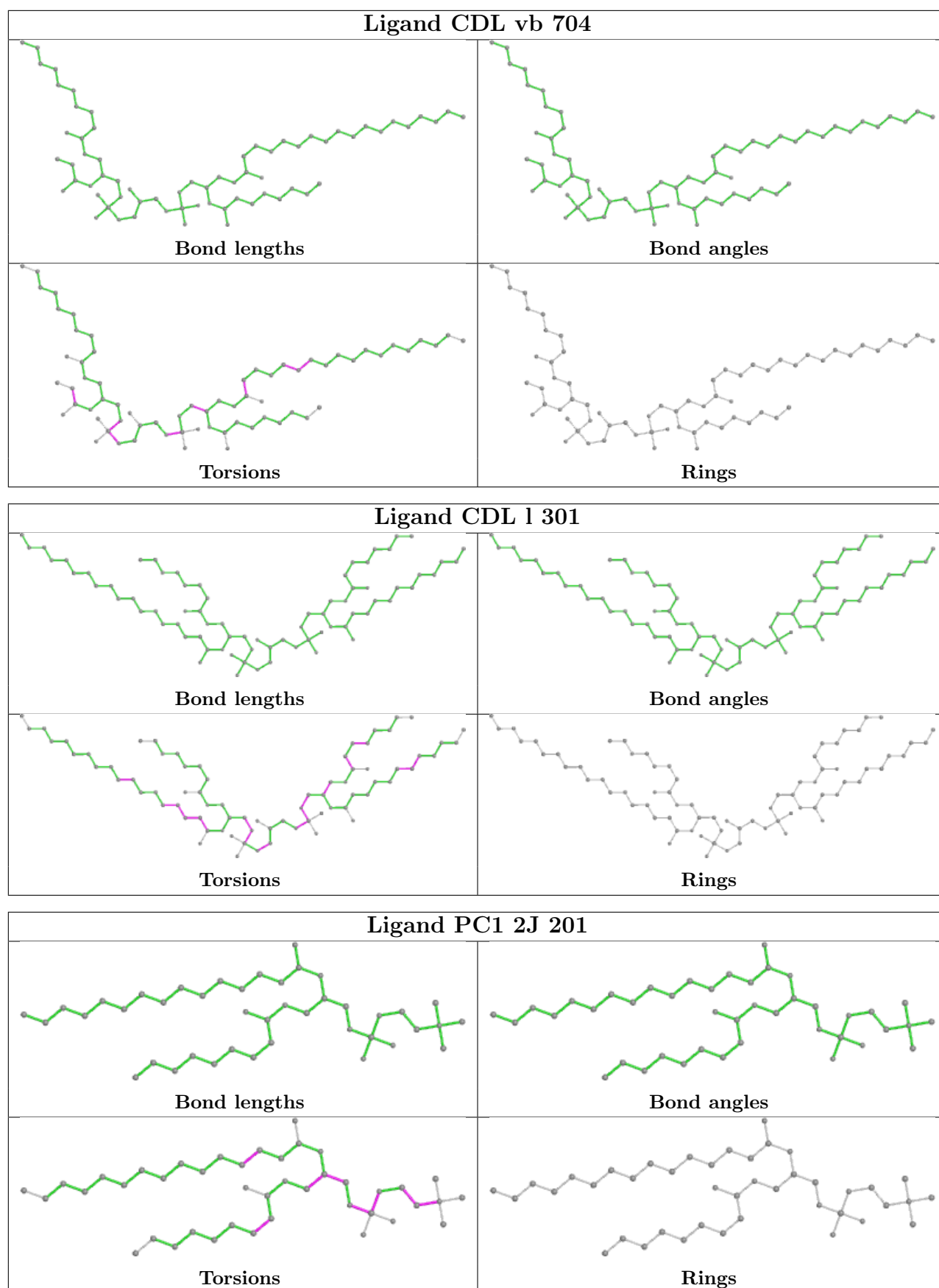


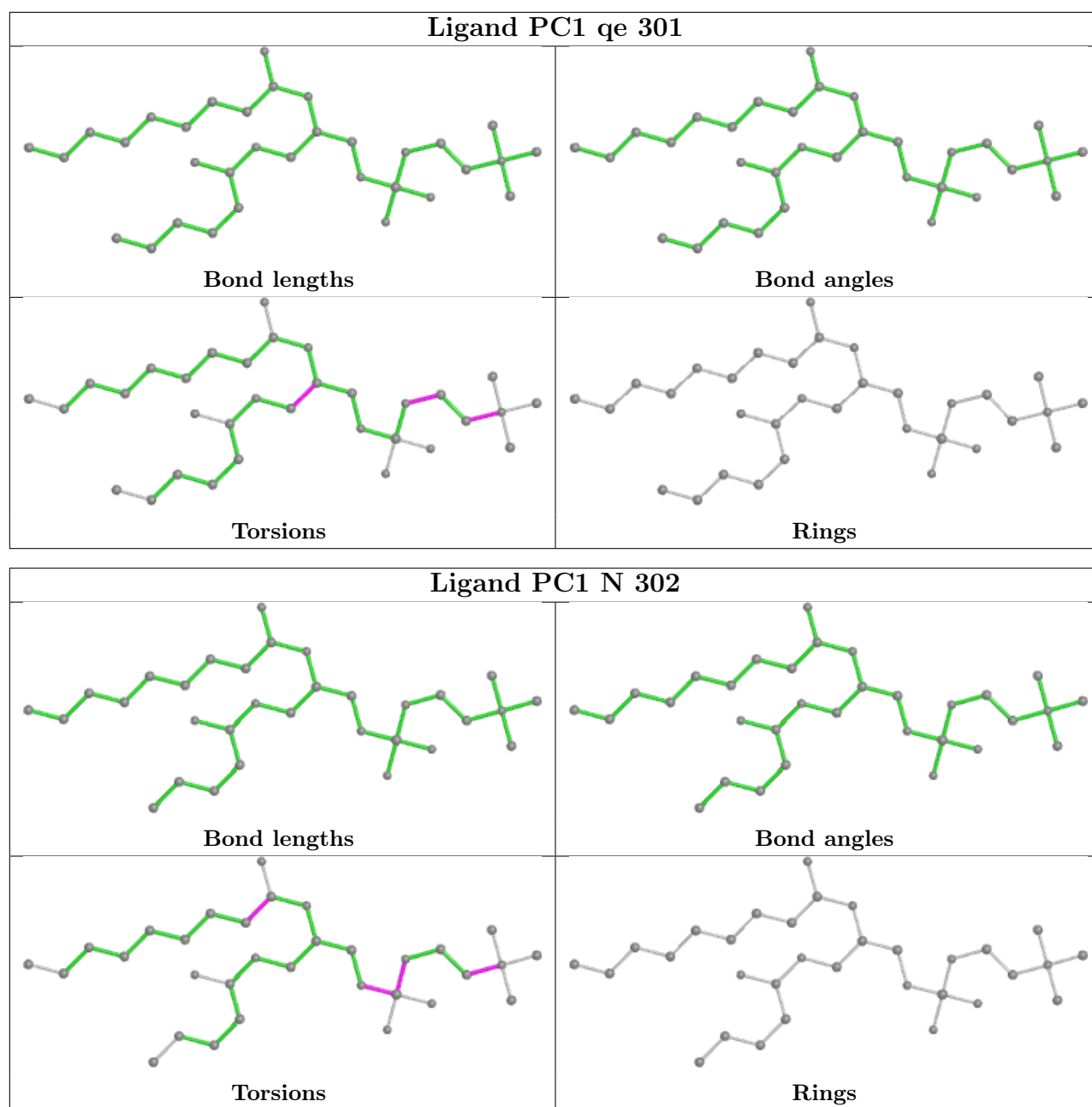


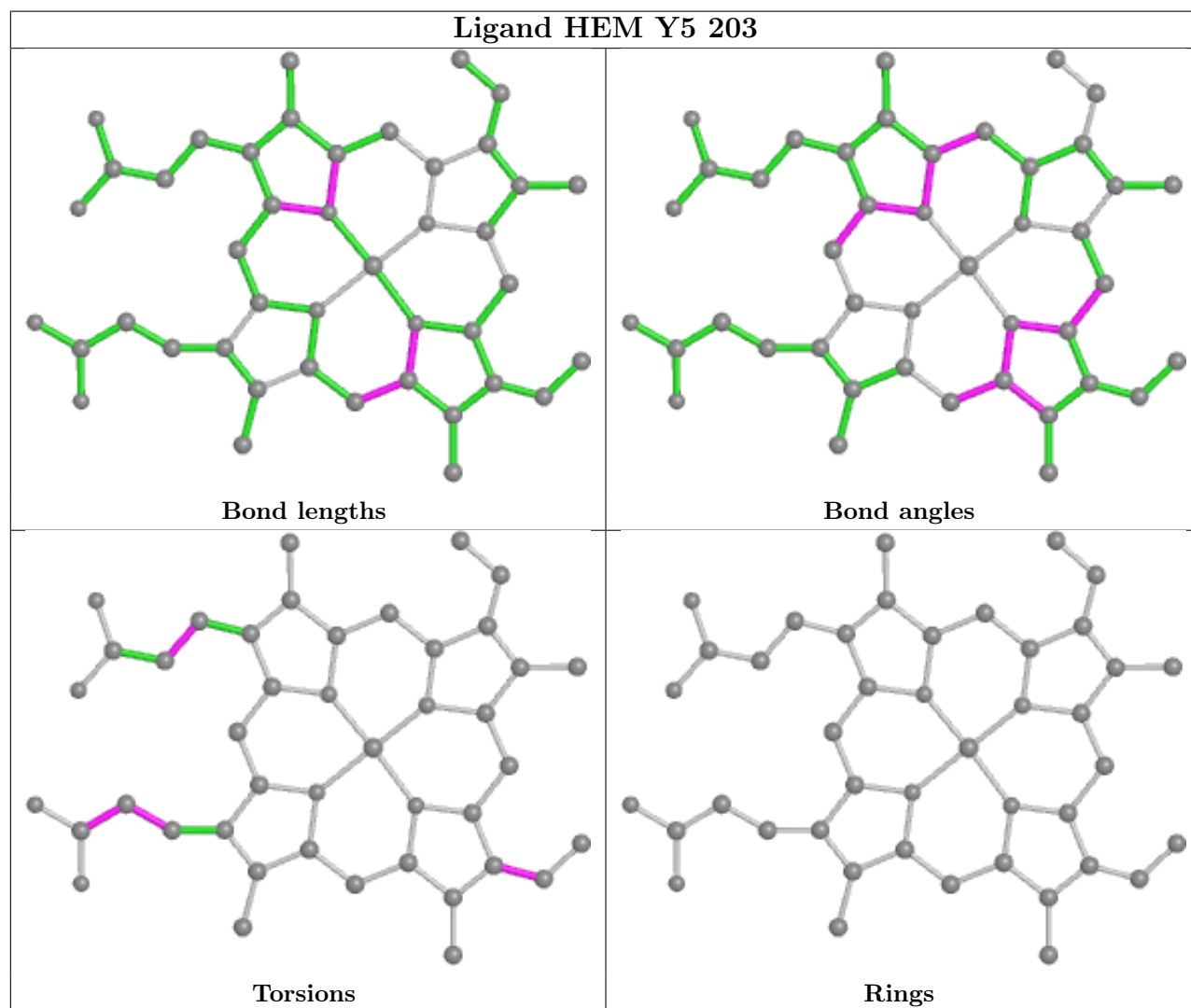
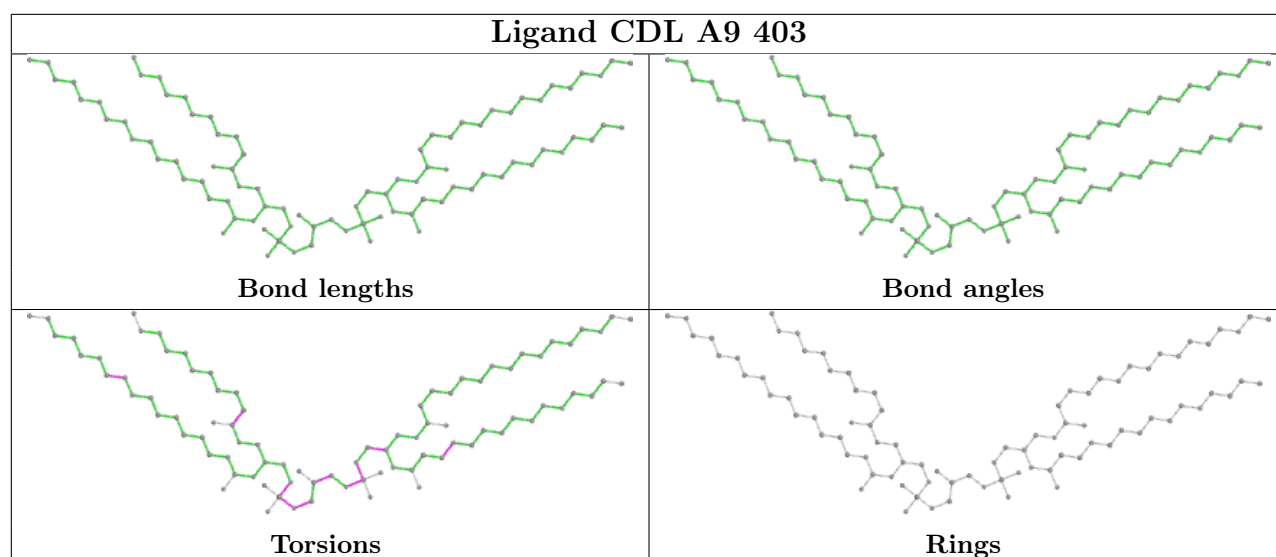


