



wwPDB EM Validation Summary Report ⓘ

Apr 3, 2025 – 06:25 pm BST

PDB ID : 6YNZ / pdb_00006ynz
EMDB ID : EMD-10861
Title : Cryo-EM structure of Tetrahymena thermophila mitochondrial ATP synthase
- F1Fo composite tetramer model
Authors : Kock Flygaard, R.; Muhleip, A.; Amunts, A.
Deposited on : 2020-04-14
Resolution : 3.10 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:

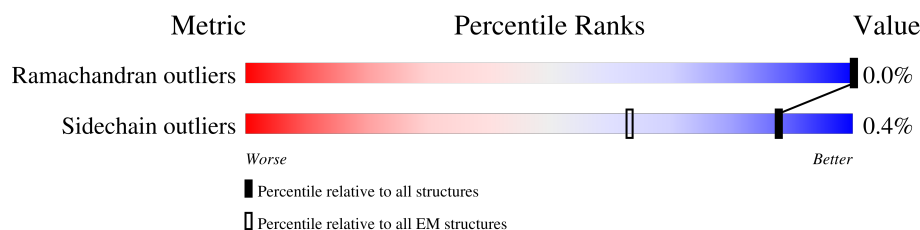
EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

1 Overall quality at a glance

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

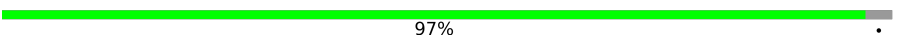
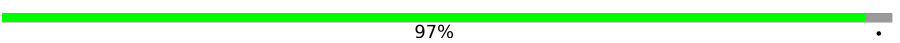
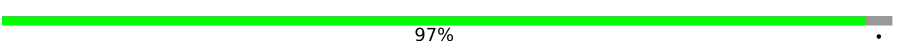
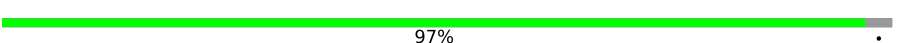
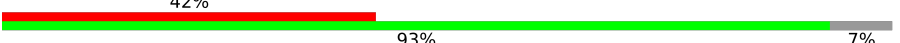




The reported resolution of this entry is 3.10 Å.

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 | A | 446 |  97% . |
| 1 | A3 | 446 |  97% . |
| 1 | a | 446 |  97% . |
| 1 | a3 | 446 |  97% . |
| 2 | B | 381 |  42% 93% 7% |
| 2 | B3 | 381 |  50% 93% 7% |
| 2 | b | 381 |  50% 93% 7% |
| 2 | b3 | 381 |  42% 93% 7% |
| 3 | D | 234 |  23% 88% 12% |

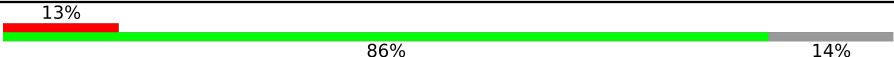

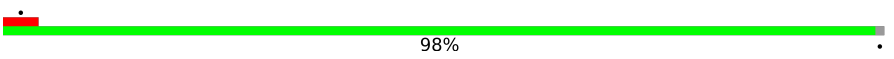
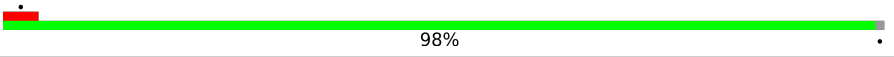
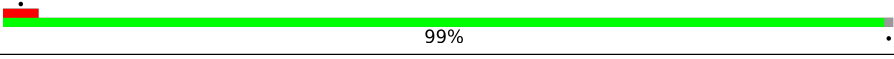
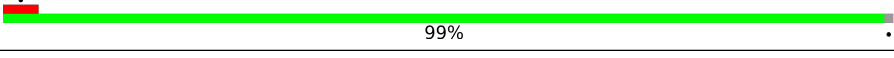
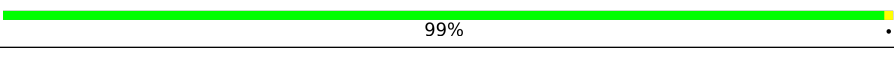
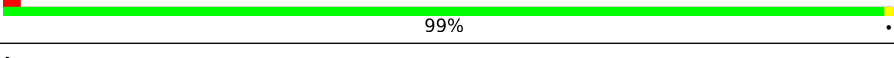
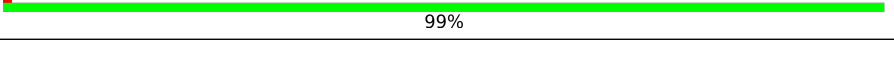
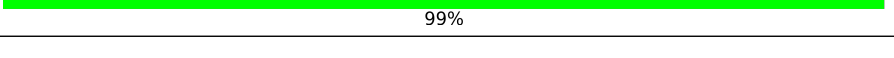
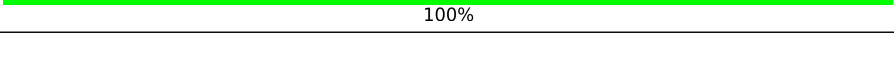
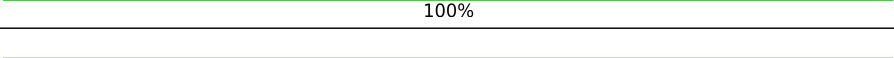
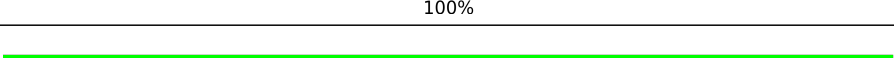
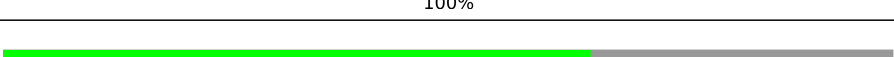

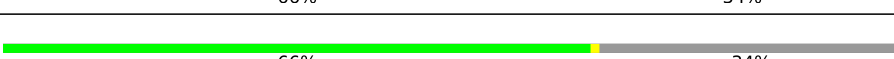
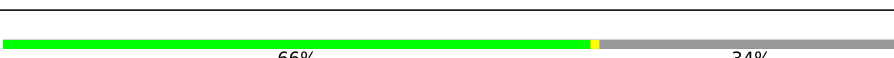
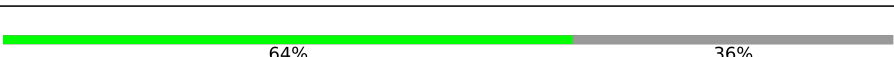
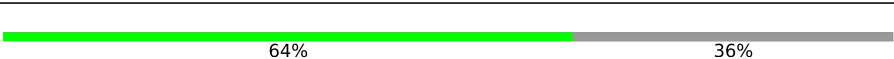


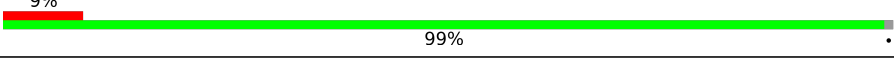
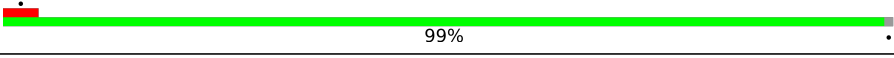
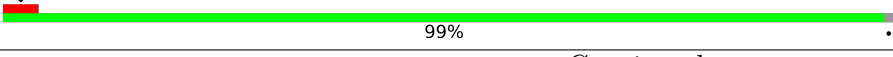

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3 | D3 | 234 | |
| 3 | d | 234 | |
| 3 | d3 | 234 | |
| 4 | F | 204 | |
| 4 | F3 | 204 | |
| 4 | f | 204 | |
| 4 | f3 | 204 | |
| 5 | I | 209 | |
| 5 | I3 | 209 | |
| 5 | i | 209 | |
| 5 | i3 | 209 | |
| 6 | K | 179 | |
| 6 | K3 | 179 | |
| 6 | k | 179 | |
| 6 | k3 | 179 | |
| 7 | C | 100 | |
| 7 | C3 | 100 | |
| 7 | c | 100 | |
| 7 | c3 | 100 | |
| 8 | G | 286 | |
| 8 | G3 | 286 | |
| 8 | g | 286 | |
| 8 | g3 | 286 | |
| 9 | H | 268 | |
| 9 | H3 | 268 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 9 | h | 268 |  |
| 9 | h3 | 268 |  |
| 10 | J | 273 |  |
| 10 | J3 | 273 |  |
| 10 | j | 273 |  |
| 10 | j3 | 273 |  |
| 11 | L | 247 |  |
| 11 | L3 | 247 |  |
| 11 | l | 247 |  |
| 11 | l3 | 247 |  |
| 12 | M | 221 |  |
| 12 | M3 | 221 |  |
| 12 | m | 221 |  |
| 12 | m3 | 221 |  |
| 13 | N | 179 |  |
| 13 | N3 | 179 |  |
| 13 | n | 179 |  |
| 13 | n3 | 179 |  |
| 14 | O | 154 |  |
| 14 | O3 | 154 |  |
| 14 | o | 154 |  |
| 14 | o3 | 154 |  |
| 15 | P | 152 |  |
| 15 | P3 | 152 |  |
| 15 | p | 152 |  |



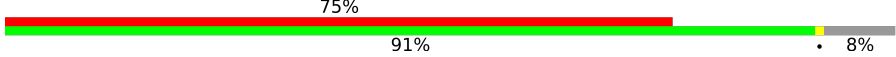
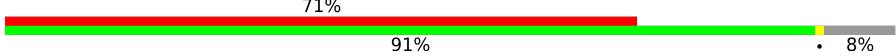
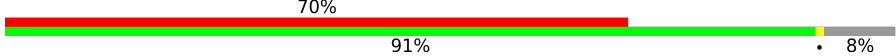
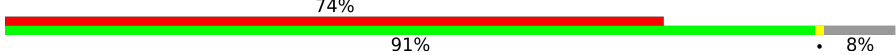
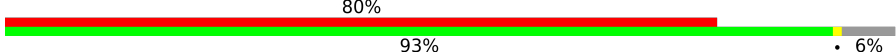
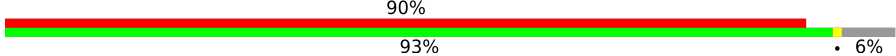
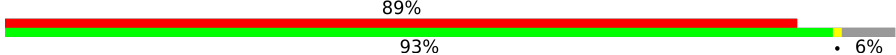
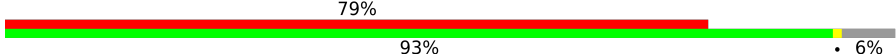
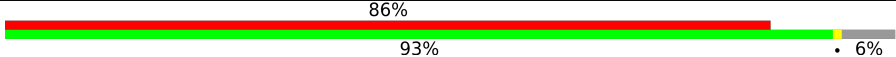

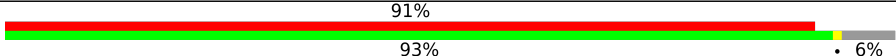
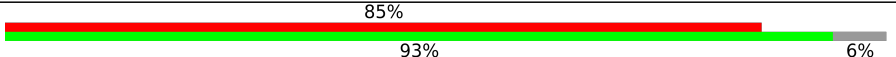
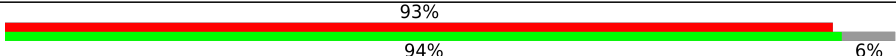
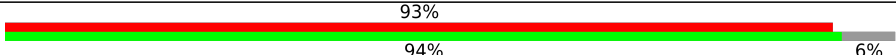
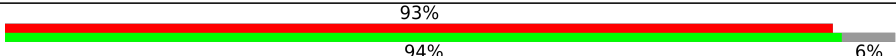
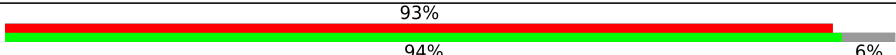
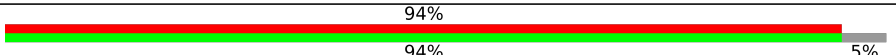
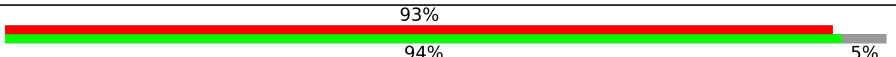
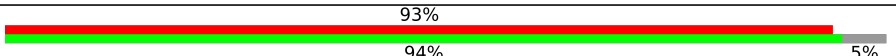
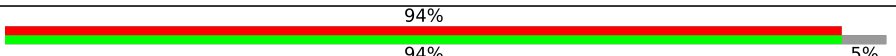
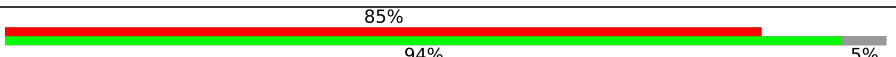
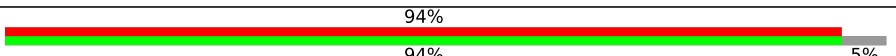
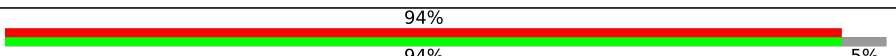
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15 | p3 | 152 | |
| 16 | Q | 152 | |
| 16 | Q3 | 152 | |
| 16 | q | 152 | |
| 16 | q3 | 152 | |
| 17 | R | 149 | |
| 17 | R3 | 149 | |
| 17 | r | 149 | |
| 17 | r3 | 149 | |
| 18 | S | 145 | |
| 18 | S3 | 145 | |
| 18 | s | 145 | |
| 18 | s3 | 145 | |
| 19 | E | 480 | |
| 19 | E3 | 480 | |
| 19 | e | 480 | |
| 19 | e3 | 480 | |
| 20 | i1 | 108 | |
| 20 | i2 | 108 | |
| 20 | i4 | 108 | |
| 20 | i5 | 108 | |
| 21 | t | 460 | |
| 21 | t3 | 460 | |
| 22 | G1 | 219 | |
| 22 | G2 | 219 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---------------------------------------------------------------------------------------------|
| 22 | G4 | 219 | 86%  |
| 22 | G5 | 219 | 86%  |
| 23 | g1 | 299 | 75%  |
| 23 | g2 | 299 | 71%  |
| 23 | g4 | 299 | 70%  |
| 23 | g5 | 299 | 74%  |
| 24 | A1 | 546 | 80%  |
| 24 | A2 | 546 | 90%  |
| 24 | A4 | 546 | 89%  |
| 24 | A5 | 546 | 79%  |
| 24 | B1 | 546 | 86%  |
| 24 | B2 | 546 | 91%  |
| 24 | B4 | 546 | 91%  |
| 24 | B5 | 546 | 85%  |
| 24 | C1 | 546 | 93%  |
| 24 | C2 | 546 | 93%  |
| 24 | C4 | 546 | 93%  |
| 24 | C5 | 546 | 93%  |
| 25 | D1 | 497 | 94%  |
| 25 | D2 | 497 | 93%  |
| 25 | D4 | 497 | 93%  |
| 25 | D5 | 497 | 94%  |
| 25 | E1 | 497 | 85%  |
| 25 | E2 | 497 | 94%  |
| 25 | E4 | 497 | 94%  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 25 | E5 | 497 | 86% 94% 5% |
| 25 | F1 | 497 | 91% 94% 6% |
| 25 | F2 | 497 | 91% 94% 6% |
| 25 | F4 | 497 | 92% 94% 6% |
| 25 | F5 | 497 | 91% 94% 6% |
| 26 | H1 | 76 | 9% 99% . |
| 26 | H2 | 76 | 5% 99% . |
| 26 | H4 | 76 | 7% 99% . |
| 26 | H5 | 76 | 9% 99% . |
| 26 | I1 | 76 | 14% 96% .. |
| 26 | I2 | 76 | . 99% . |
| 26 | I4 | 76 | 5% 96% .. |
| 26 | I5 | 76 | 14% 99% . |
| 26 | J1 | 76 | 24% 99% . |
| 26 | J2 | 76 | 8% 99% . |
| 26 | J4 | 76 | 8% 99% . |
| 26 | J5 | 76 | 26% 99% . |
| 26 | K1 | 76 | 32% 99% . |
| 26 | K2 | 76 | 13% 97% .. |
| 26 | K4 | 76 | 14% 99% . |
| 26 | K5 | 76 | 33% 97% .. |
| 26 | L1 | 76 | 30% 99% . |
| 26 | L2 | 76 | 12% 99% . |
| 26 | L4 | 76 | 12% 99% . |
| 26 | L5 | 76 | 30% 99% . |

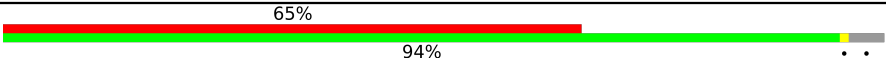
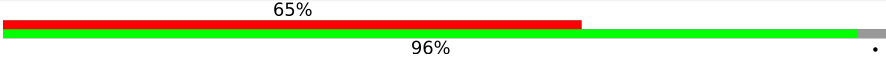
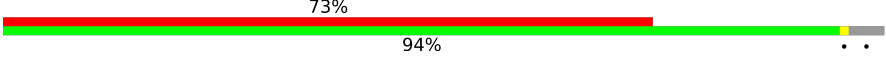
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|-----------------------------------------------------------|
| 26 | M1 | 76 | <div> <div>24%</div> <div>99%</div> </div> |
| 26 | M2 | 76 | <div> <div>9%</div> <div>99%</div> </div> |
| 26 | M4 | 76 | <div> <div>9%</div> <div>99%</div> </div> |
| 26 | M5 | 76 | <div> <div>24%</div> <div>99%</div> </div> |
| 26 | N1 | 76 | <div> <div>21%</div> <div>99%</div> </div> |
| 26 | N2 | 76 | <div> <div>11%</div> <div>99%</div> </div> |
| 26 | N4 | 76 | <div> <div>11%</div> <div>99%</div> </div> |
| 26 | N5 | 76 | <div> <div>20%</div> <div>99%</div> </div> |
| 26 | O1 | 76 | <div> <div>28%</div> <div>99%</div> </div> |
| 26 | O2 | 76 | <div> <div>12%</div> <div>99%</div> </div> |
| 26 | O4 | 76 | <div> <div>11%</div> <div>99%</div> </div> |
| 26 | O5 | 76 | <div> <div>22%</div> <div>99%</div> </div> |
| 26 | P1 | 76 | <div> <div>11%</div> <div>99%</div> </div> |
| 26 | P2 | 76 | <div> <div>12%</div> <div>99%</div> </div> |
| 26 | P4 | 76 | <div> <div>13%</div> <div>99%</div> </div> |
| 26 | P5 | 76 | <div> <div>12%</div> <div>99%</div> </div> |
| 26 | Q1 | 76 | <div> <div>9%</div> <div>99%</div> </div> |
| 26 | Q2 | 76 | <div> <div>5%</div> <div>99%</div> </div> |
| 26 | Q4 | 76 | <div> <div>7%</div> <div>99%</div> </div> |
| 26 | Q5 | 76 | <div> <div>12%</div> <div>99%</div> </div> |
| 27 | d1 | 158 | <div> <div>51%</div> <div>84%</div> <div>15%</div> </div> |
| 27 | d2 | 158 | <div> <div>45%</div> <div>84%</div> <div>15%</div> </div> |
| 27 | d4 | 158 | <div> <div>47%</div> <div>84%</div> <div>15%</div> </div> |
| 27 | d5 | 158 | <div> <div>51%</div> <div>84%</div> <div>15%</div> </div> |
| 28 | e1 | 71 | <div> <div>73%</div> <div>96%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---------------------------------------------------------------------------------------------------|
| 28 | e2 | 71 |  65% 94% . . |
| 28 | e4 | 71 |  65% 96% . |
| 28 | e5 | 71 |  73% 94% . . |

2 Entry composition [i](#)

There are 37 unique types of molecules in this entry. The entry contains 571866 atoms, of which 287810 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 Ymf66.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 1 | a | 433 | Total | C | H | N | O | S | 0 | 0 |
| | | | 7155 | 2453 | 3527 | 526 | 633 | 16 | | |
| 1 | A | 433 | Total | C | H | N | O | S | 0 | 0 |
| | | | 7157 | 2453 | 3529 | 526 | 633 | 16 | | |
| 1 | a3 | 433 | Total | C | H | N | O | S | 0 | 0 |
| | | | 7155 | 2453 | 3527 | 526 | 633 | 16 | | |
| 1 | A3 | 433 | Total | C | H | N | O | S | 0 | 0 |
| | | | 7157 | 2453 | 3529 | 526 | 633 | 16 | | |

- Molecule 2 is a protein called subunit b.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 2 | b | 354 | Total | C | H | N | O | S | 0 | 0 |
| | | | 5726 | 1845 | 2851 | 487 | 531 | 12 | | |
| 2 | B | 354 | Total | C | H | N | O | S | 0 | 0 |
| | | | 5724 | 1845 | 2849 | 487 | 531 | 12 | | |
| 2 | b3 | 354 | Total | C | H | N | O | S | 0 | 0 |
| | | | 5726 | 1845 | 2851 | 487 | 531 | 12 | | |
| 2 | B3 | 354 | Total | C | H | N | O | S | 0 | 0 |
| | | | 5724 | 1845 | 2849 | 487 | 531 | 12 | | |

- Molecule 3 is a protein called subunit d.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 3 | d | 206 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3274 | 1065 | 1598 | 274 | 332 | 5 | | |
| 3 | D | 206 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3274 | 1065 | 1598 | 274 | 332 | 5 | | |
| 3 | d3 | 206 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3274 | 1065 | 1598 | 274 | 332 | 5 | | |
| 3 | D3 | 206 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3274 | 1065 | 1598 | 274 | 332 | 5 | | |

- Molecule 4 is a protein called subunit f.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 4 | f | 200 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3373 | 1095 | 1691 | 299 | 278 | 10 | | |
| 4 | F | 200 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3374 | 1095 | 1692 | 299 | 278 | 10 | | |
| 4 | f3 | 200 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3373 | 1095 | 1691 | 299 | 278 | 10 | | |
| 4 | F3 | 200 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3374 | 1095 | 1692 | 299 | 278 | 10 | | |

- Molecule 5 is a protein called subunit i/j.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 5 | i | 209 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3462 | 1121 | 1742 | 304 | 285 | 10 | | |
| 5 | I | 209 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3460 | 1121 | 1740 | 304 | 285 | 10 | | |
| 5 | i3 | 209 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3462 | 1121 | 1742 | 304 | 285 | 10 | | |
| 5 | I3 | 209 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3460 | 1121 | 1740 | 304 | 285 | 10 | | |

- Molecule 6 is a protein called subunit k.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|----|---------|-------|
| 6 | k | 179 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2902 | 939 | 1429 | 257 | 266 | 11 | | |
| 6 | K | 179 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2903 | 939 | 1430 | 257 | 266 | 11 | | |
| 6 | k3 | 179 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2902 | 939 | 1429 | 257 | 266 | 11 | | |
| 6 | K3 | 179 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2903 | 939 | 1430 | 257 | 266 | 11 | | |

- Molecule 7 is a protein called Ymf56.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 7 | c | 96 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1671 | 565 | 830 | 131 | 143 | 2 | | |
| 7 | C | 96 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1671 | 565 | 830 | 131 | 143 | 2 | | |
| 7 | c3 | 96 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1671 | 565 | 830 | 131 | 143 | 2 | | |

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| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 7 | C3 | 96 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1671 | 565 | 830 | 131 | 143 | 2 | | |

- Molecule 8 is a protein called ATPTT3.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 8 | g | 256 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4338 | 1474 | 2118 | 348 | 388 | 10 | | |
| 8 | G | 256 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4338 | 1474 | 2118 | 348 | 388 | 10 | | |
| 8 | g3 | 256 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4338 | 1474 | 2118 | 348 | 388 | 10 | | |
| 8 | G3 | 256 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4338 | 1474 | 2118 | 348 | 388 | 10 | | |