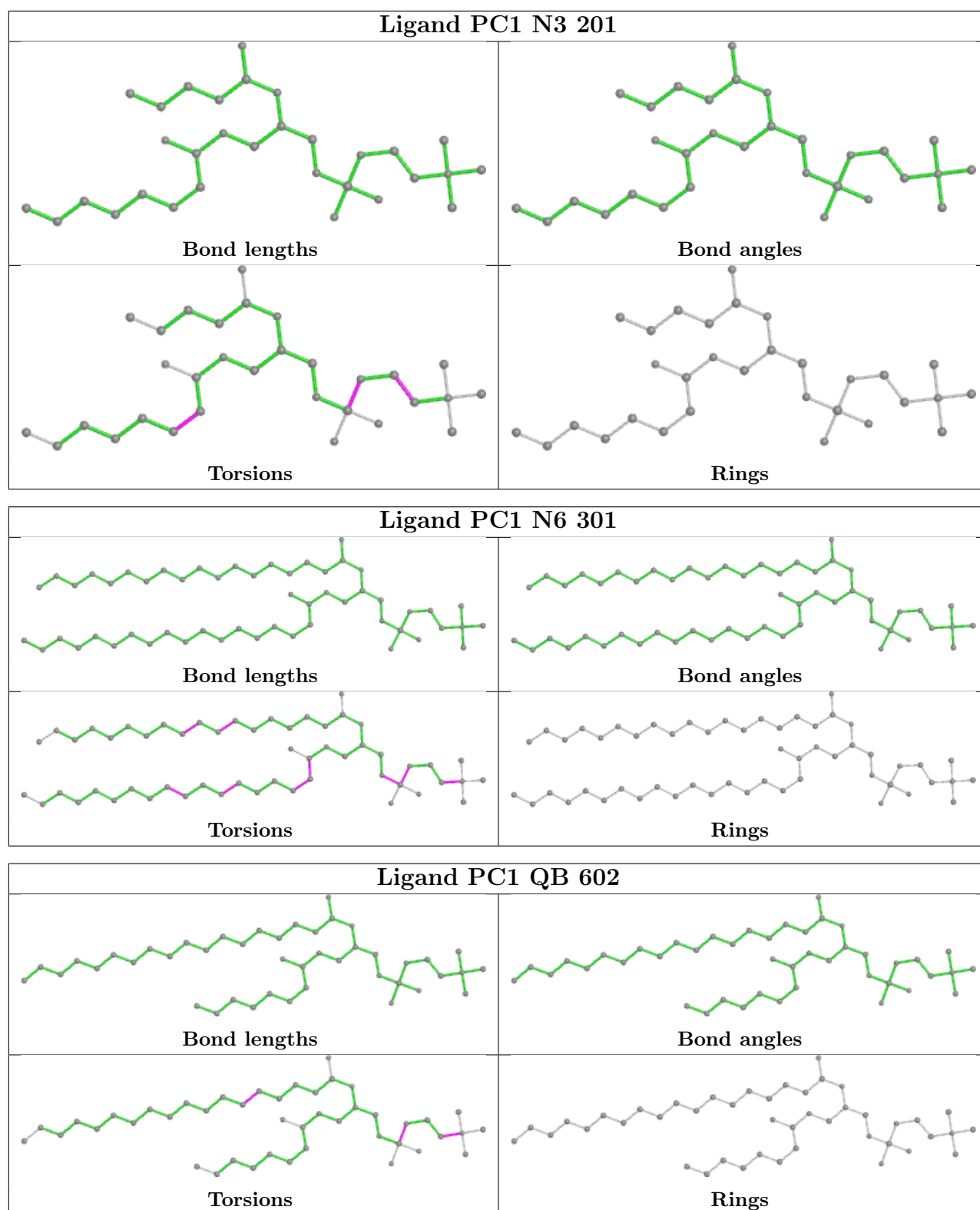


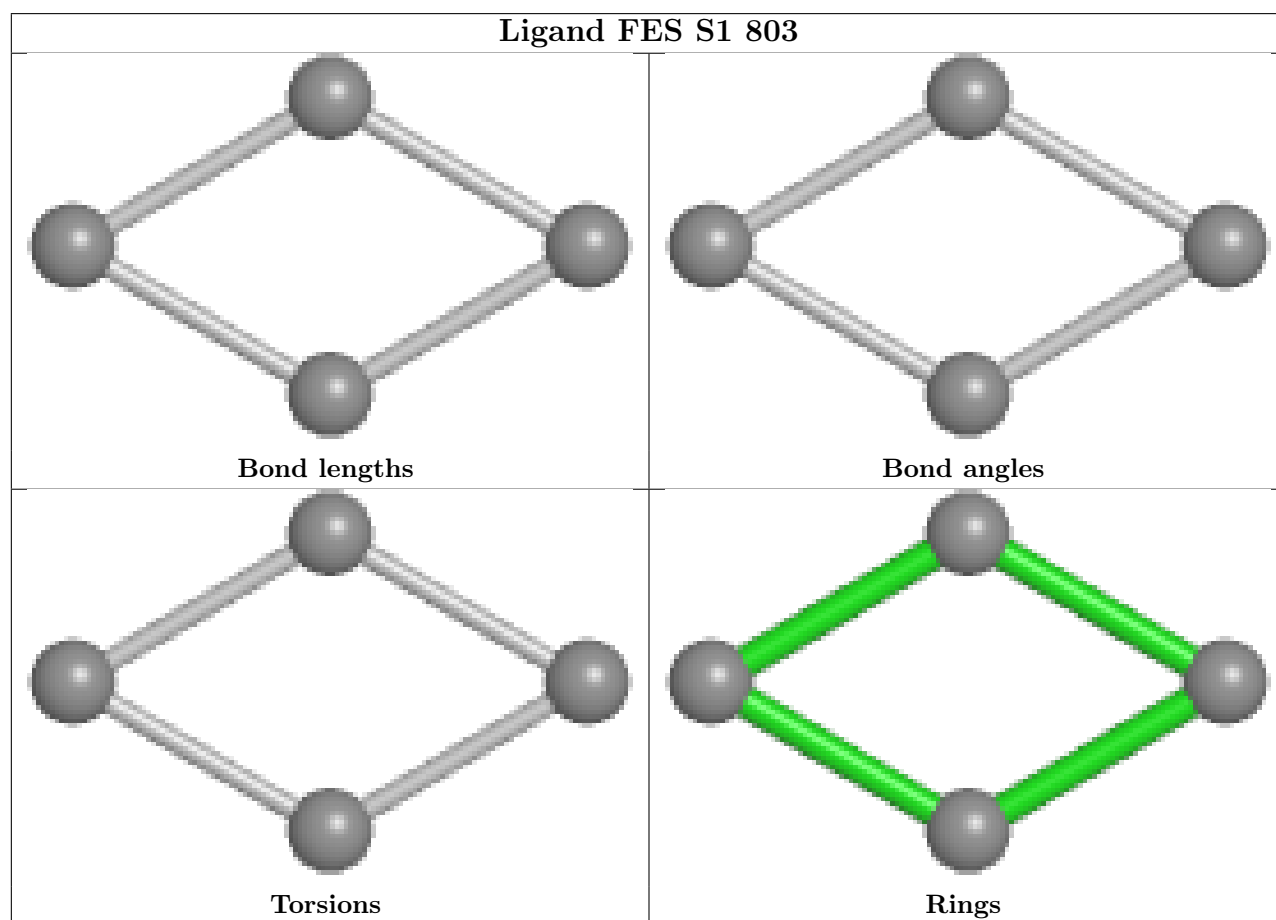
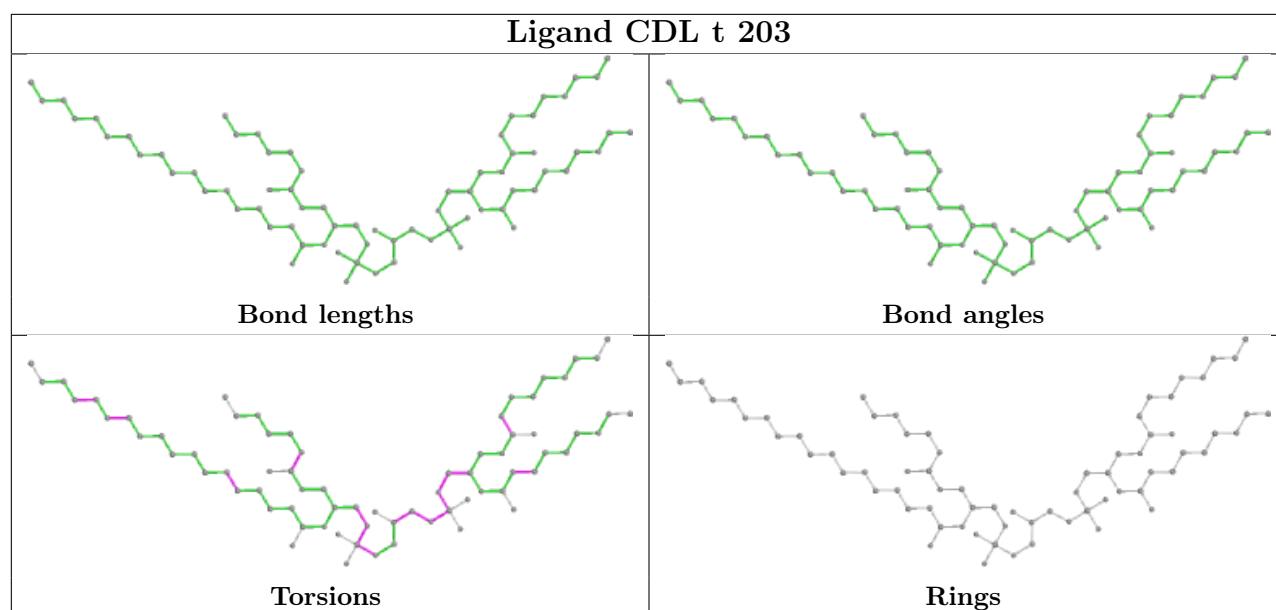


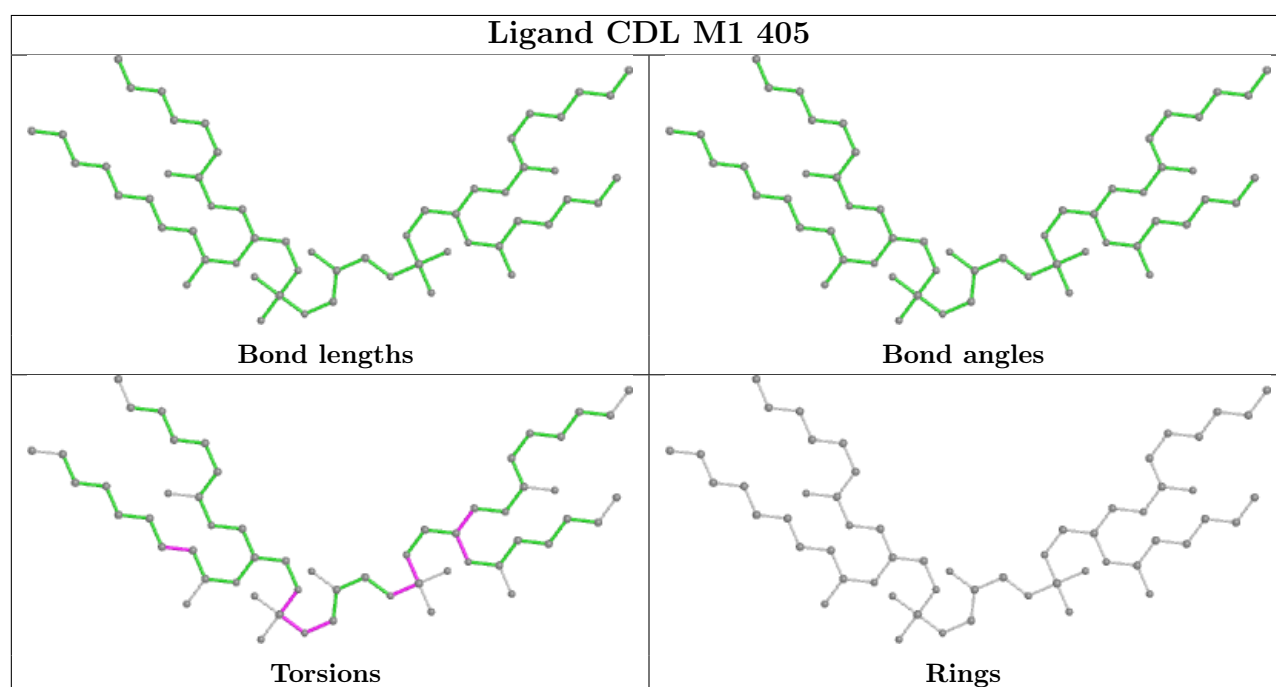
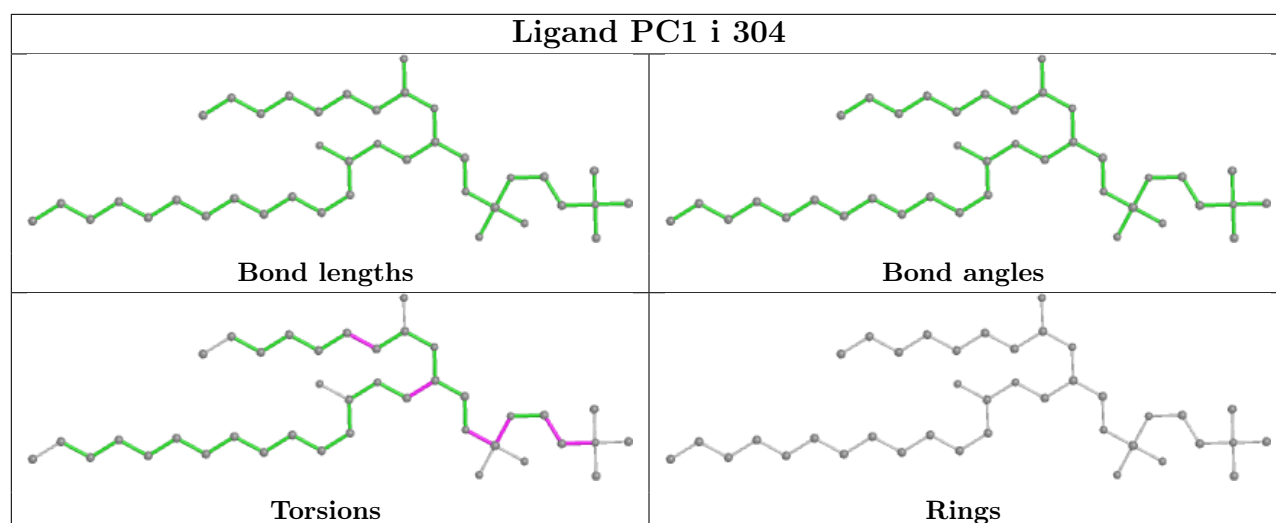