- Molecule 9 is a protein called ATPTT4.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 9 | h | 231 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3836 | 1236 | 1883 | 361 | 350 | 6 | | |
| 9 | H | 231 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3836 | 1236 | 1883 | 361 | 350 | 6 | | |
| 9 | h3 | 231 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3836 | 1236 | 1883 | 361 | 350 | 6 | | |
| 9 | H3 | 231 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3836 | 1236 | 1883 | 361 | 350 | 6 | | |

- Molecule 10 is a protein called ATPTT5.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 10 | j | 269 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4346 | 1381 | 2147 | 406 | 404 | 8 | | |
| 10 | J | 269 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4346 | 1381 | 2147 | 406 | 404 | 8 | | |
| 10 | j3 | 269 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4346 | 1381 | 2147 | 406 | 404 | 8 | | |
| 10 | J3 | 269 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4346 | 1381 | 2147 | 406 | 404 | 8 | | |

- Molecule 11 is a protein called ATPTT6.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 11 | l | 246 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4070 | 1344 | 1999 | 360 | 361 | 6 | | |
| 11 | L | 246 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4070 | 1344 | 1999 | 360 | 361 | 6 | | |
| 11 | l3 | 246 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4070 | 1344 | 1999 | 360 | 361 | 6 | | |
| 11 | L3 | 246 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4070 | 1344 | 1999 | 360 | 361 | 6 | | |

- Molecule 12 is a protein called ATPTT7.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 12 | m | 221 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3696 | 1205 | 1835 | 313 | 336 | 7 | | |
| 12 | M | 221 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3696 | 1205 | 1835 | 313 | 336 | 7 | | |
| 12 | m3 | 221 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3696 | 1205 | 1835 | 313 | 336 | 7 | | |
| 12 | M3 | 221 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3696 | 1205 | 1835 | 313 | 336 | 7 | | |

- Molecule 13 is a protein called ATPTT8.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 13 | n | 119 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1960 | 655 | 962 | 164 | 173 | 6 | | |
| 13 | N | 119 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1960 | 655 | 962 | 164 | 173 | 6 | | |
| 13 | n3 | 119 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1960 | 655 | 962 | 164 | 173 | 6 | | |
| 13 | N3 | 119 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1960 | 655 | 962 | 164 | 173 | 6 | | |

- Molecule 14 is a protein called ATPTT9.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 14 | o | 99 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1599 | 507 | 794 | 145 | 147 | 6 | | |
| 14 | O | 99 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1599 | 507 | 794 | 145 | 147 | 6 | | |
| 14 | o3 | 99 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1599 | 507 | 794 | 145 | 147 | 6 | | |

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| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 14 | O3 | 99 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1599 | 507 | 794 | 145 | 147 | 6 | | |

- Molecule 15 is a protein called ATPTT10.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 15 | p | 150 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2413 | 788 | 1196 | 204 | 224 | 1 | | |
| 15 | P | 150 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2413 | 788 | 1196 | 204 | 224 | 1 | | |
| 15 | p3 | 150 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2413 | 788 | 1196 | 204 | 224 | 1 | | |
| 15 | P3 | 150 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2413 | 788 | 1196 | 204 | 224 | 1 | | |

- Molecule 16 is a protein called ATPTT11.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 16 | q | 108 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1749 | 556 | 874 | 149 | 169 | 1 | | |
| 16 | Q | 108 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1749 | 556 | 874 | 149 | 169 | 1 | | |
| 16 | q3 | 108 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1749 | 556 | 874 | 149 | 169 | 1 | | |
| 16 | Q3 | 108 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1749 | 556 | 874 | 149 | 169 | 1 | | |

- Molecule 17 is a protein called ATPTT12.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 17 | r | 145 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2373 | 776 | 1180 | 201 | 212 | 4 | | |
| 17 | R | 140 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2288 | 750 | 1134 | 194 | 206 | 4 | | |
| 17 | r3 | 145 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2373 | 776 | 1180 | 201 | 212 | 4 | | |
| 17 | R3 | 140 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2288 | 750 | 1134 | 194 | 206 | 4 | | |

- Molecule 18 is a protein called ATPTT13.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 18 | s | 124 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2025 | 648 | 1009 | 174 | 189 | 5 | | |
| 18 | S | 125 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2039 | 652 | 1016 | 175 | 191 | 5 | | |
| 18 | s3 | 124 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2025 | 648 | 1009 | 174 | 189 | 5 | | |
| 18 | S3 | 125 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2039 | 652 | 1016 | 175 | 191 | 5 | | |

- Molecule 19 is a protein called ATPTT1.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 19 | e | 417 | Total | C | H | N | O | S | 0 | 0 |
| | | | 6681 | 2171 | 3286 | 602 | 614 | 8 | | |
| 19 | E | 417 | Total | C | H | N | O | S | 0 | 0 |
| | | | 6681 | 2171 | 3286 | 602 | 614 | 8 | | |
| 19 | e3 | 417 | Total | C | H | N | O | S | 0 | 0 |
| | | | 6681 | 2171 | 3286 | 602 | 614 | 8 | | |
| 19 | E3 | 417 | Total | C | H | N | O | S | 0 | 0 |
| | | | 6681 | 2171 | 3286 | 602 | 614 | 8 | | |

- Molecule 20 is a protein called Inhibitor of F1 (IF1).

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 20 | i2 | 64 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1112 | 351 | 556 | 97 | 107 | 1 | | |
| 20 | i1 | 68 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1167 | 368 | 582 | 103 | 113 | 1 | | |
| 20 | i5 | 64 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1112 | 351 | 556 | 97 | 107 | 1 | | |
| 20 | i4 | 68 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1167 | 368 | 582 | 103 | 113 | 1 | | |

- Molecule 21 is a protein called ATPTT2.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 21 | t | 365 | Total | C | H | N | O | S | 0 | 0 |
| | | | 5889 | 1925 | 2876 | 533 | 544 | 11 | | |
| 21 | t3 | 365 | Total | C | H | N | O | S | 0 | 0 |
| | | | 5889 | 1925 | 2876 | 533 | 544 | 11 | | |

- Molecule 22 is a protein called Oligomycin sensitivity-conferring protein (OSCP).

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 22 | G1 | 188 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3000 | 942 | 1515 | 252 | 287 | 4 | | |
| 22 | G2 | 188 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3000 | 942 | 1515 | 252 | 287 | 4 | | |
| 22 | G4 | 188 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3000 | 942 | 1515 | 252 | 287 | 4 | | |
| 22 | G5 | 188 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3000 | 942 | 1515 | 252 | 287 | 4 | | |

- Molecule 23 is a protein called ATP synthase subunit gamma.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 23 | g1 | 275 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4332 | 1343 | 2206 | 373 | 400 | 10 | | |
| 23 | g2 | 275 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4332 | 1343 | 2206 | 373 | 400 | 10 | | |
| 23 | g4 | 275 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4332 | 1343 | 2206 | 373 | 400 | 10 | | |
| 23 | g5 | 275 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4332 | 1343 | 2206 | 373 | 400 | 10 | | |

- Molecule 24 is a protein called ATP synthase subunit alpha.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 24 | C1 | 513 | Total | C | H | N | O | S | 0 | 0 |
| | | | 7980 | 2481 | 4058 | 685 | 739 | 17 | | |
| 24 | B1 | 511 | Total | C | H | N | O | S | 0 | 0 |
| | | | 7934 | 2469 | 4030 | 681 | 737 | 17 | | |
| 24 | A1 | 512 | Total | C | H | N | O | S | 0 | 0 |
| | | | 7946 | 2472 | 4037 | 682 | 738 | 17 | | |
| 24 | C2 | 513 | Total | C | H | N | O | S | 0 | 0 |
| | | | 7980 | 2481 | 4058 | 685 | 739 | 17 | | |
| 24 | B2 | 511 | Total | C | H | N | O | S | 0 | 0 |
| | | | 7934 | 2469 | 4030 | 681 | 737 | 17 | | |
| 24 | A2 | 512 | Total | C | H | N | O | S | 0 | 0 |
| | | | 7946 | 2472 | 4037 | 682 | 738 | 17 | | |
| 24 | C4 | 513 | Total | C | H | N | O | S | 0 | 0 |
| | | | 7980 | 2481 | 4058 | 685 | 739 | 17 | | |
| 24 | B4 | 511 | Total | C | H | N | O | S | 0 | 0 |
| | | | 7934 | 2469 | 4030 | 681 | 737 | 17 | | |
| 24 | A4 | 512 | Total | C | H | N | O | S | 0 | 0 |
| | | | 7946 | 2472 | 4037 | 682 | 738 | 17 | | |
| 24 | C5 | 513 | Total | C | H | N | O | S | 0 | 0 |
| | | | 7980 | 2481 | 4058 | 685 | 739 | 17 | | |

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| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 24 | B5 | 511 | Total | C | H | N | O | S | 0 | 0 |
| | | | 7934 | 2469 | 4030 | 681 | 737 | 17 | | |
| 24 | A5 | 512 | Total | C | H | N | O | S | 0 | 0 |
| | | | 7946 | 2472 | 4037 | 682 | 738 | 17 | | |

- Molecule 25 is a protein called ATP synthase subunit beta.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 25 | D1 | 470 | Total | C | H | N | O | S | 0 | 0 |
| | | | 7135 | 2243 | 3581 | 612 | 688 | 11 | | |
| 25 | F1 | 469 | Total | C | H | N | O | S | 0 | 0 |
| | | | 7113 | 2237 | 3568 | 610 | 687 | 11 | | |
| 25 | E1 | 470 | Total | C | H | N | O | S | 0 | 0 |
| | | | 7135 | 2243 | 3581 | 612 | 688 | 11 | | |
| 25 | D2 | 470 | Total | C | H | N | O | S | 0 | 0 |
| | | | 7135 | 2243 | 3581 | 612 | 688 | 11 | | |
| 25 | F2 | 469 | Total | C | H | N | O | S | 0 | 0 |
| | | | 7113 | 2237 | 3568 | 610 | 687 | 11 | | |
| 25 | E2 | 470 | Total | C | H | N | O | S | 0 | 0 |
| | | | 7135 | 2243 | 3581 | 612 | 688 | 11 | | |
| 25 | D4 | 470 | Total | C | H | N | O | S | 0 | 0 |
| | | | 7135 | 2243 | 3581 | 612 | 688 | 11 | | |
| 25 | F4 | 469 | Total | C | H | N | O | S | 0 | 0 |
| | | | 7113 | 2237 | 3568 | 610 | 687 | 11 | | |
| 25 | E4 | 470 | Total | C | H | N | O | S | 0 | 0 |
| | | | 7135 | 2243 | 3581 | 612 | 688 | 11 | | |
| 25 | D5 | 470 | Total | C | H | N | O | S | 0 | 0 |
| | | | 7135 | 2243 | 3581 | 612 | 688 | 11 | | |
| 25 | F5 | 469 | Total | C | H | N | O | S | 0 | 0 |
| | | | 7113 | 2237 | 3568 | 610 | 687 | 11 | | |
| 25 | E5 | 470 | Total | C | H | N | O | S | 0 | 0 |
| | | | 7135 | 2243 | 3581 | 612 | 688 | 11 | | |

- Molecule 26 is a protein called ATP synthase F0 subunit 9.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 26 | P1 | 75 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1148 | 377 | 587 | 84 | 94 | 6 | | |
| 26 | O1 | 75 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1148 | 377 | 587 | 84 | 94 | 6 | | |
| 26 | N1 | 75 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1148 | 377 | 587 | 84 | 94 | 6 | | |

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| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|---------|---------|--------|---------|-------|
| 26 | M1 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | L1 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | K1 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | J1 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | I1 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | H1 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | Q1 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | P2 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | O2 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | N2 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | M2 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | L2 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | K2 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | J2 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | I2 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | H2 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | Q2 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | P4 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | O4 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | N4 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | M4 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|---------|---------|--------|---------|-------|
| 26 | L4 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | K4 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | J4 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | I4 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | H4 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | Q4 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | P5 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | O5 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | N5 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | M5 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | L5 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | K5 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | J5 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | I5 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | H5 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |
| 26 | Q5 | 75 | Total 1148 | C 377 | H 587 | N 84 | O 94 | S 6 | 0 | 0 |

- Molecule 27 is a protein called subunit delta.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 27 | d1 | 134 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2144 | 674 | 1082 | 185 | 200 | 3 | | |
| 27 | d2 | 134 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2144 | 674 | 1082 | 185 | 200 | 3 | | |
| 27 | d4 | 134 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2144 | 674 | 1082 | 185 | 200 | 3 | | |

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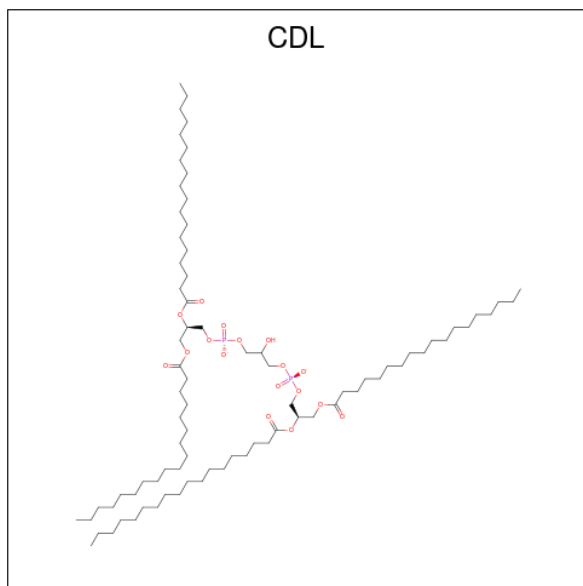
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| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 27 | d5 | 134 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2144 | 674 | 1082 | 185 | 200 | 3 | | |

- Molecule 28 is a protein called subunit epsilon.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 28 | e1 | 68 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1096 | 347 | 559 | 94 | 95 | 1 | | |
| 28 | e2 | 68 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1096 | 347 | 559 | 94 | 95 | 1 | | |
| 28 | e4 | 68 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1096 | 347 | 559 | 94 | 95 | 1 | | |
| 28 | e5 | 68 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1096 | 347 | 559 | 94 | 95 | 1 | | |

- Molecule 29 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|-----|----|---|---------|
| 29 | a | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 29 | b | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 29 | f | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 29 | f | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|--------------|---------|----------|---------|--------|---------|
| 29 | f | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | i | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | k | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | g | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | j | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | j | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | l | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | l | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | p | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | r | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | A | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | B | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | B | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | B | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | B | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | F | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | F | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | I | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | I | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | K | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | K | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |

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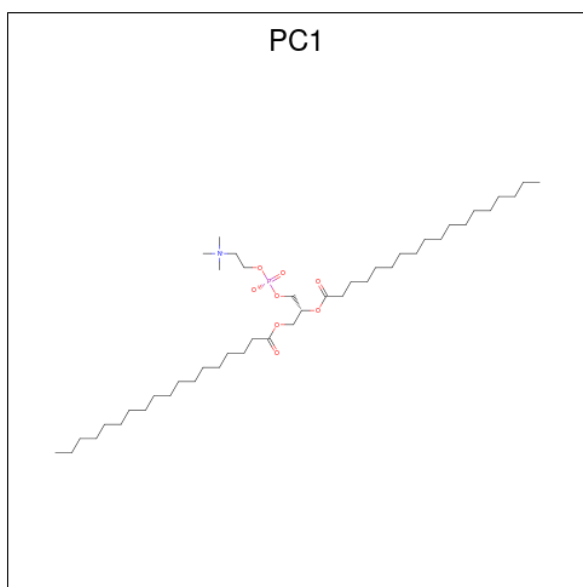
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|--------------|---------|----------|---------|--------|---------|
| 29 | J | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | J | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | L | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | L | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | P | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | a3 | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | a3 | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | b3 | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | f3 | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | f3 | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | f3 | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | f3 | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | i3 | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | i3 | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | k3 | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | g3 | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | j3 | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | j3 | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | l3 | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | l3 | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | p3 | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | A3 | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|--------------|---------|----------|---------|--------|---------|
| 29 | B3 | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | B3 | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | B3 | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | B3 | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | F3 | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | I3 | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | I3 | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | I3 | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | K3 | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | K3 | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | J3 | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | J3 | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | L3 | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |
| 29 | P3 | 1 | Total 256 | C 81 | H 156 | O 17 | P 2 | 0 |

- Molecule 30 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



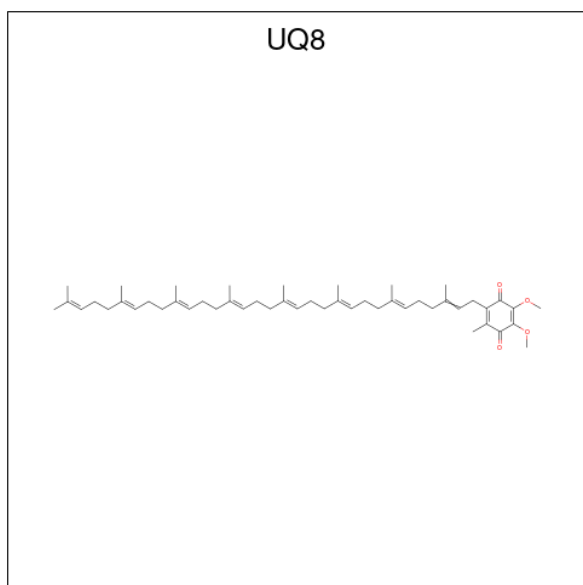
| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---|---------|
| 30 | d | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 30 | g | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 30 | g | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 30 | D | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 30 | G | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 30 | G | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 30 | d3 | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 30 | g3 | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 30 | g3 | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 30 | D3 | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 30 | G3 | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 30 | G3 | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |

- Molecule 31 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



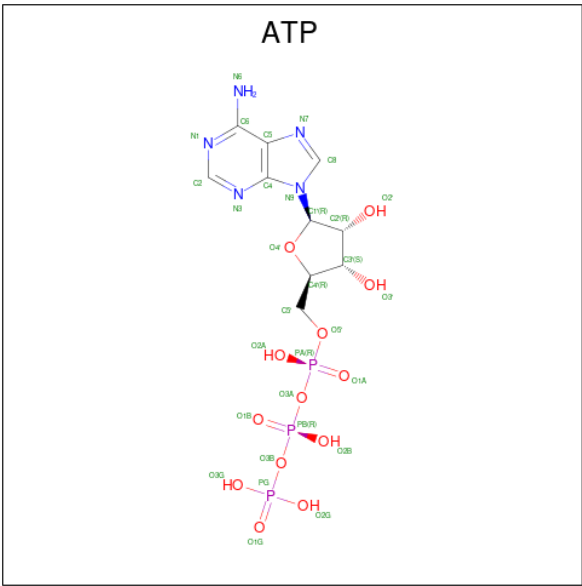
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 31 | f | 1 | Total | O | P | 0 |
| | | | 5 | 4 | 1 | |
| 31 | F | 1 | Total | O | P | 0 |
| | | | 5 | 4 | 1 | |
| 31 | f3 | 1 | Total | O | P | 0 |
| | | | 5 | 4 | 1 | |
| 31 | F3 | 1 | Total | O | P | 0 |
| | | | 5 | 4 | 1 | |

- Molecule 32 is Ubiquinone-8 (CCD ID: UQ8) (formula: C₄₉H₇₄O₄).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 32 | i | 1 | Total | C | H | O | 0 |
| | | | 127 | 49 | 74 | 4 | |
| 32 | I | 1 | Total | C | H | O | 0 |
| | | | 127 | 49 | 74 | 4 | |
| 32 | i3 | 1 | Total | C | H | O | 0 |
| | | | 127 | 49 | 74 | 4 | |
| 32 | I3 | 1 | Total | C | H | O | 0 |
| | | | 127 | 49 | 74 | 4 | |

- Molecule 33 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|----|---|---------|
| 33 | g | 1 | Total | C | H | N | O | P | 0 |
| | | | 42 | 10 | 11 | 5 | 13 | 3 | |
| 33 | G | 1 | Total | C | H | N | O | P | 0 |
| | | | 42 | 10 | 11 | 5 | 13 | 3 | |
| 33 | C1 | 1 | Total | C | H | N | O | P | 0 |
| | | | 42 | 10 | 11 | 5 | 13 | 3 | |
| 33 | B1 | 1 | Total | C | H | N | O | P | 0 |
| | | | 42 | 10 | 11 | 5 | 13 | 3 | |
| 33 | A1 | 1 | Total | C | H | N | O | P | 0 |
| | | | 42 | 10 | 11 | 5 | 13 | 3 | |
| 33 | C2 | 1 | Total | C | H | N | O | P | 0 |
| | | | 42 | 10 | 11 | 5 | 13 | 3 | |
| 33 | B2 | 1 | Total | C | H | N | O | P | 0 |
| | | | 42 | 10 | 11 | 5 | 13 | 3 | |
| 33 | A2 | 1 | Total | C | H | N | O | P | 0 |
| | | | 42 | 10 | 11 | 5 | 13 | 3 | |

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| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|--------|---------|
| 33 | g3 | 1 | Total 42 | C 10 | H 11 | N 5 | O 13 | P 3 | 0 |
| 33 | G3 | 1 | Total 42 | C 10 | H 11 | N 5 | O 13 | P 3 | 0 |
| 33 | C4 | 1 | Total 42 | C 10 | H 11 | N 5 | O 13 | P 3 | 0 |
| 33 | B4 | 1 | Total 42 | C 10 | H 11 | N 5 | O 13 | P 3 | 0 |
| 33 | A4 | 1 | Total 42 | C 10 | H 11 | N 5 | O 13 | P 3 | 0 |
| 33 | C5 | 1 | Total 42 | C 10 | H 11 | N 5 | O 13 | P 3 | 0 |
| 33 | B5 | 1 | Total 42 | C 10 | H 11 | N 5 | O 13 | P 3 | 0 |
| 33 | A5 | 1 | Total 42 | C 10 | H 11 | N 5 | O 13 | P 3 | 0 |

- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

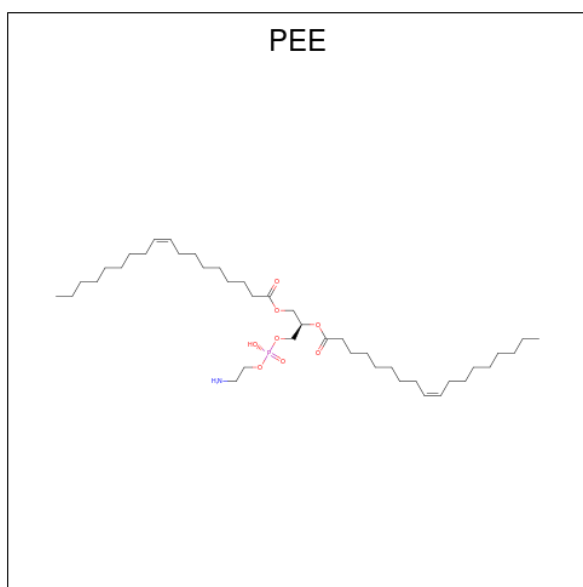
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|---------|---------|
| 34 | g | 1 | Total 1 | Mg 1 | 0 |
| 34 | G | 1 | Total 1 | Mg 1 | 0 |
| 34 | C1 | 1 | Total 1 | Mg 1 | 0 |
| 34 | D1 | 1 | Total 1 | Mg 1 | 0 |
| 34 | B1 | 1 | Total 1 | Mg 1 | 0 |
| 34 | A1 | 1 | Total 1 | Mg 1 | 0 |
| 34 | E1 | 1 | Total 1 | Mg 1 | 0 |
| 34 | C2 | 1 | Total 1 | Mg 1 | 0 |
| 34 | D2 | 1 | Total 1 | Mg 1 | 0 |
| 34 | B2 | 1 | Total 1 | Mg 1 | 0 |
| 34 | A2 | 1 | Total 1 | Mg 1 | 0 |