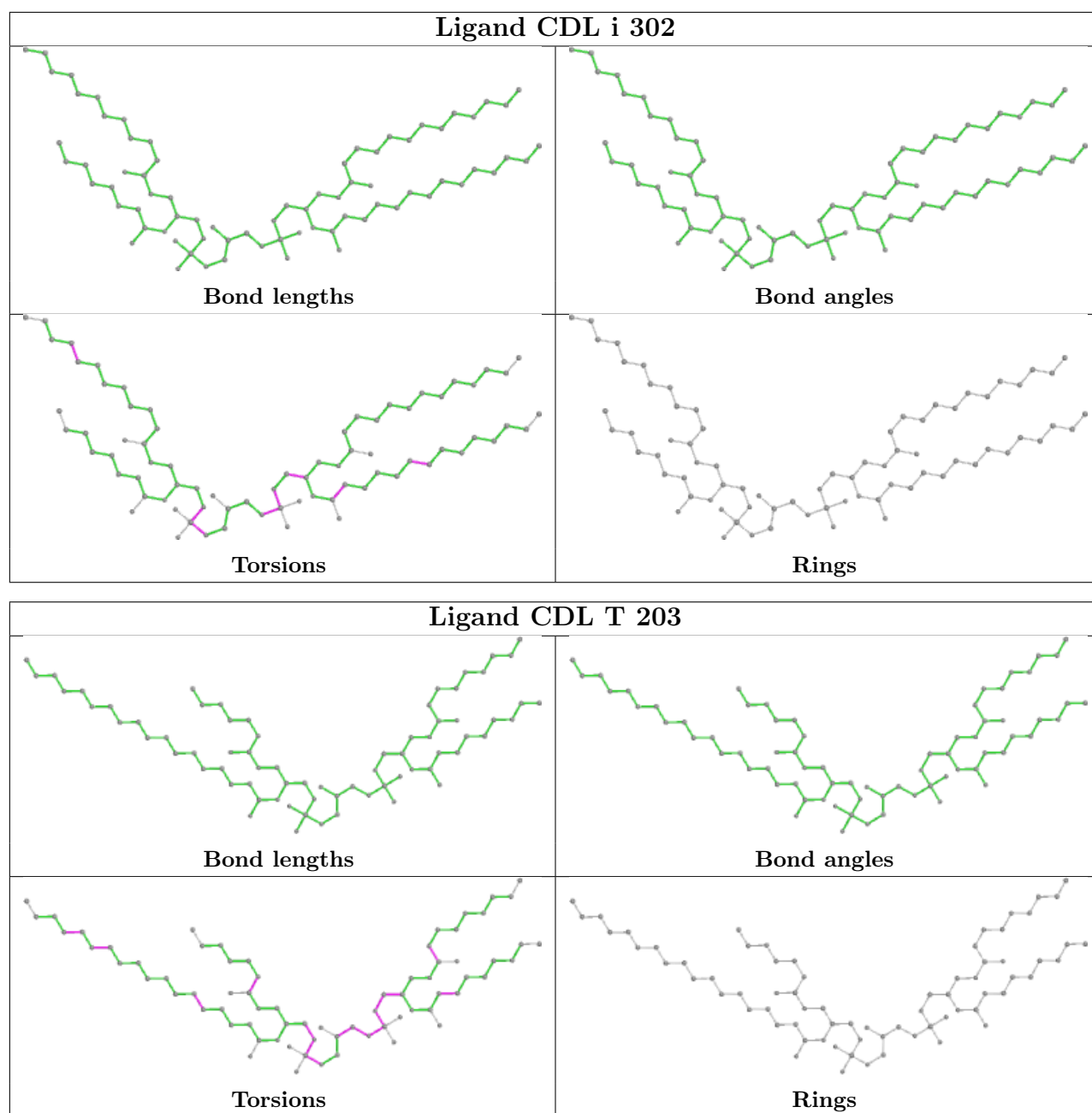


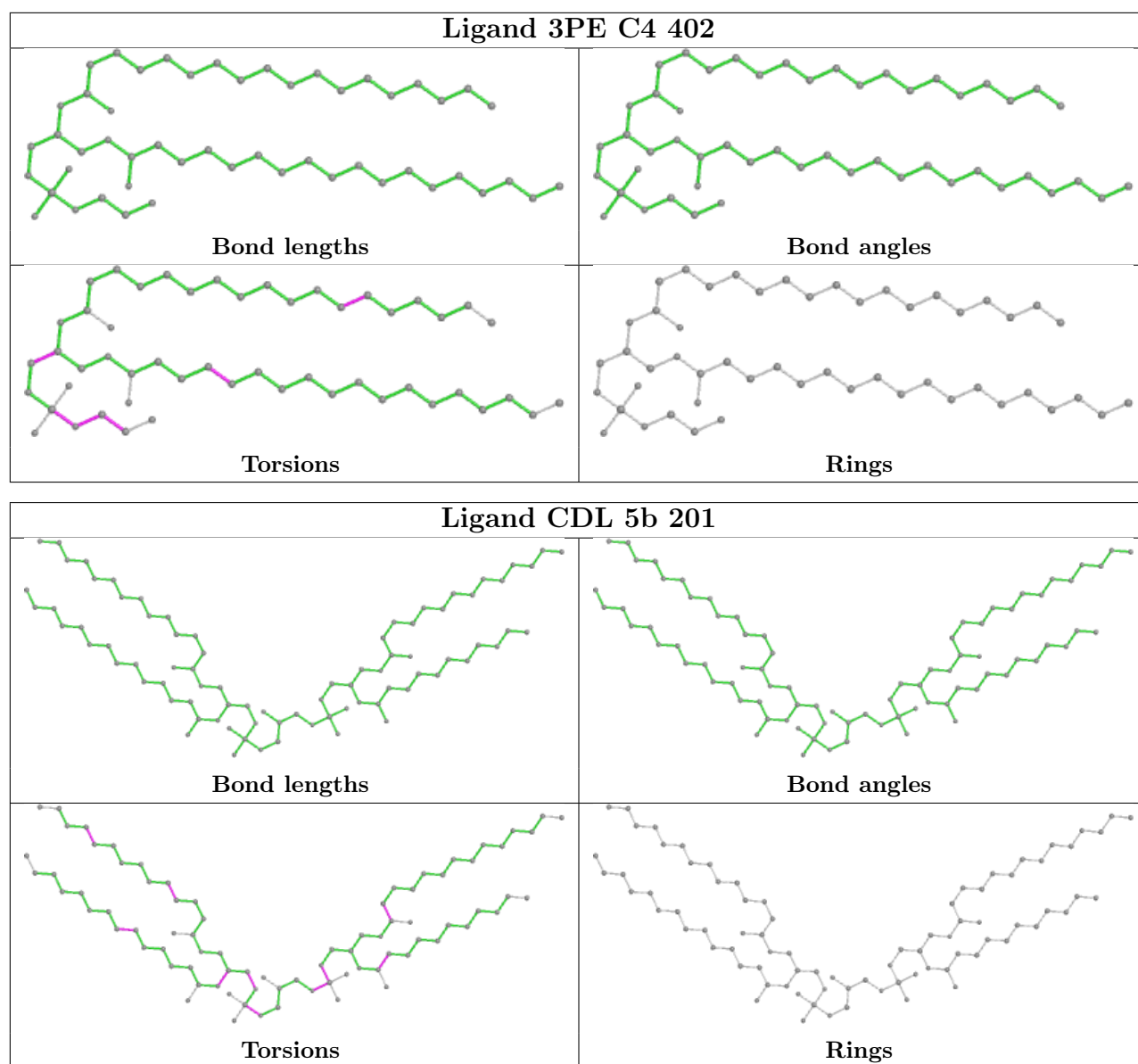


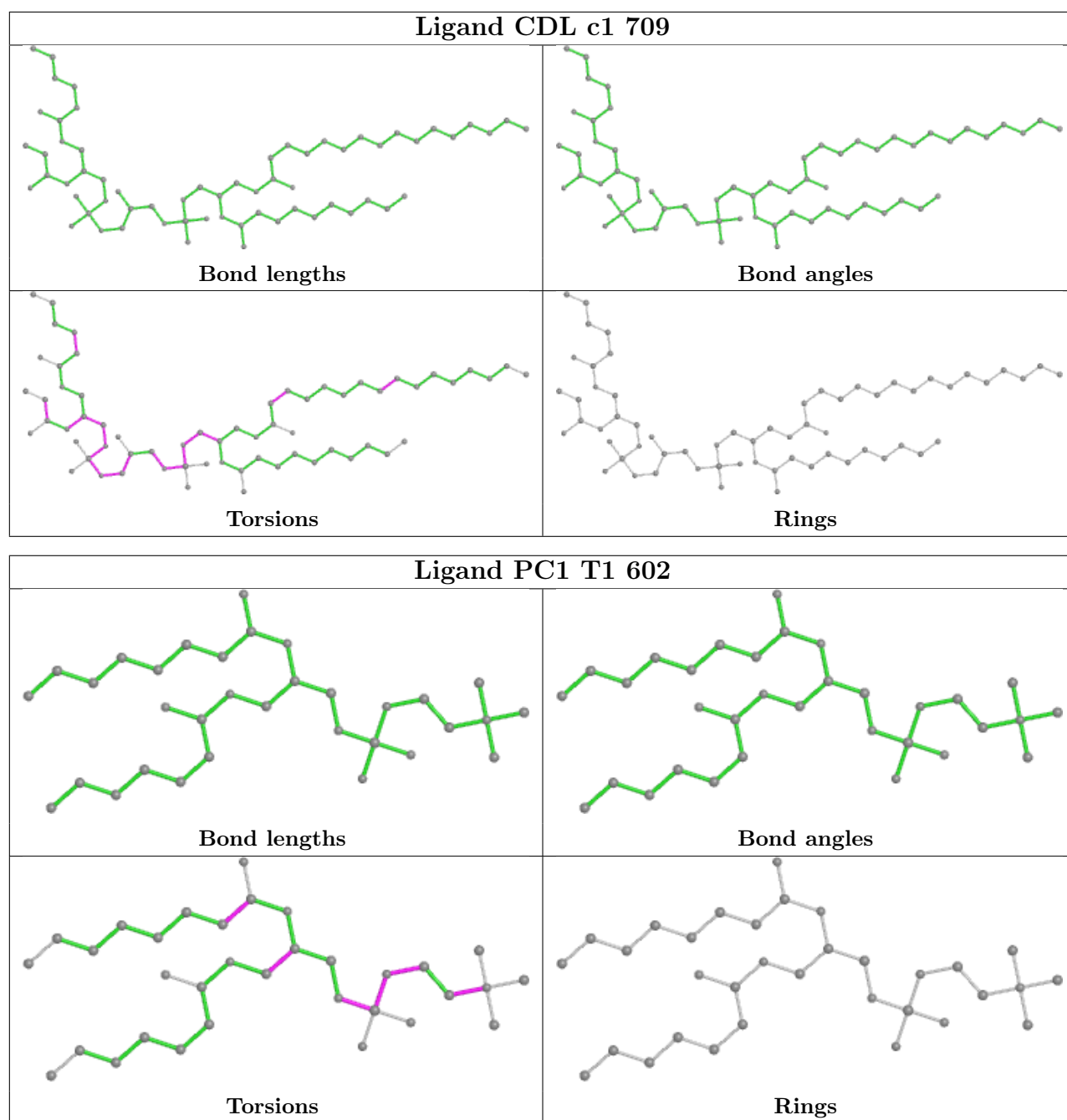












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

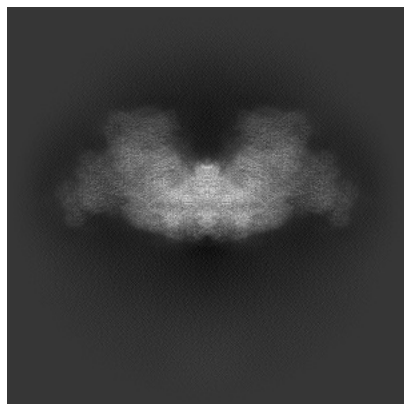
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34373. These allow visual inspection of the internal detail of the map and identification of artifacts.

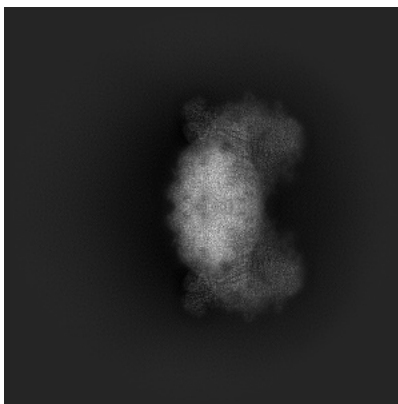
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

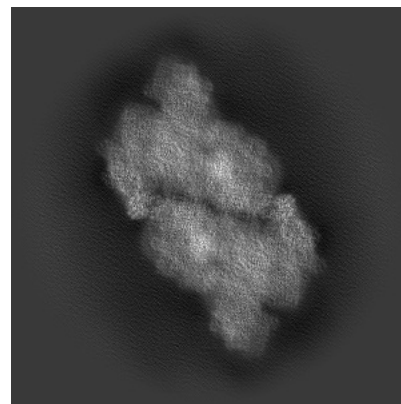
6.1.1 Primary map



X

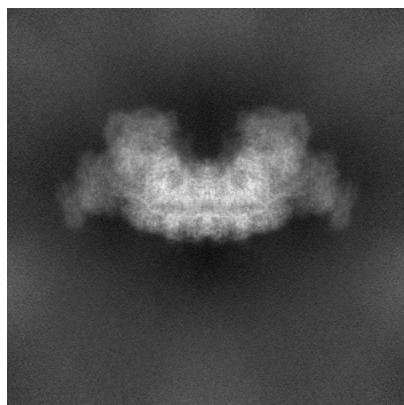


Y

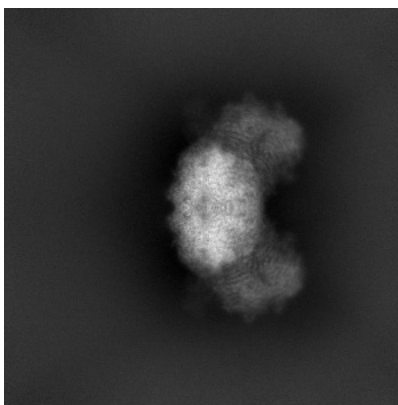


Z

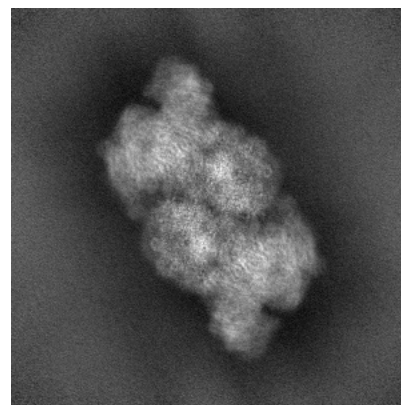
6.1.2 Raw map



X



Y

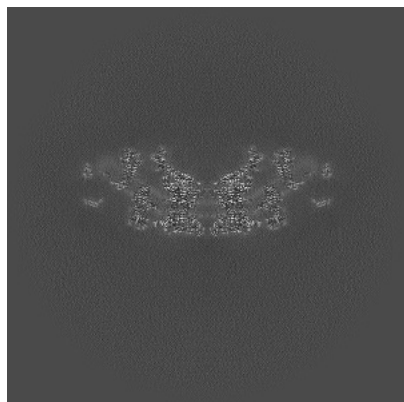


Z

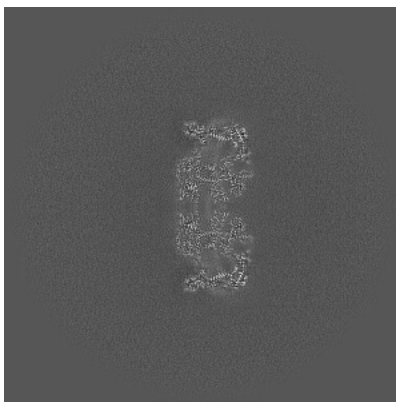
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

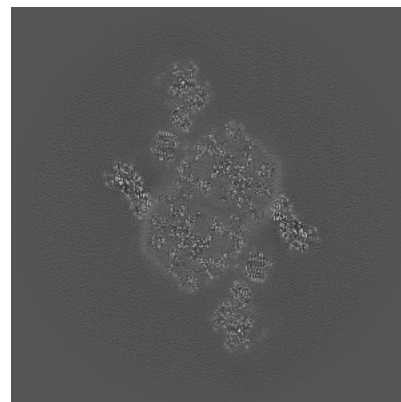
6.2.1 Primary map



X Index: 420

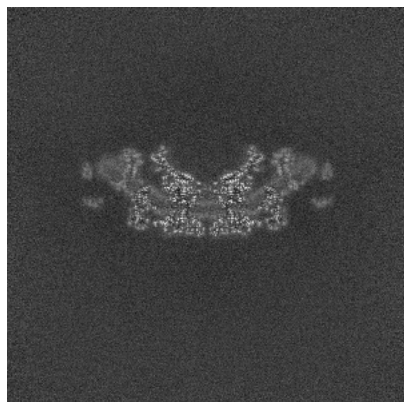


Y Index: 420

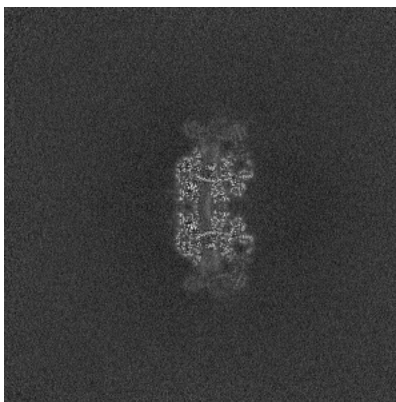


Z Index: 420

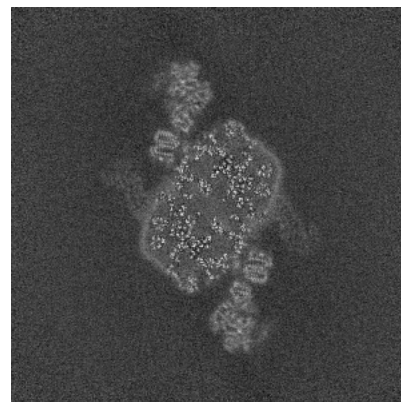
6.2.2 Raw map



X Index: 420



Y Index: 420

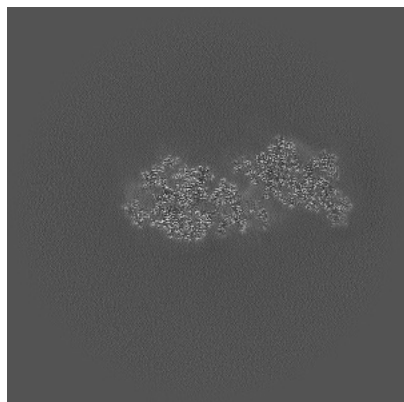


Z Index: 420

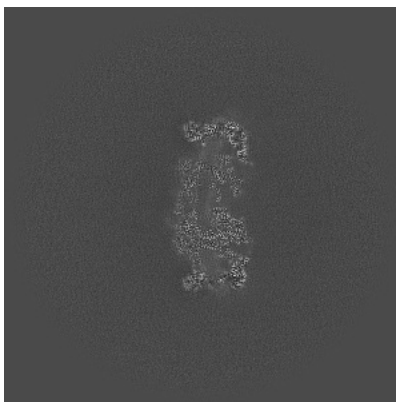
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