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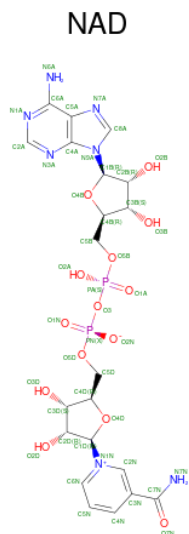
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|---------|---------|
| 34 | E2 | 1 | Total 1 | Mg 1 | 0 |
| 34 | g3 | 1 | Total 1 | Mg 1 | 0 |
| 34 | G3 | 1 | Total 1 | Mg 1 | 0 |
| 34 | C4 | 1 | Total 1 | Mg 1 | 0 |
| 34 | D4 | 1 | Total 1 | Mg 1 | 0 |
| 34 | B4 | 1 | Total 1 | Mg 1 | 0 |
| 34 | A4 | 1 | Total 1 | Mg 1 | 0 |
| 34 | E4 | 1 | Total 1 | Mg 1 | 0 |
| 34 | C5 | 1 | Total 1 | Mg 1 | 0 |
| 34 | D5 | 1 | Total 1 | Mg 1 | 0 |
| 34 | B5 | 1 | Total 1 | Mg 1 | 0 |
| 34 | A5 | 1 | Total 1 | Mg 1 | 0 |
| 34 | E5 | 1 | Total 1 | Mg 1 | 0 |

- Molecule 35 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



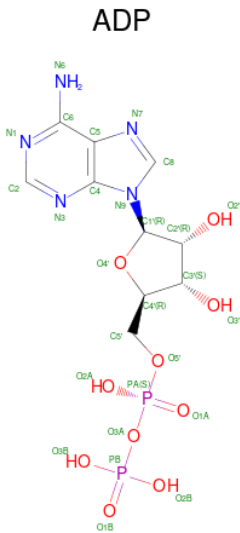
| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---|---------|
| 35 | m | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 35 | A | 1 | Total | C | H | N | O | P | 0 |
| | | | 123 | 38 | 75 | 1 | 8 | 1 | |
| 35 | J | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 35 | L | 1 | Total | C | H | N | O | P | 0 |
| | | | 123 | 38 | 75 | 1 | 8 | 1 | |
| 35 | a3 | 1 | Total | C | H | N | O | P | 0 |
| | | | 123 | 38 | 75 | 1 | 8 | 1 | |
| 35 | j3 | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 35 | l3 | 1 | Total | C | H | N | O | P | 0 |
| | | | 123 | 38 | 75 | 1 | 8 | 1 | |
| 35 | L3 | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |

- Molecule 36 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|--------|---------|
| 36 | e | 1 | Total 70 | C 21 | H 26 | N 7 | O 14 | P 2 | 0 |
| 36 | E | 1 | Total 70 | C 21 | H 26 | N 7 | O 14 | P 2 | 0 |
| 36 | e3 | 1 | Total 70 | C 21 | H 26 | N 7 | O 14 | P 2 | 0 |
| 36 | E3 | 1 | Total 70 | C 21 | H 26 | N 7 | O 14 | P 2 | 0 |

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

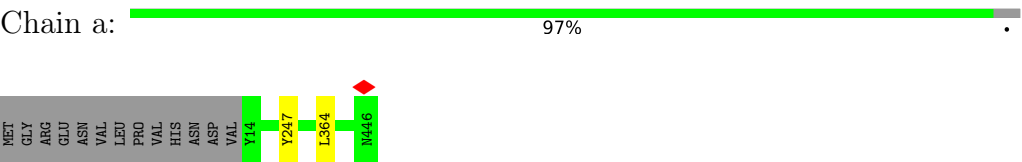


| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|--------|---------|
| 37 | D1 | 1 | Total 38 | C 10 | H 11 | N 5 | O 10 | P 2 | 0 |
| 37 | B1 | 1 | Total 38 | C 10 | H 11 | N 5 | O 10 | P 2 | 0 |
| 37 | D2 | 1 | Total 38 | C 10 | H 11 | N 5 | O 10 | P 2 | 0 |
| 37 | B2 | 1 | Total 38 | C 10 | H 11 | N 5 | O 10 | P 2 | 0 |
| 37 | D4 | 1 | Total 38 | C 10 | H 11 | N 5 | O 10 | P 2 | 0 |
| 37 | B4 | 1 | Total 38 | C 10 | H 11 | N 5 | O 10 | P 2 | 0 |
| 37 | D5 | 1 | Total 38 | C 10 | H 11 | N 5 | O 10 | P 2 | 0 |
| 37 | B5 | 1 | Total 38 | C 10 | H 11 | N 5 | O 10 | P 2 | 0 |

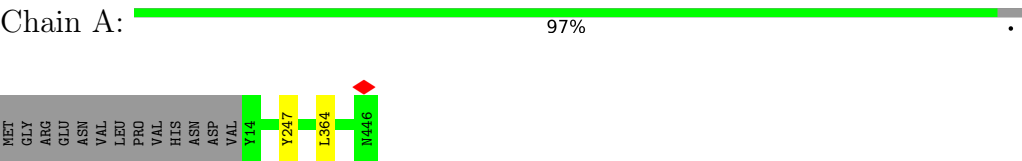
3 Residue-property plots [i](#)

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.

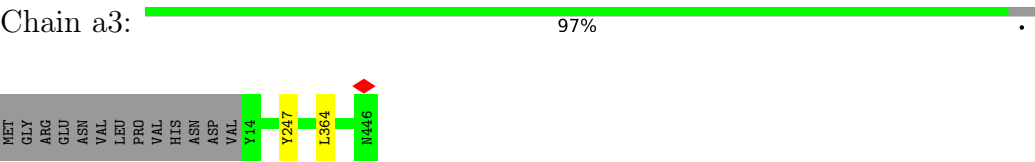
• Molecule 1: Ymf66



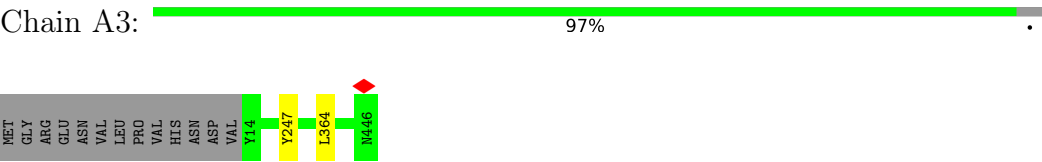
• Molecule 1: Ymf66



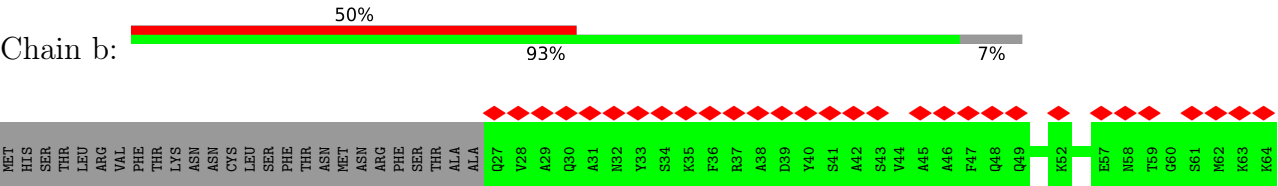
• Molecule 1: Ymf66

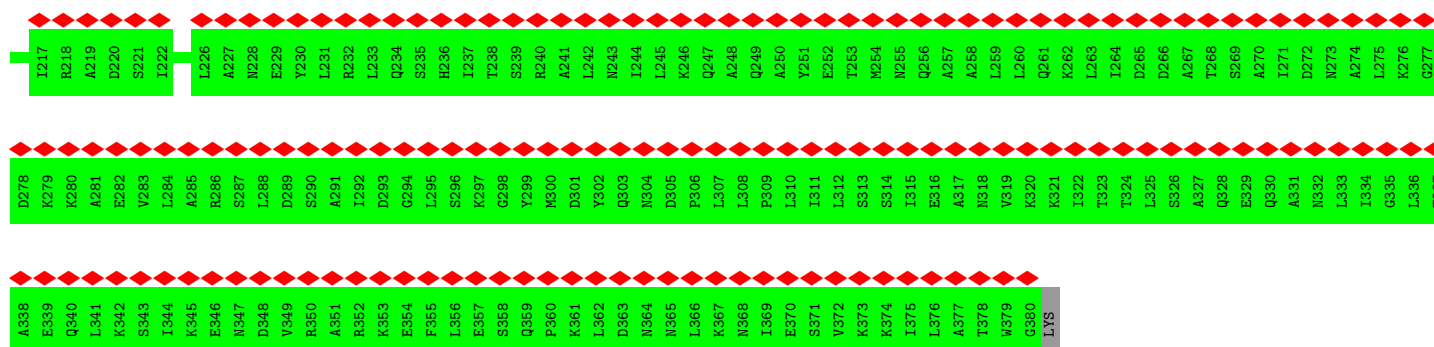


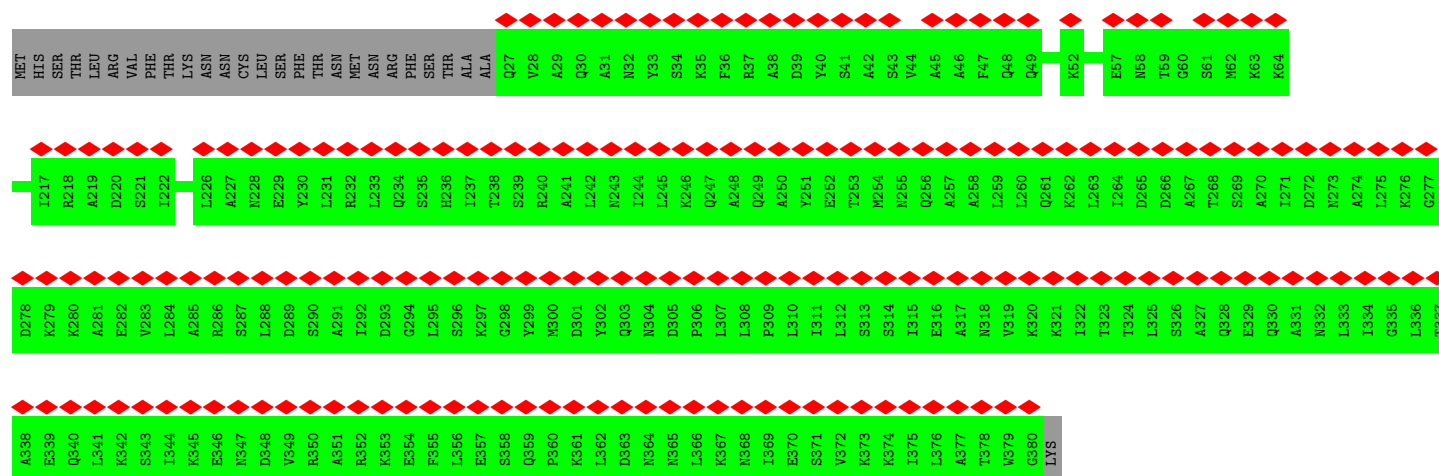
• Molecule 1: Ymf66



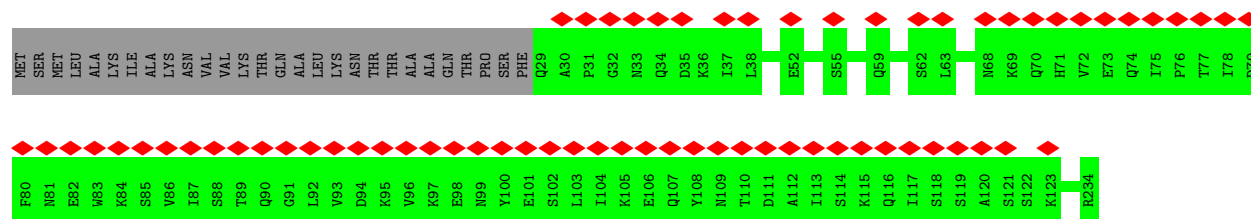
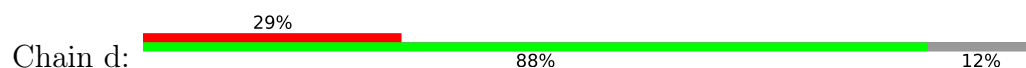
• Molecule 2: subunit b



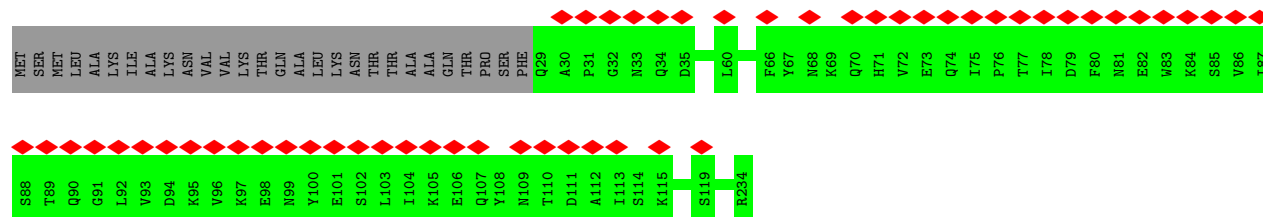
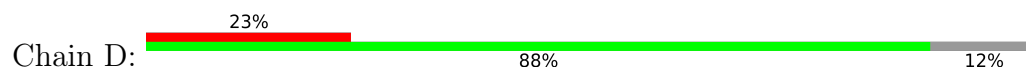




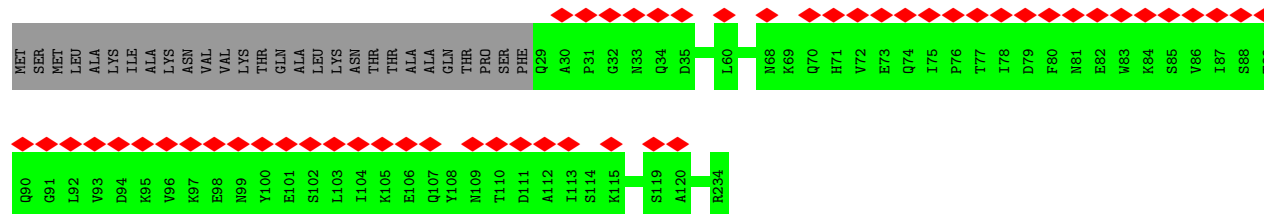
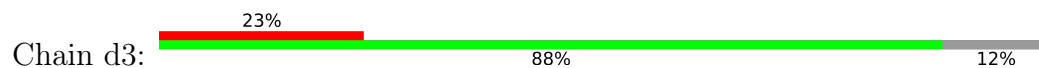
• Molecule 3: subunit d



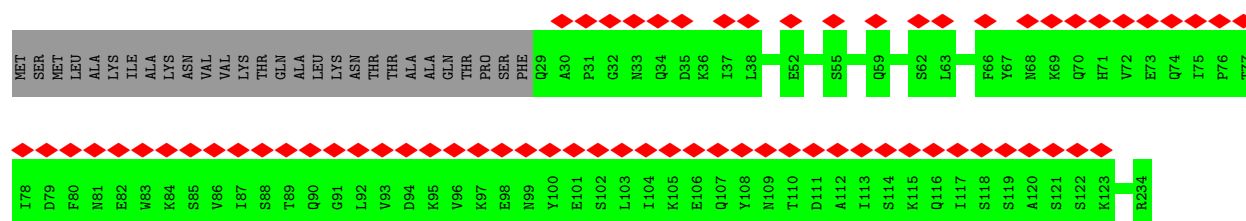
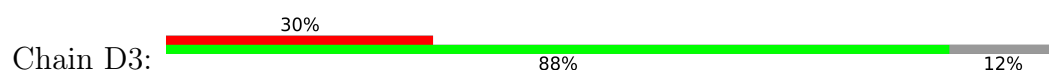
• Molecule 3: subunit d



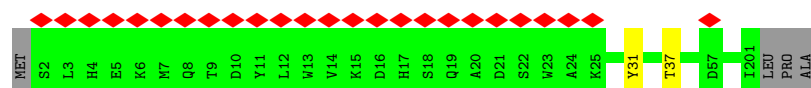
• Molecule 3: subunit d



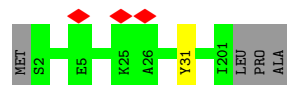
• Molecule 3: subunit d



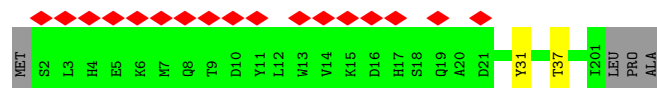
- Molecule 4: subunit f



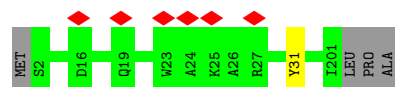
- Molecule 4: subunit f



- Molecule 4: subunit f



- Molecule 4: subunit f

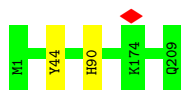


- Molecule 5: subunit i/j

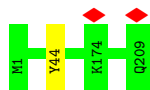


- Molecule 5: subunit i/j





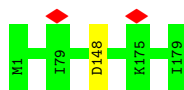
- Molecule 5: subunit i/j



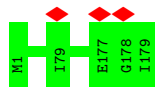
- Molecule 5: subunit i/j



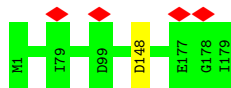
- Molecule 6: subunit k



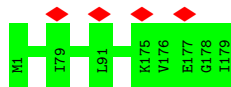
- Molecule 6: subunit k



- Molecule 6: subunit k



- Molecule 6: subunit k



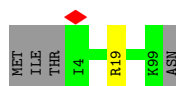
- Molecule 7: Ymf56

Chain c:  95%



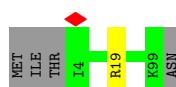
• Molecule 7: Ymf56

Chain C:  95%



• Molecule 7: Ymf56

Chain c3:  95%




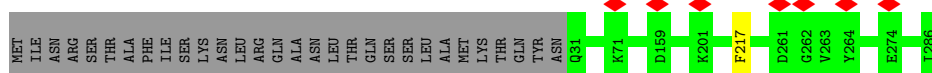
• Molecule 7: Ymf56

Chain C3:  95%



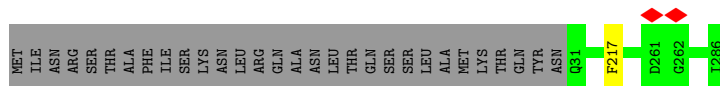
• Molecule 8: ATPTT3

Chain g:  89% 10%




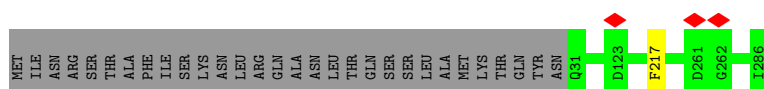
• Molecule 8: ATPTT3

Chain G:  89% 10%

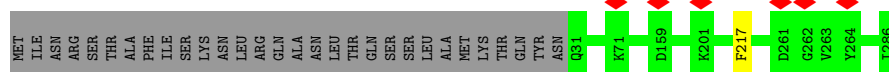
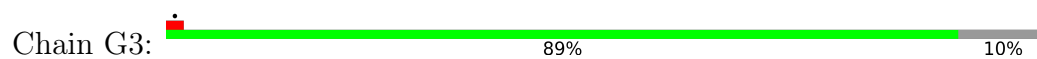


• Molecule 8: ATPTT3

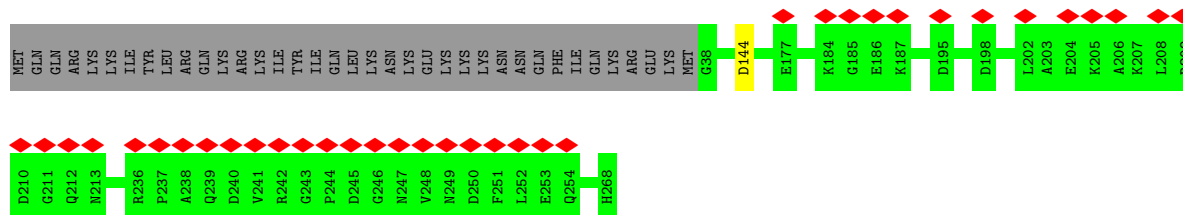
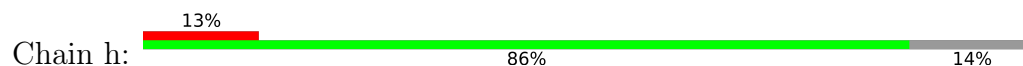
Chain g3:  89% 10%



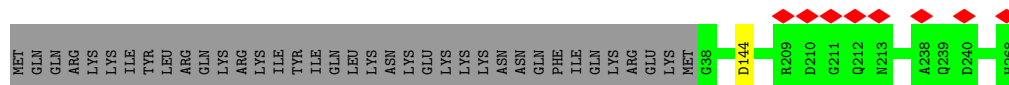
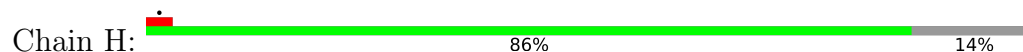
• Molecule 8: ATPTT3



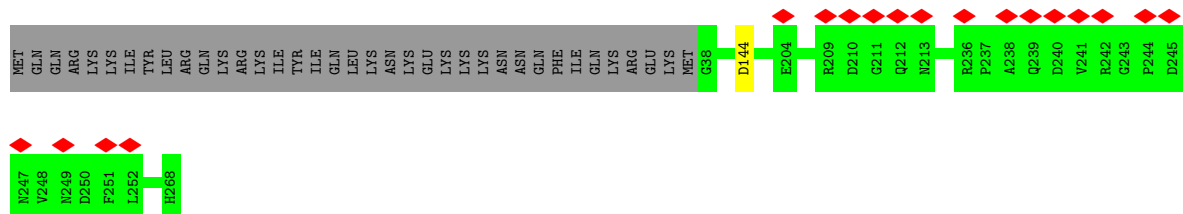
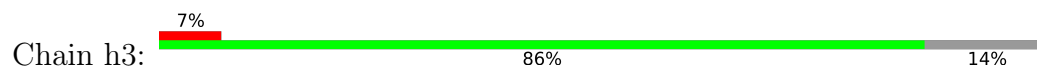
• Molecule 9: ATPTT4



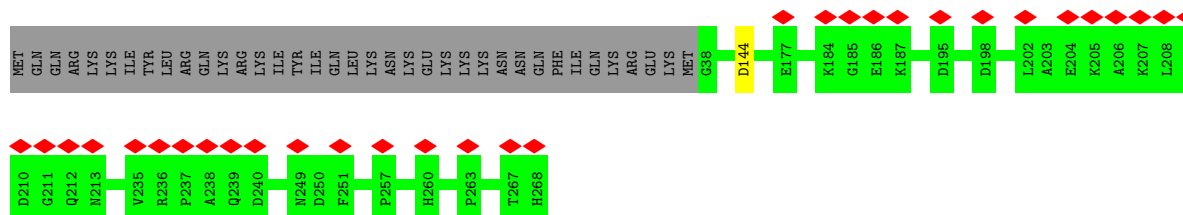
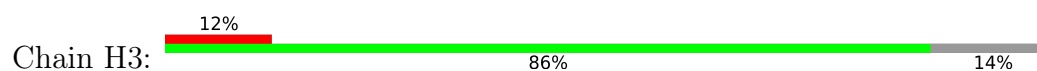
• Molecule 9: ATPTT4