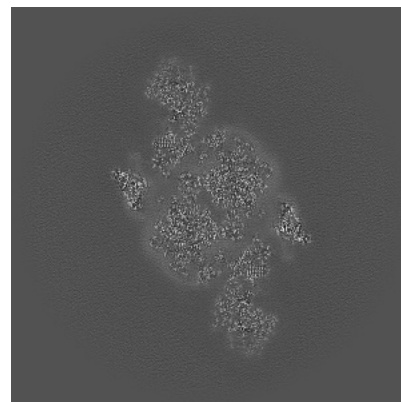
6.3.1 Primary map



X Index: 378

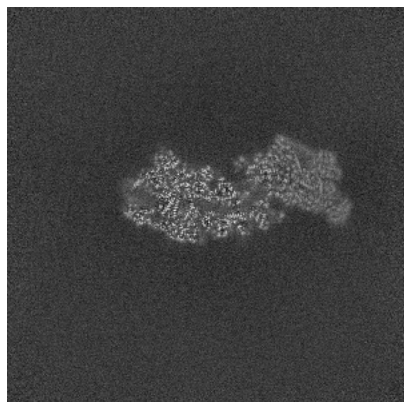


Y Index: 412

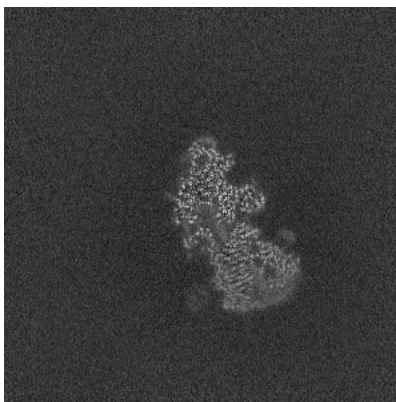


Z Index: 439

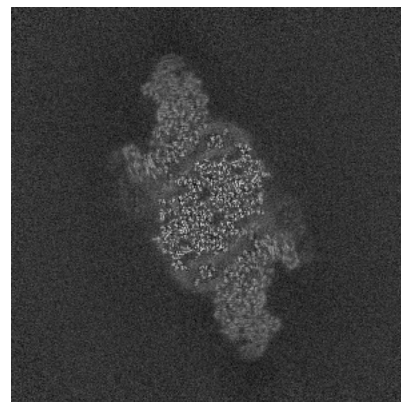
6.3.2 Raw map



X Index: 384



Y Index: 508

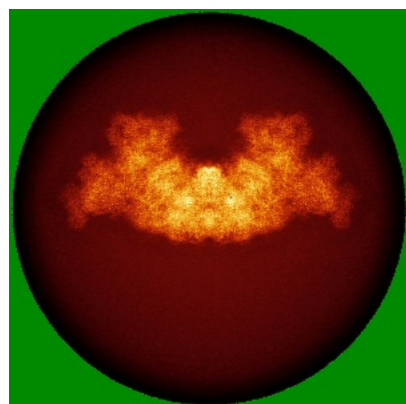


Z Index: 453

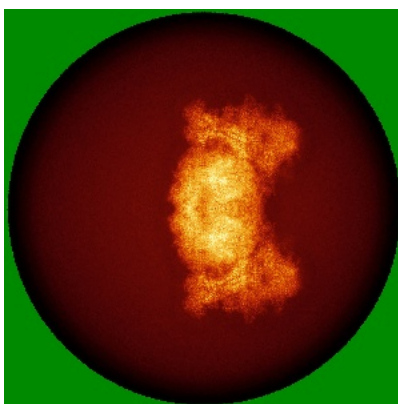
The images above show the largest variance slices of the map in three orthogonal directions.

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

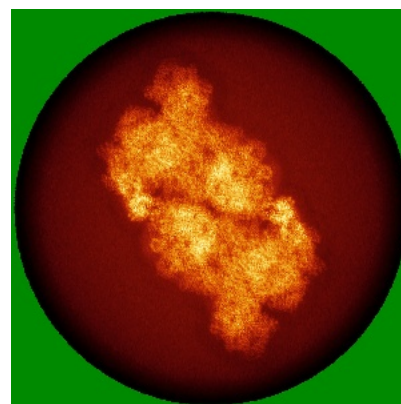
6.4.1 Primary map



X

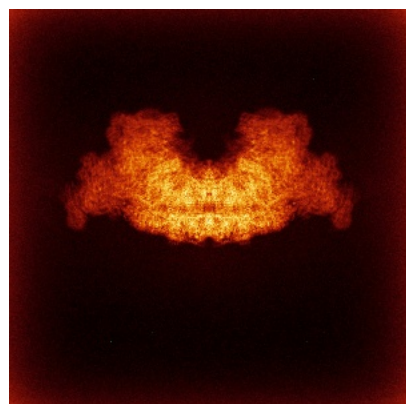


Y

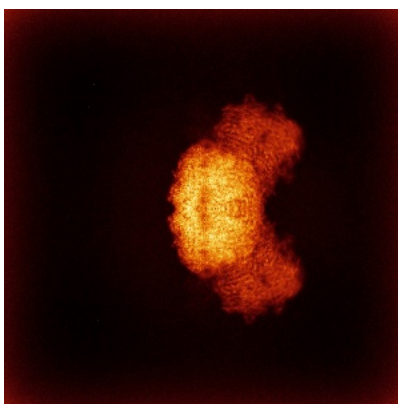


Z

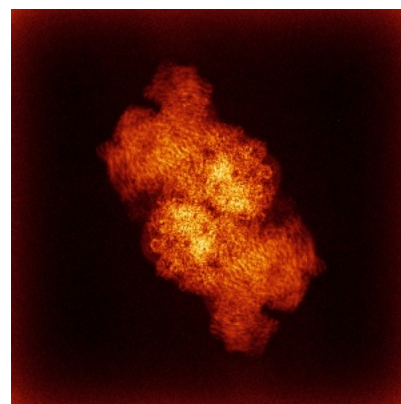
6.4.2 Raw map



X



Y

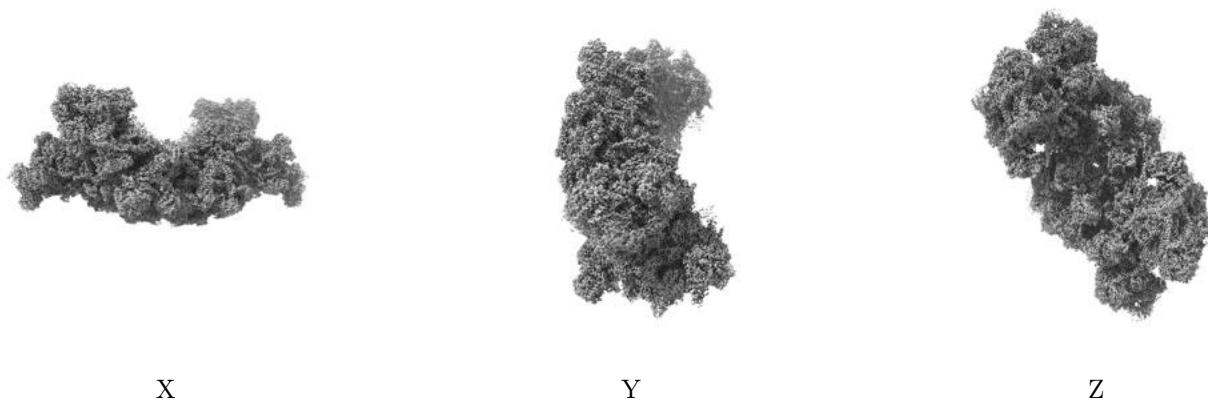


Z

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

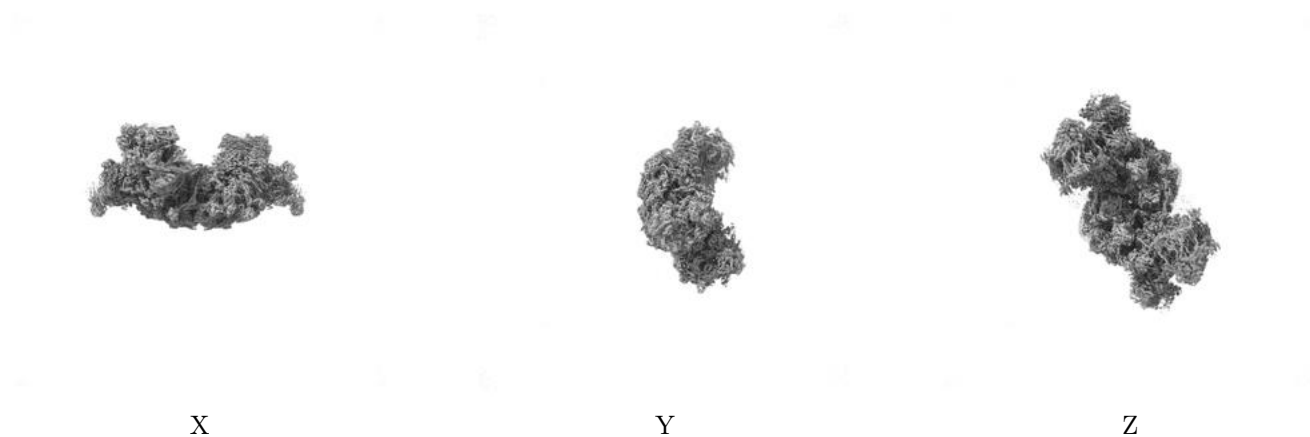
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

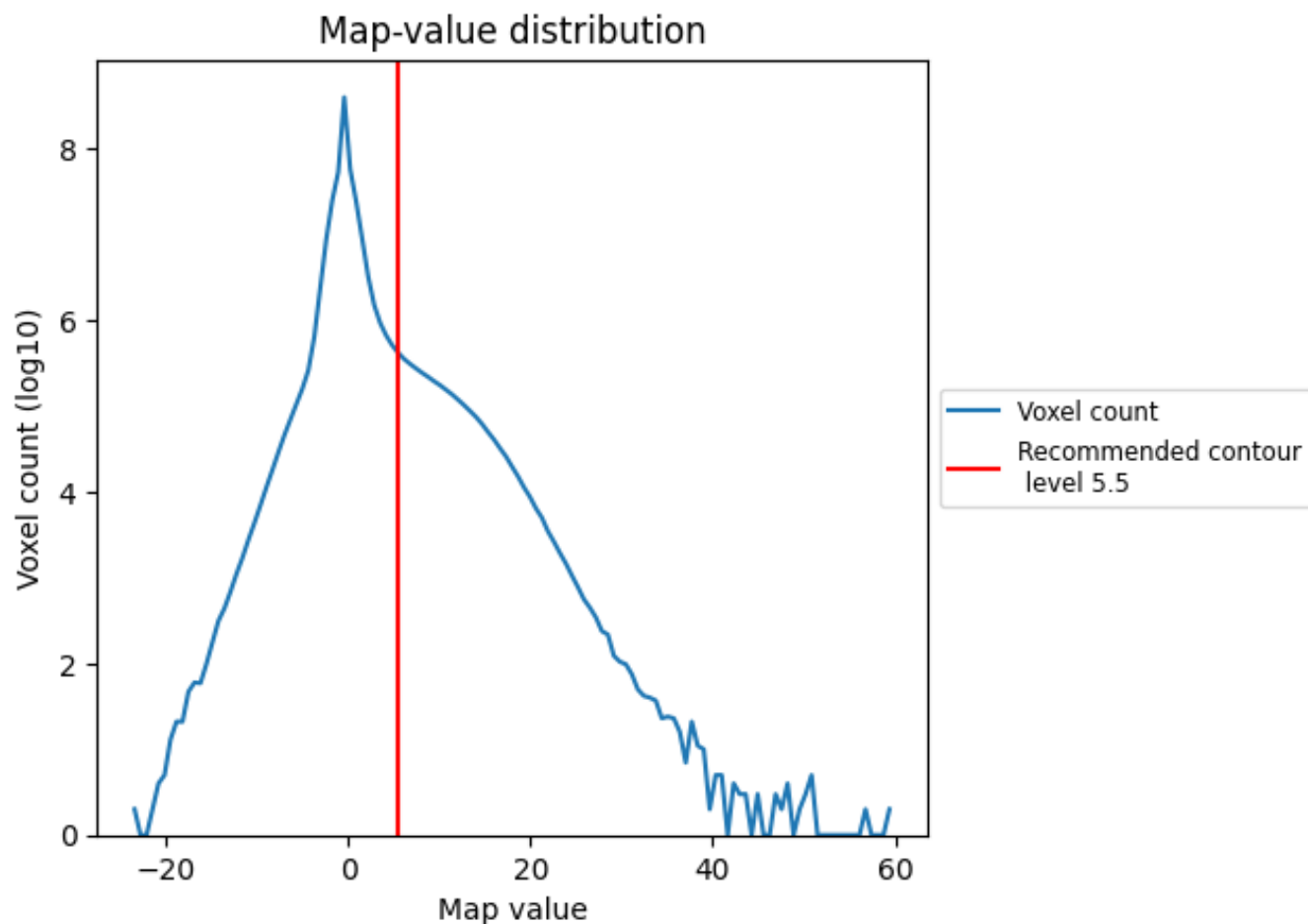
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

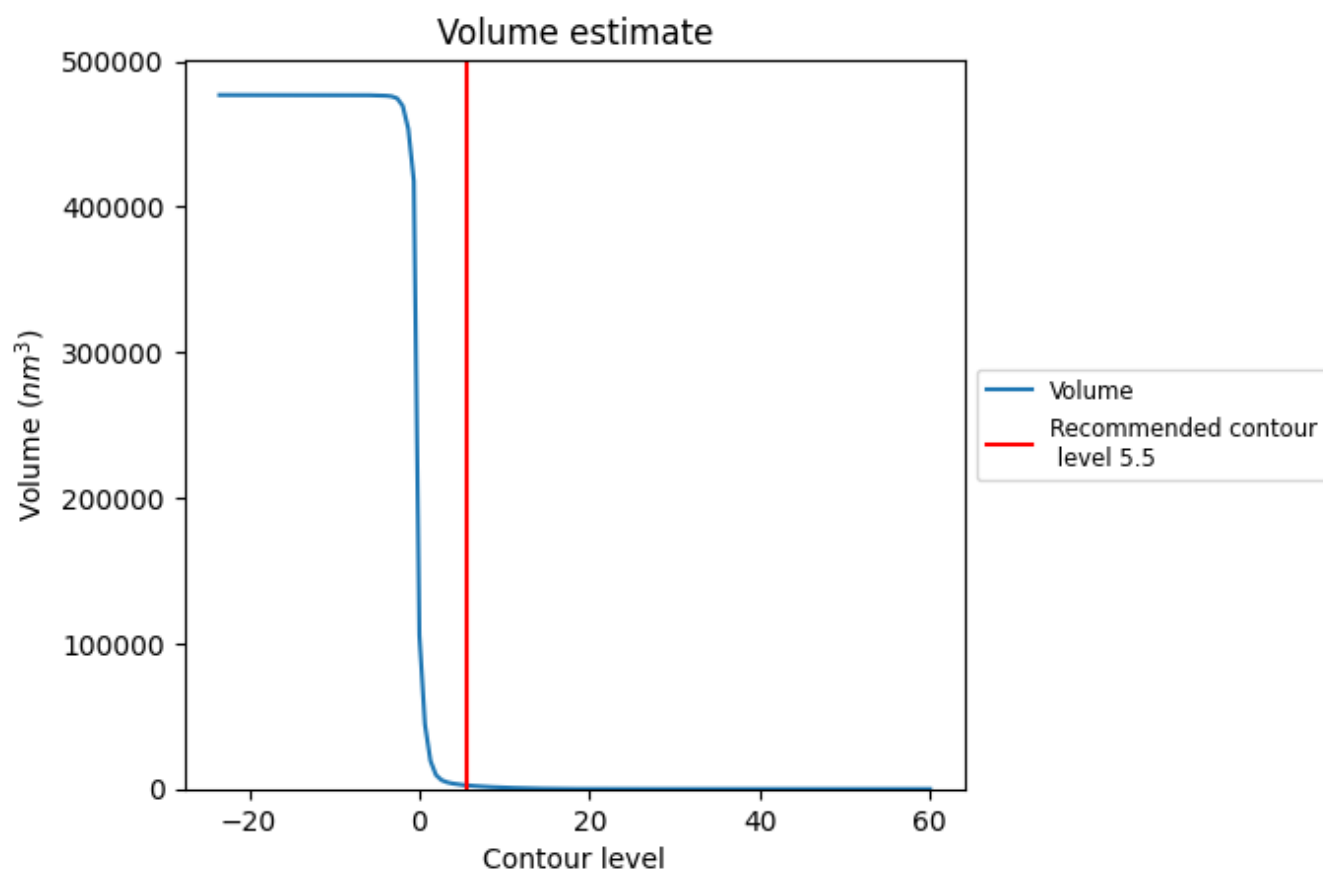
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

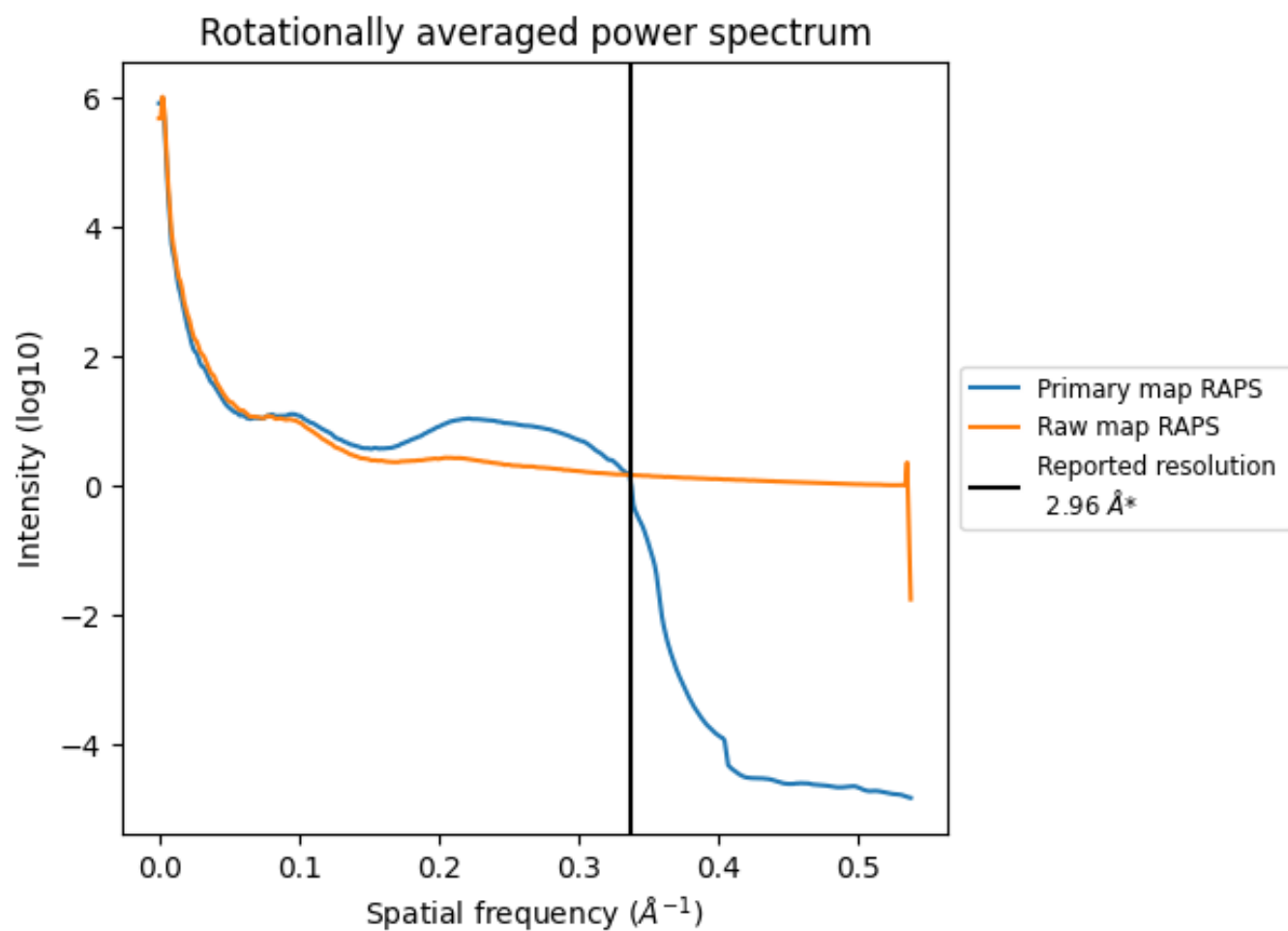
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2536 nm^3 ; this corresponds to an approximate mass of 2290 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 ⓘ

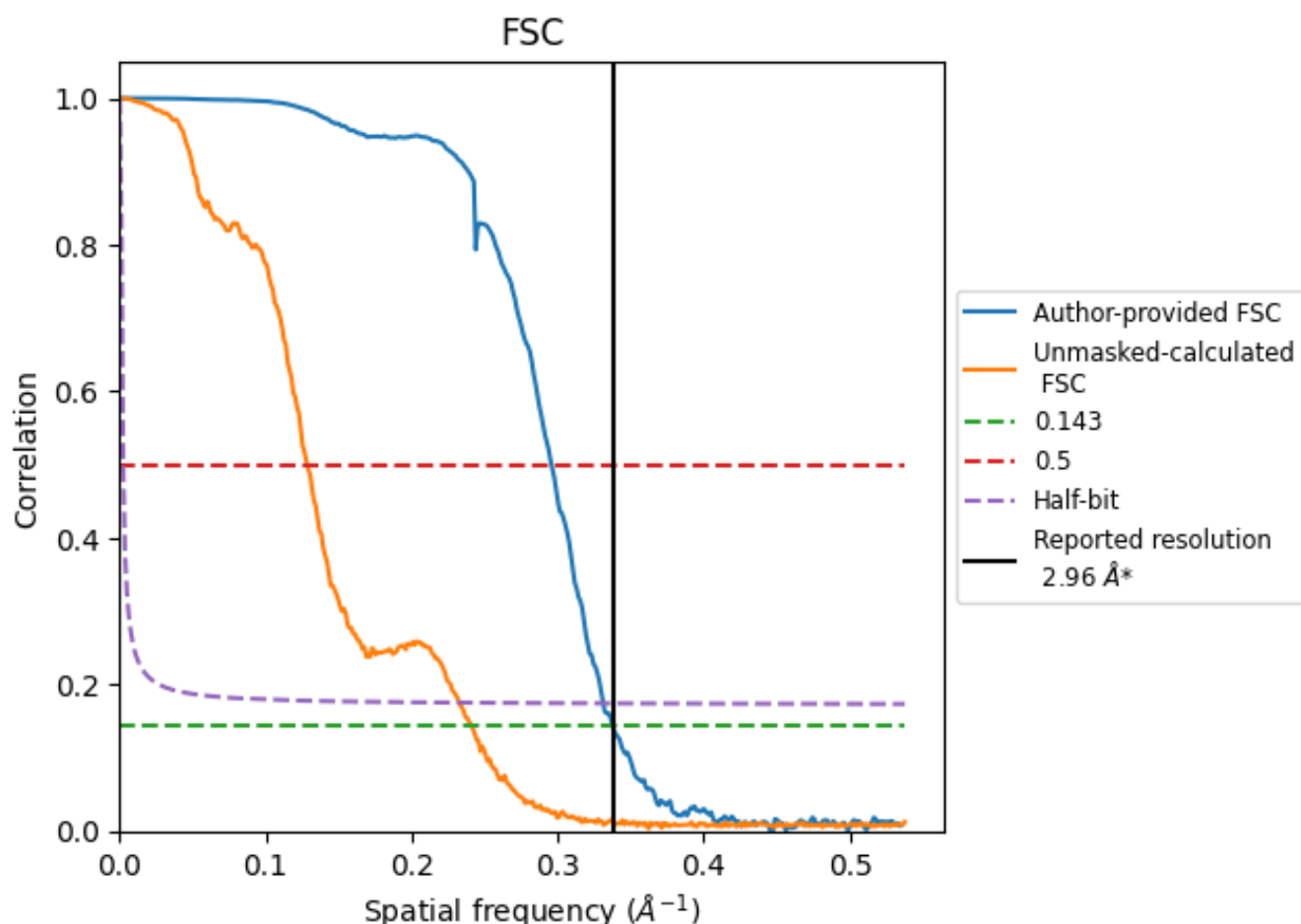


*Reported resolution corresponds to spatial frequency of 0.338 Å⁻¹

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 0.338 \AA^{-1}

8.2 Resolution estimates [i](#)

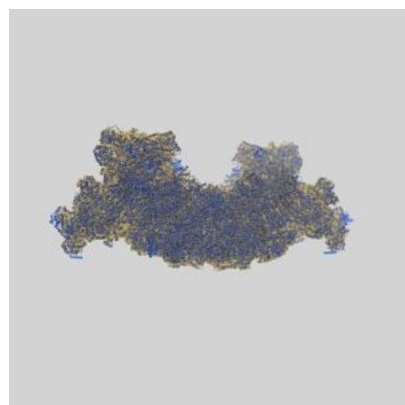
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 2.96 | - | - |
| Author-provided FSC curve | 2.96 | 3.38 | 3.02 |
| Unmasked-calculated* | 4.15 | 7.78 | 4.30 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.15 differs from the reported value 2.96 by more than 10 %

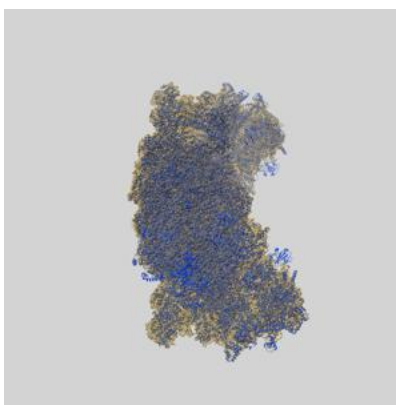
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34373 and PDB model 8GYM. Per-residue inclusion information can be found in [section 3](#) on [page 81](#).