• Molecule 9: ATPTT4

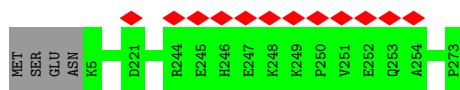


• Molecule 9: ATPTT4

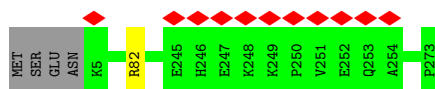


• Molecule 10: ATPTT5

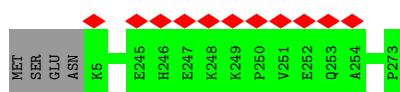




- Molecule 10: ATPTT5



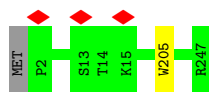
- Molecule 10: ATPTT5



- Molecule 10: ATPTT5



- Molecule 11: ATPTT6



- Molecule 11: ATPTT6



- Molecule 11: ATPTT6



- Molecule 11: ATPTT6



- Molecule 13: ATPTT8

Chain N3:  66% 34%

T61 L179

- Molecule 14: ATPPT9

Chain o:  64% 36%

[illegible]

- Molecule 14: ATPPT9

Chain 0:  64% 36%

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|
| MET | LYS | GLN | GLN | LYS | LYS | ILE | ASN | LYS | LEU | LEU | LYS | LYS | LYS | LYS | GLY | VAL | GLN | ASP | LYS | TYR | TYR | TYR | SER | LYS | ILE | LEU | LEU | LEU | LEU | ASP | GLN | GLU | GLU | GLY | GLY | LYS | LYS | LYS | ARG | ASN | ASN | LYS | LYS | GLY | GLU | LYS | LYS | LYS | LEU | LEU | LEU | GLU | GLU | GLU | M55 | K153 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|

- Molecule 14: ATPTT9

Chain o3: 64% 36%

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Met | Lys | Lys | Gln | Lys | Lys | Asn | Lys | Leu | Leu | Lys | Lys | Asn | Lys | Gly | Val | Gln | Asp | Lys | Lys | Trp | Lys | Lys | Trp | Leu | Ser | Ser | Lys | Lys | Leu | Lys | Leu | Lys | Leu | Leu | Lys | Lys | Arg | Arg | Lys | Asn | Lys | Lys | Lys | Gln | Glu | Glu | Lys | Met |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- Molecule 14: ATPTT9

Chain O3: 

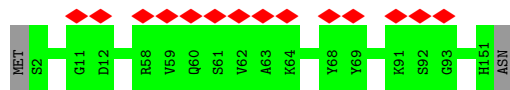
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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|
| MET | GLN | GLN | GLN | LYS | LYS | ASN | LYS | LEU | LEU | LYS | LYS | ASN | ASN | GLY | VAL | GLN | GLN | ASP | LYS | LYS | TYR | TYR | TYR | LYS | LEU | LEU | LEU | LEU | ASP | GLN | GLU | ILE | ILE | GLY | GLY | LYS | LYS | LYS | LYS | ASN | ASN | ARG | LYS | LYS | LYS | LYS | ASN | ASN | GLU | GLU | LYS | LYS | GLN | GLN | GLU | GLU | LEU | LEU | ILE | ILE | LYS | LYS | VAL | M55 | K153 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|

- Molecule 15: ATPTT10

Chain p: 99%

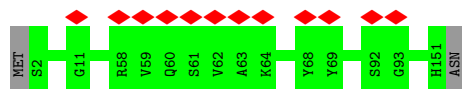
- Molecule 15: ATPTT10

Chain P:  9% 99%



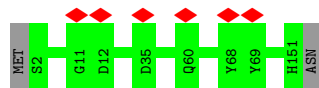
- Molecule 15: ATPTT10

Chain p3:  8% 99%



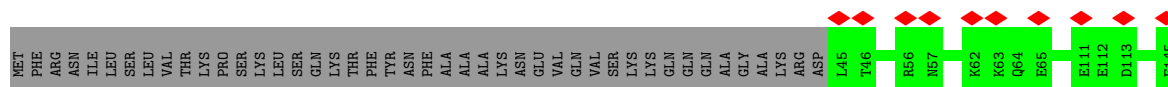
- Molecule 15: ATPTT10

Chain P3:  99%



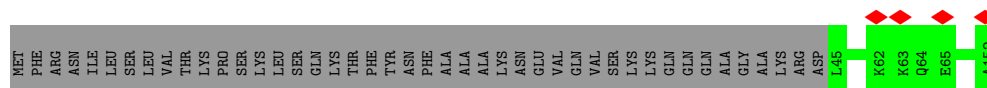
- Molecule 16: ATPTT11

Chain q:  8% 71% 29%



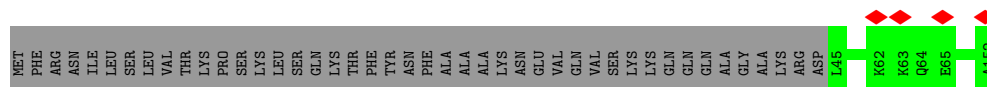
- Molecule 16: ATPTT11

Chain Q:  71% 29%

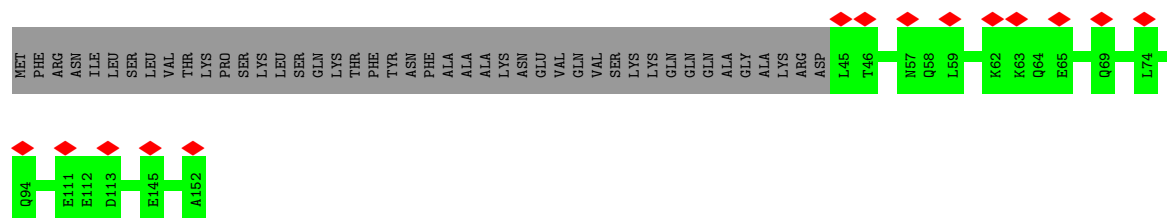
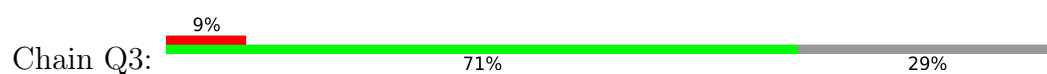


- Molecule 16: ATPTT11

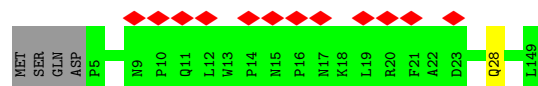
Chain q3:  71% 29%



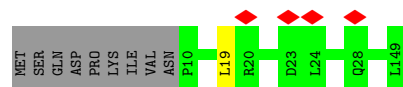
- Molecule 16: ATPTT11



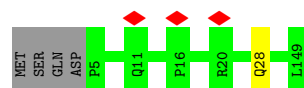
• Molecule 17: ATPTT12



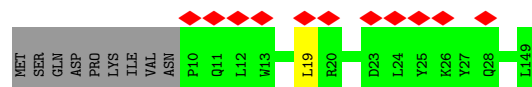
• Molecule 17: ATPTT12



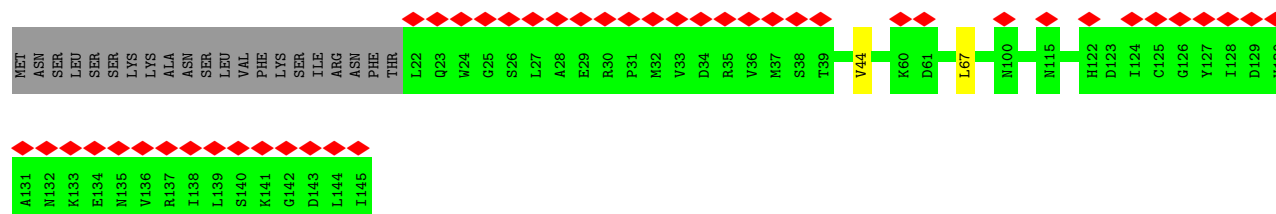
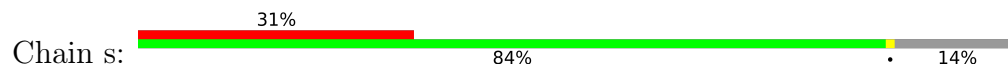
• Molecule 17: ATPTT12



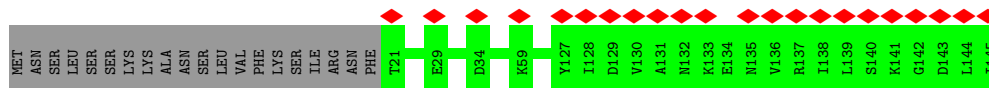
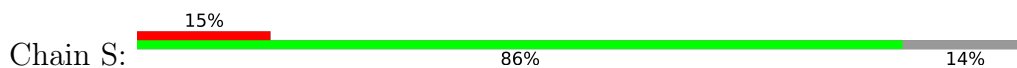
• Molecule 17: ATPTT12



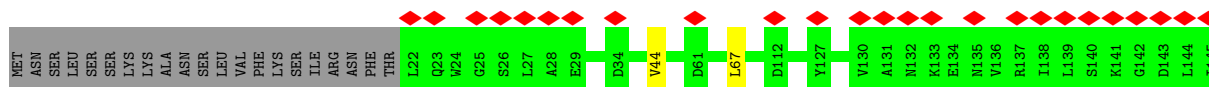
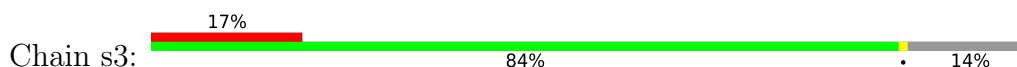
• Molecule 18: ATPTT13



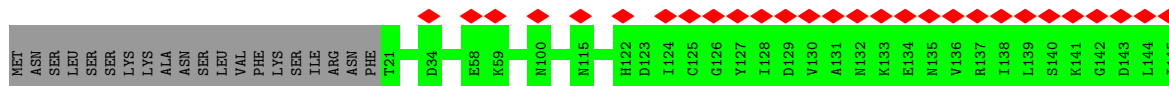
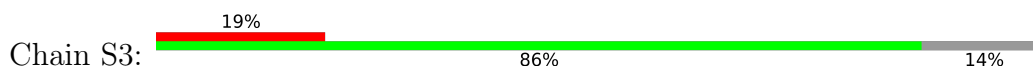
- Molecule 18: ATPTT13



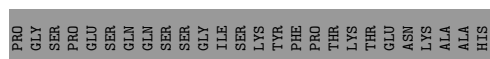
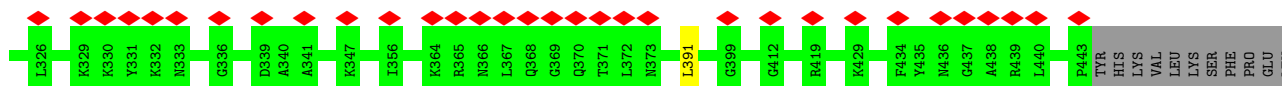
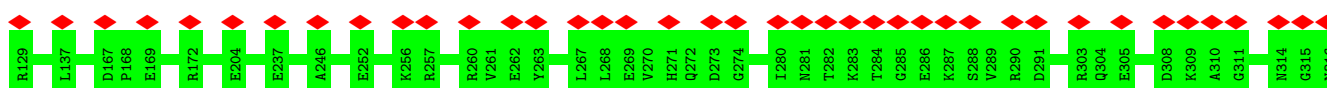
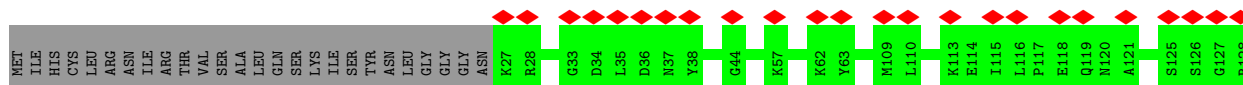
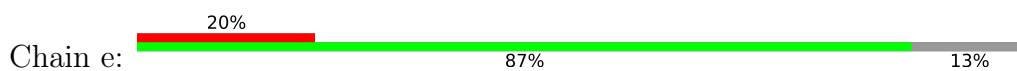
- Molecule 18: ATPTT13