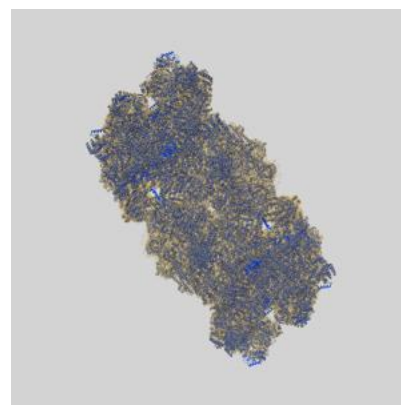
9.1 Map-model overlay [i](#)



X



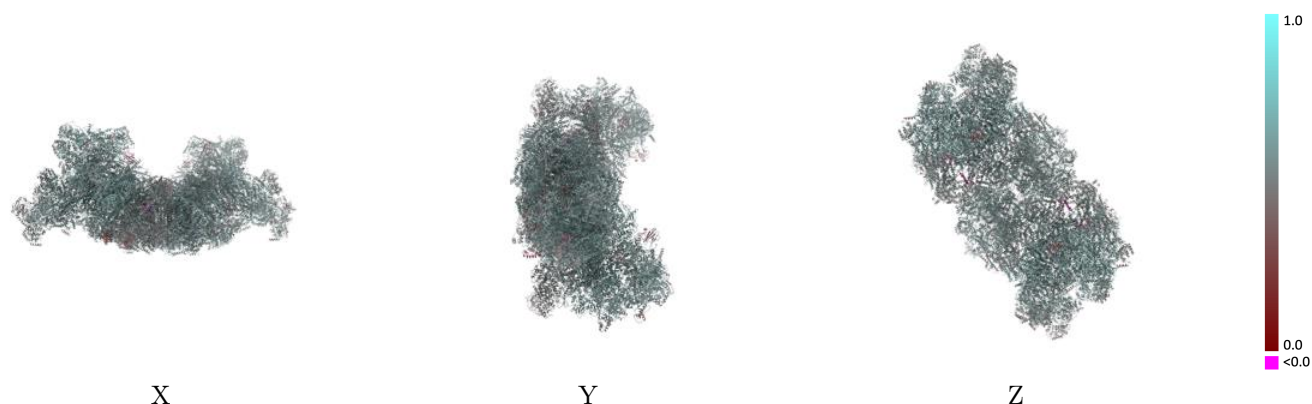
Y



Z

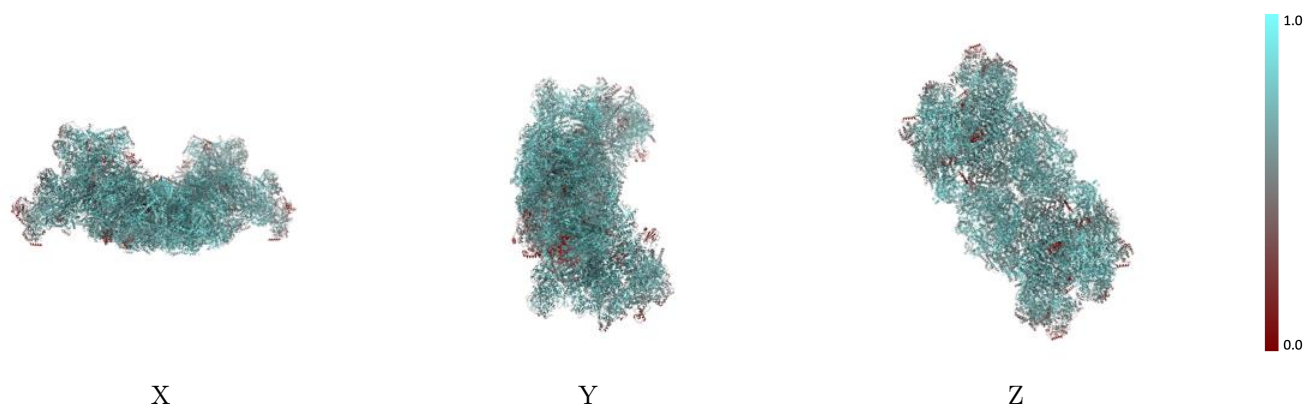
The images above show the 3D surface view of the map at the recommended contour level 5.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



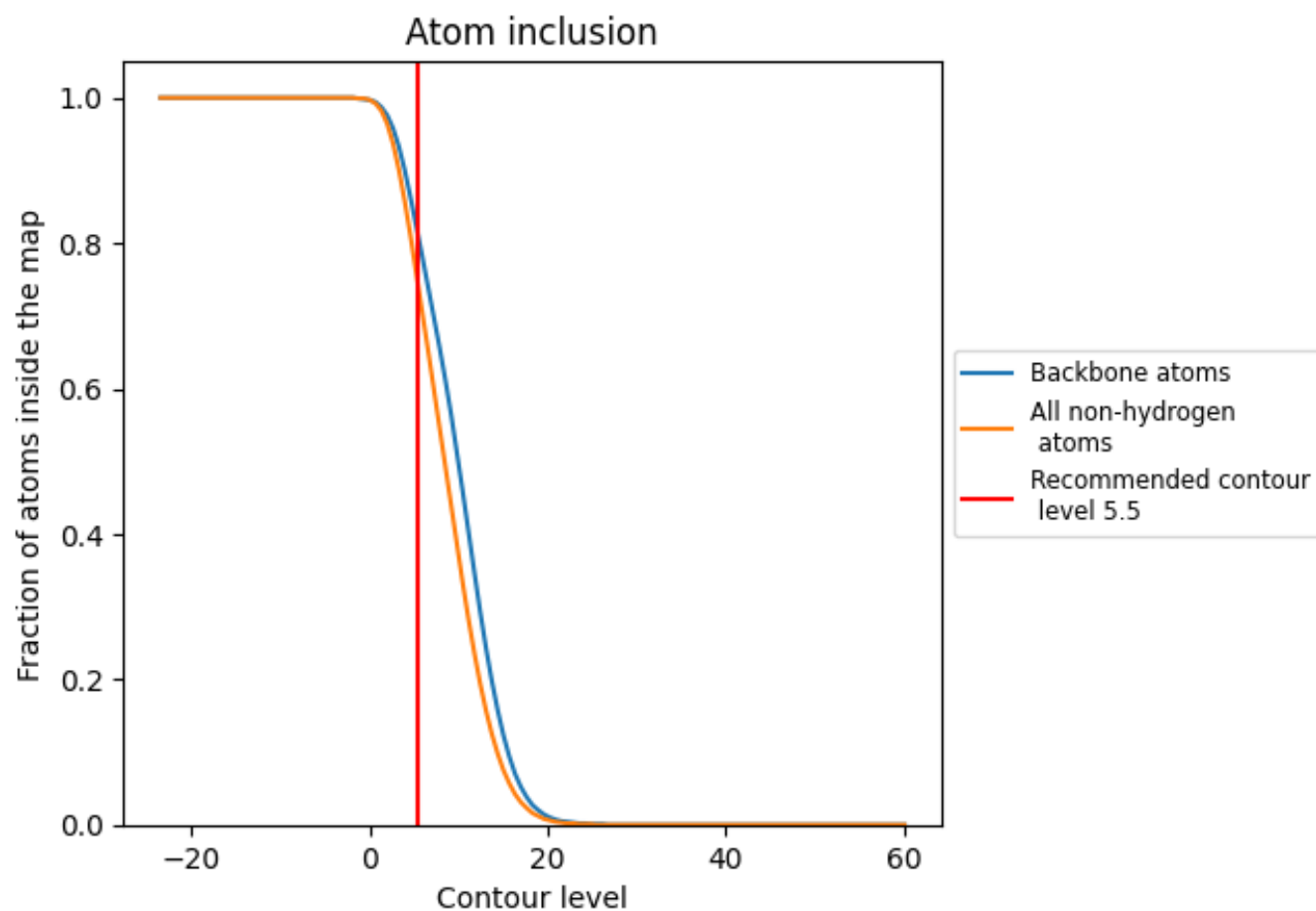
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5.5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 74% 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 (5.5) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.7380 |  0.5560 |
| 1B |  0.8100 |  0.6000 |
| 1T |  0.7970 |  0.5540 |
| 1b |  0.8100 |  0.6010 |
| 1t |  0.7970 |  0.5530 |
| 2B |  0.8340 |  0.6060 |
| 2E |  0.7130 |  0.4660 |
| 2F |  0.8130 |  0.5170 |
| 2G |  0.7650 |  0.5060 |
| 2H |  0.8350 |  0.4880 |
| 2I |  0.7720 |  0.4860 |
| 2J |  0.7800 |  0.4930 |
| 2K |  0.8000 |  0.5180 |
| 2L |  0.8300 |  0.4930 |
| 2M |  0.8460 |  0.5290 |
| 2N |  0.8180 |  0.5170 |
| 2O |  0.8480 |  0.5140 |
| 2T |  0.6780 |  0.5240 |
| 2b |  0.8340 |  0.6030 |
| 2e |  0.7130 |  0.4670 |
| 2f |  0.8130 |  0.5150 |
| 2g |  0.7650 |  0.5060 |
| 2h |  0.8350 |  0.4860 |
| 2i |  0.7730 |  0.4880 |
| 2j |  0.7870 |  0.4970 |
| 2k |  0.8000 |  0.5180 |
| 2l |  0.8300 |  0.5010 |
| 2m |  0.8470 |  0.5300 |
| 2n |  0.8120 |  0.5150 |
| 2o |  0.8480 |  0.5160 |
| 2t |  0.6780 |  0.5220 |
| 3T |  0.6390 |  0.5110 |
| 3t |  0.6410 |  0.5070 |
| 4A |  0.8030 |  0.5730 |
| 4L |  0.8160 |  0.5960 |























































































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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| 4T |  0.8030 |  0.5430 |
| 4a |  0.8020 |  0.5680 |
| 4l |  0.8170 |  0.5960 |
| 4t |  0.8030 |  0.5460 |
| 5B |  0.7820 |  0.5970 |
| 5T |  0.6840 |  0.5250 |
| 5b |  0.7810 |  0.5960 |
| 5t |  0.6800 |  0.5300 |
| 6A |  0.8000 |  0.5630 |
| 6B |  0.8530 |  0.5760 |
| 6C |  0.7880 |  0.5460 |
| 6L |  0.7550 |  0.5430 |
| 6T |  0.7230 |  0.5270 |
| 6a |  0.8000 |  0.5630 |
| 6b |  0.8530 |  0.5740 |
| 6c |  0.7880 |  0.5450 |
| 6l |  0.7550 |  0.5450 |
| 6t |  0.7200 |  0.5280 |
| 7A |  0.8230 |  0.5770 |
| 7C |  0.8020 |  0.5650 |
| 7L |  0.8110 |  0.5670 |
| 7a |  0.8240 |  0.5780 |
| 7c |  0.8040 |  0.5640 |
| 7l |  0.8110 |  0.5640 |
| A |  0.8140 |  0.5690 |
| A1 |  0.7460 |  0.5910 |
| A2 |  0.6140 |  0.5310 |
| A3 |  0.8070 |  0.5960 |
| A5 |  0.7480 |  0.5650 |
| A6 |  0.8350 |  0.5950 |
| A7 |  0.6910 |  0.5550 |
| A8 |  0.7900 |  0.5900 |
| A9 |  0.7510 |  0.5680 |
| AB |  0.7580 |  0.5870 |
| AC |  0.7490 |  0.5770 |
| AL |  0.7400 |  0.5780 |
| AM |  0.7610 |  0.5800 |
| AN |  0.7360 |  0.5850 |
| B |  0.5360 |  0.4790 |
| B2 |  0.6960 |  0.5670 |
| B3 |  0.6410 |  0.5610 |
| B4 |  0.7660 |  0.5910 |





















































































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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| B6 |  0.7870 |  0.5940 |
| B7 |  0.7590 |  0.5710 |
| B8 |  0.7060 |  0.5770 |
| B9 |  0.7830 |  0.5890 |
| BL |  0.8200 |  0.5960 |
| BM |  0.6820 |  0.5620 |
| BP |  0.7100 |  0.5410 |
| C |  0.4500 |  0.4230 |
| C1 |  0.8230 |  0.5670 |
| C2 |  0.8340 |  0.5700 |
| C3 |  0.7730 |  0.5490 |
| C4 |  0.7500 |  0.5810 |
| D |  0.7370 |  0.5490 |
| E |  0.7730 |  0.5550 |
| F |  0.7790 |  0.5610 |
| FS |  0.7890 |  0.5670 |
| FX |  0.8450 |  0.5990 |
| G |  0.8250 |  0.5680 |
| G1 |  0.8580 |  0.6060 |
| G2 |  0.8070 |  0.5940 |
| G3 |  0.7790 |  0.5810 |
| H |  0.6900 |  0.5160 |
| I |  0.7220 |  0.5430 |
| J |  0.7560 |  0.5670 |
| J1 |  0.7330 |  0.5750 |
| K |  0.7890 |  0.5600 |
| L |  0.7830 |  0.5580 |
| M |  0.7720 |  0.5630 |
| M1 |  0.7860 |  0.5530 |
| M2 |  0.7850 |  0.5500 |
| M3 |  0.7710 |  0.5560 |
| N |  0.7960 |  0.5660 |
| N1 |  0.7590 |  0.5790 |
| N2 |  0.8230 |  0.6010 |
| N3 |  0.7750 |  0.5840 |
| N4 |  0.8290 |  0.5950 |
| N5 |  0.6770 |  0.5150 |
| N6 |  0.7900 |  0.5960 |
| O |  0.8560 |  0.5710 |
| P |  0.7370 |  0.5430 |
| P1 |  0.7020 |  0.5790 |
| P2 |  0.7180 |  0.5760 |

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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| Q |  0.8470 |  0.5690 |
| QA |  0.6990 |  0.5610 |
| QB |  0.7790 |  0.5830 |
| QC |  0.7760 |  0.5860 |
| QD |  0.8320 |  0.5990 |
| QE |  0.5560 |  0.4870 |
| QF |  0.7010 |  0.5690 |
| QG |  0.6230 |  0.5470 |
| QH |  0.7790 |  0.5940 |
| QI |  0.7670 |  0.5880 |
| QJ |  0.7840 |  0.5900 |
| QL |  0.5640 |  0.5540 |
| QM |  0.8240 |  0.5780 |
| Qa |  0.6180 |  0.5490 |
| Qb |  0.6790 |  0.5640 |
| Qc |  0.7540 |  0.5790 |
| Qd |  0.7980 |  0.5920 |
| Qe |  0.4930 |  0.4760 |
| Qf |  0.5330 |  0.5100 |
| Qg |  0.6420 |  0.5560 |
| Qh |  0.7650 |  0.5860 |
| Qi |  0.6550 |  0.5710 |
| Qj |  0.7230 |  0.5720 |
| Ql |  0.6760 |  0.5620 |
| Qm |  0.8470 |  0.5880 |
| R |  0.7850 |  0.5500 |
| S |  0.7080 |  0.5310 |
| S1 |  0.6940 |  0.5540 |
| S2 |  0.7990 |  0.5820 |
| S3 |  0.7890 |  0.5780 |
| S4 |  0.7180 |  0.5620 |
| S5 |  0.7760 |  0.5920 |
| S6 |  0.6510 |  0.5490 |
| S7 |  0.8210 |  0.5870 |
| S8 |  0.8030 |  0.5750 |
| SA |  0.6350 |  0.4790 |
| SB |  0.7420 |  0.5030 |
| SC |  0.7570 |  0.5080 |
| SD |  0.8830 |  0.5460 |
| T |  0.7860 |  0.5680 |
| T1 |  0.6060 |  0.5210 |
| T2 |  0.2910 |  0.4730 |





















































































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| Chain | Atom inclusion | Q-score |
|-------|----------------|---------|
| T3 | 0.5540 | 0.5370 |
| T4 | 0.5530 | 0.5240 |
| T5 | 0.7240 | 0.5610 |
| T6 | 0.7870 | 0.5900 |
| T7 | 0.7060 | 0.5710 |
| T8 | 0.7610 | 0.5850 |
| T9 | 0.7880 | 0.5790 |
| TA | 0.7180 | 0.5600 |
| TB | 0.7710 | 0.5940 |
| TC | 0.7300 | 0.5840 |
| TD | 0.6320 | 0.5650 |
| TE | 0.6940 | 0.5760 |
| TF | 0.6720 | 0.5510 |
| TG | 0.5440 | 0.5120 |
| TH | 0.7770 | 0.5800 |
| TX | 0.7640 | 0.5840 |
| U | 0.7460 | 0.5510 |
| U1 | 0.8220 | 0.5400 |
| U2 | 0.8820 | 0.5480 |
| V | 0.7800 | 0.5590 |
| V1 | 0.5920 | 0.5300 |
| V2 | 0.4610 | 0.5070 |
| VB | 0.8000 | 0.5600 |
| W | 0.7380 | 0.5490 |
| X | 0.8620 | 0.5820 |
| X1 | 0.7930 | 0.5900 |
| Y | 0.9100 | 0.5900 |
| Y0 | 0.8650 | 0.5800 |
| Y5 | 0.7220 | 0.5380 |
| Y7 | 0.7200 | 0.5360 |
| Z | 0.7160 | 0.5390 |
| Z1 | 0.8050 | 0.5550 |
| a | 0.8120 | 0.5700 |
| a1 | 0.7720 | 0.5880 |
| a2 | 0.6120 | 0.5300 |
| a3 | 0.8090 | 0.6020 |
| a5 | 0.7490 | 0.5670 |
| a6 | 0.8370 | 0.5940 |
| a7 | 0.6910 | 0.5550 |
| a8 | 0.7900 | 0.5880 |
| a9 | 0.7500 | 0.5670 |
| ab | 0.7580 | 0.5870 |





















































































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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| ac |  0.7490 |  0.5750 |
| al |  0.7400 |  0.5760 |
| am |  0.7620 |  0.5790 |
| an |  0.7370 |  0.5850 |
| b |  0.5360 |  0.4790 |
| b2 |  0.6950 |  0.5670 |
| b3 |  0.6420 |  0.5600 |
| b4 |  0.7660 |  0.5880 |
| b6 |  0.7880 |  0.5920 |
| b7 |  0.7600 |  0.5750 |
| b8 |  0.7040 |  0.5770 |
| b9 |  0.7820 |  0.5860 |
| bl |  0.8200 |  0.5960 |
| bm |  0.6820 |  0.5610 |
| bp |  0.7080 |  0.5410 |
| c |  0.4490 |  0.4230 |
| c1 |  0.8230 |  0.5670 |
| c2 |  0.8330 |  0.5690 |
| c3 |  0.7740 |  0.5480 |
| c4 |  0.7540 |  0.5830 |
| d |  0.7360 |  0.5480 |
| e |  0.7750 |  0.5530 |
| f |  0.7810 |  0.5600 |
| fs |  0.7870 |  0.5670 |
| fx |  0.8440 |  0.5970 |
| g |  0.8250 |  0.5670 |
| g1 |  0.8570 |  0.6070 |
| g2 |  0.8090 |  0.5930 |
| g3 |  0.7790 |  0.5790 |
| h |  0.6890 |  0.5160 |
| i |  0.7200 |  0.5430 |
| j |  0.7560 |  0.5640 |
| j1 |  0.7320 |  0.5760 |
| k |  0.7900 |  0.5590 |
| l |  0.7840 |  0.5570 |
| m |  0.7700 |  0.5630 |
| m1 |  0.7870 |  0.5530 |
| m2 |  0.7850 |  0.5500 |
| m3 |  0.7710 |  0.5570 |
| n |  0.7940 |  0.5640 |
| n1 |  0.7590 |  0.5790 |
| n2 |  0.8240 |  0.6010 |

















































































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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| n3 |  0.7750 |  0.5850 |
| n4 |  0.8280 |  0.5930 |
| n5 |  0.6780 |  0.5150 |
| n6 |  0.7890 |  0.5940 |
| o |  0.8550 |  0.5720 |
| p |  0.7360 |  0.5410 |
| p1 |  0.7020 |  0.5790 |
| p2 |  0.7160 |  0.5760 |
| q |  0.8240 |  0.5630 |
| qA |  0.6980 |  0.5610 |
| qB |  0.7800 |  0.5820 |
| qC |  0.7770 |  0.5840 |
| qD |  0.8340 |  0.5980 |
| qE |  0.5560 |  0.4890 |
| qF |  0.6960 |  0.5650 |
| qG |  0.6220 |  0.5450 |
| qH |  0.7790 |  0.5920 |
| qI |  0.7670 |  0.5870 |
| qJ |  0.7900 |  0.5910 |
| qL |  0.5640 |  0.5510 |
| qM |  0.8240 |  0.5800 |
| qa |  0.6180 |  0.5470 |
| qb |  0.6800 |  0.5640 |
| qc |  0.7530 |  0.5790 |
| qd |  0.7980 |  0.5920 |
| qe |  0.4950 |  0.4750 |
| qf |  0.5280 |  0.5110 |
| qg |  0.6410 |  0.5570 |
| qh |  0.7670 |  0.5860 |
| qi |  0.6550 |  0.5690 |
| qj |  0.7230 |  0.5720 |
| ql |  0.6680 |  0.5630 |
| qm |  0.8470 |  0.5840 |
| r |  0.7840 |  0.5500 |
| s |  0.7080 |  0.5290 |
| s1 |  0.6950 |  0.5540 |
| s2 |  0.7980 |  0.5800 |
| s3 |  0.7890 |  0.5770 |
| s4 |  0.7160 |  0.5620 |
| s5 |  0.7770 |  0.5870 |
| s6 |  0.6500 |  0.5460 |
| s7 |  0.8220 |  0.5870 |

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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| s8 |  0.8020 |  0.5740 |
| sa |  0.6340 |  0.4790 |
| sb |  0.7440 |  0.5050 |
| sc |  0.7550 |  0.5110 |
| sd |  0.8830 |  0.5450 |
| t |  0.7870 |  0.5670 |
| t1 |  0.6050 |  0.5210 |
| t2 |  0.2900 |  0.4720 |
| t3 |  0.5550 |  0.5360 |
| t4 |  0.5520 |  0.5230 |
| t5 |  0.7220 |  0.5620 |
| t6 |  0.7830 |  0.5920 |
| t7 |  0.7010 |  0.5710 |
| t8 |  0.7590 |  0.5860 |
| t9 |  0.7880 |  0.5770 |
| ta |  0.7210 |  0.5600 |
| tb |  0.7710 |  0.5970 |
| tc |  0.7330 |  0.5820 |
| td |  0.6110 |  0.5660 |
| te |  0.6960 |  0.5730 |
| tf |  0.6720 |  0.5500 |
| tg |  0.5390 |  0.5120 |
| th |  0.7760 |  0.5780 |
| tx |  0.7640 |  0.5840 |
| u |  0.7460 |  0.5510 |
| u1 |  0.8220 |  0.5380 |
| u2 |  0.8820 |  0.5380 |
| v |  0.7790 |  0.5600 |
| v1 |  0.5920 |  0.5300 |
| v2 |  0.4630 |  0.5090 |
| vb |  0.8100 |  0.5620 |
| w |  0.7390 |  0.5480 |
| x |  0.8590 |  0.5840 |
| x1 |  0.7950 |  0.5880 |
| y |  0.9100 |  0.5900 |
| y0 |  0.8660 |  0.5810 |
| y5 |  0.7220 |  0.5370 |
| y7 |  0.7210 |  0.5360 |
| z |  0.7180 |  0.5420 |
| z1 |  0.8030 |  0.5530 |