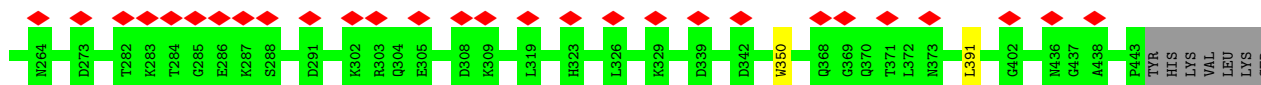
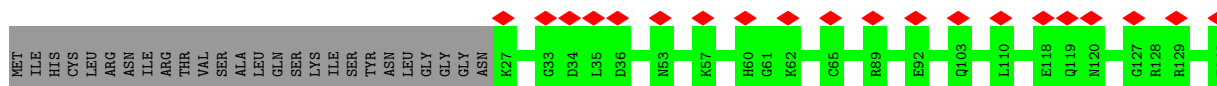
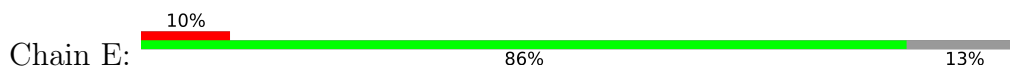
- Molecule 18: ATPTT13



- Molecule 19: ATPTT1



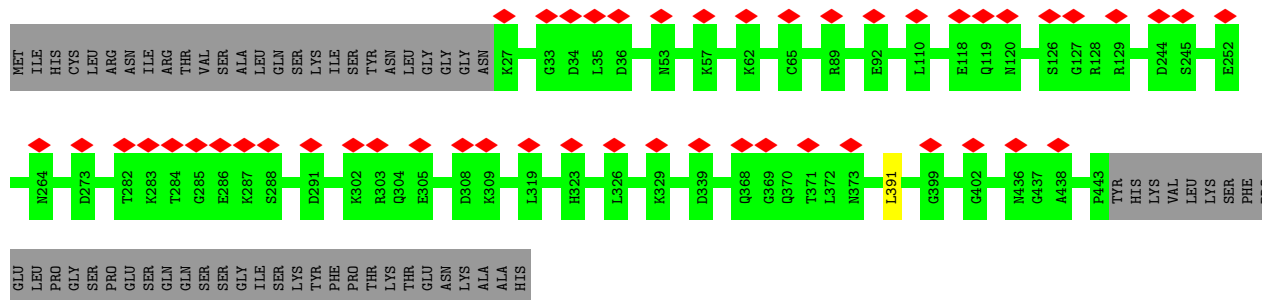
- Molecule 19: ATPTT1



PHE
PRO
GLU
LEU
PRO
PRO
GLY
SER
PRO
GLU
SER
GLN
GLN
SER
SER
GLY
SER
LYS
LYS
TYR
PHE
PRO
THR
LYS
GLY
THR
GLY
ASN
LYS
ALA
ALA
HIS

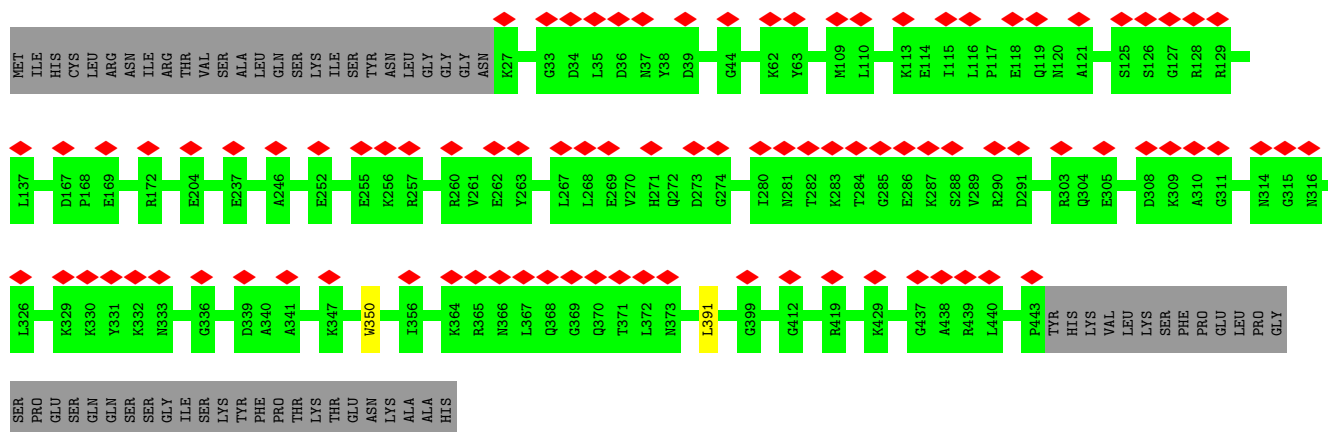
• Molecule 19: ATPPTT1

Chain e3: 10% 87% 13%



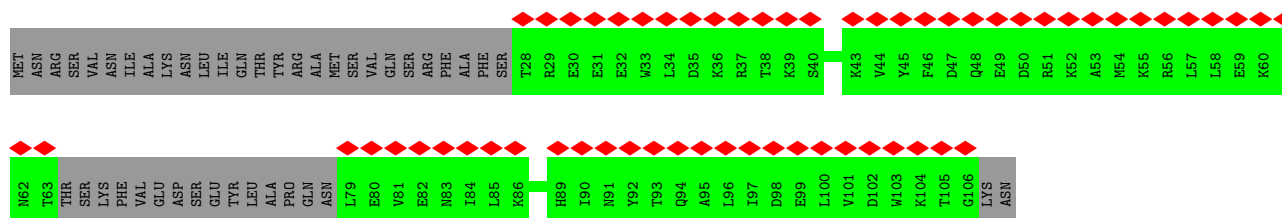
• Molecule 19: ATPPTT1

Chain E3: 19% 86% 13%



• Molecule 20: Inhibitor of F1 (IF1)

Chain i2: 56% 59% 41%

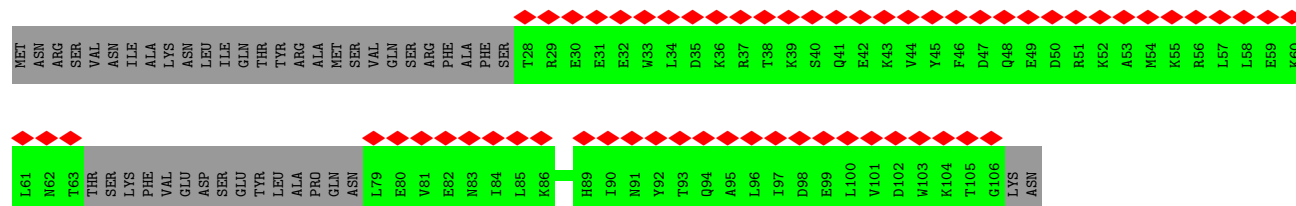


• Molecule 20: Inhibitor of F1 (IF1)

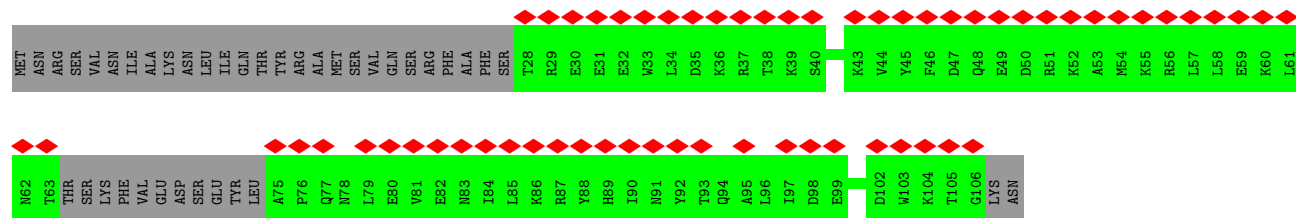
Chain i1: 60% 63% 37%



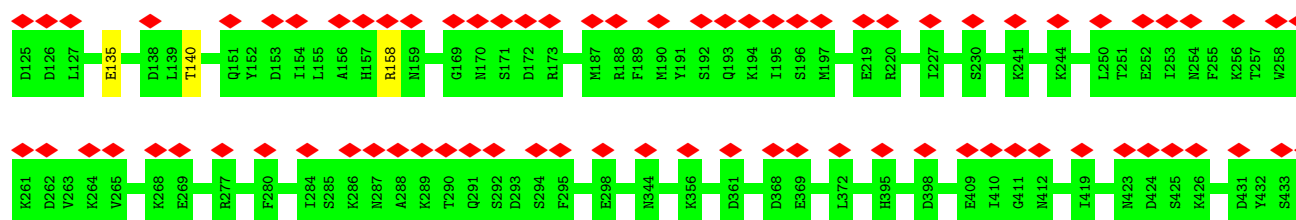
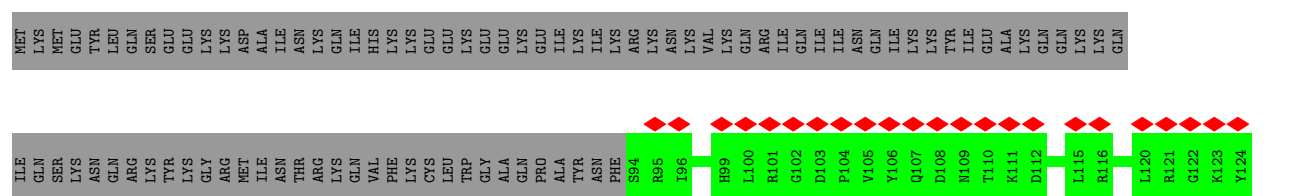
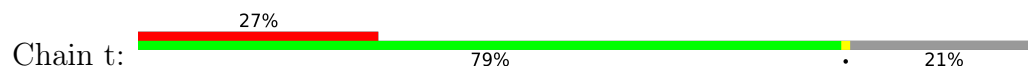
• Molecule 20: Inhibitor of F1 (IF1)



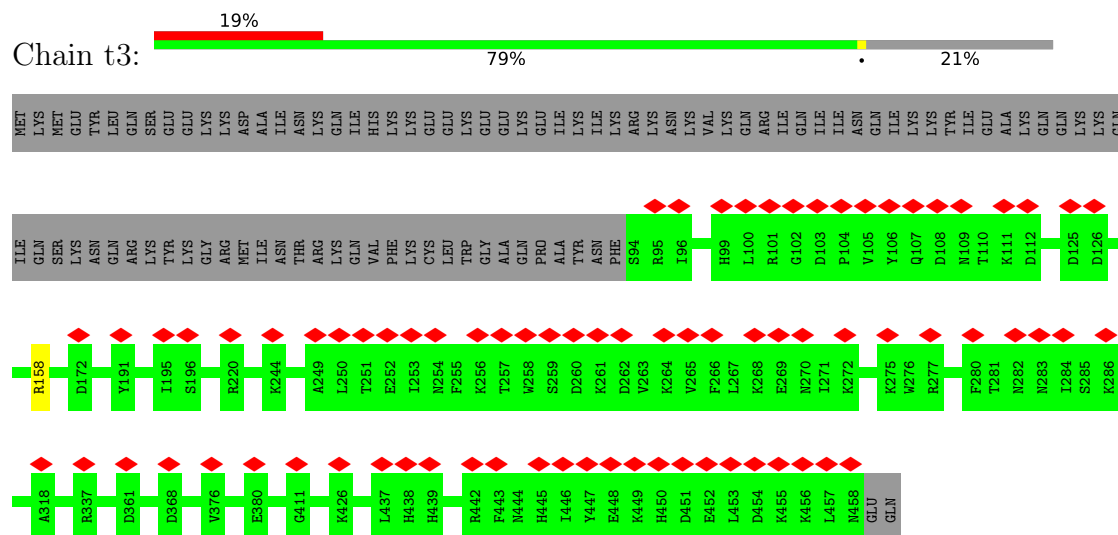
• Molecule 20: Inhibitor of F1 (IF1)



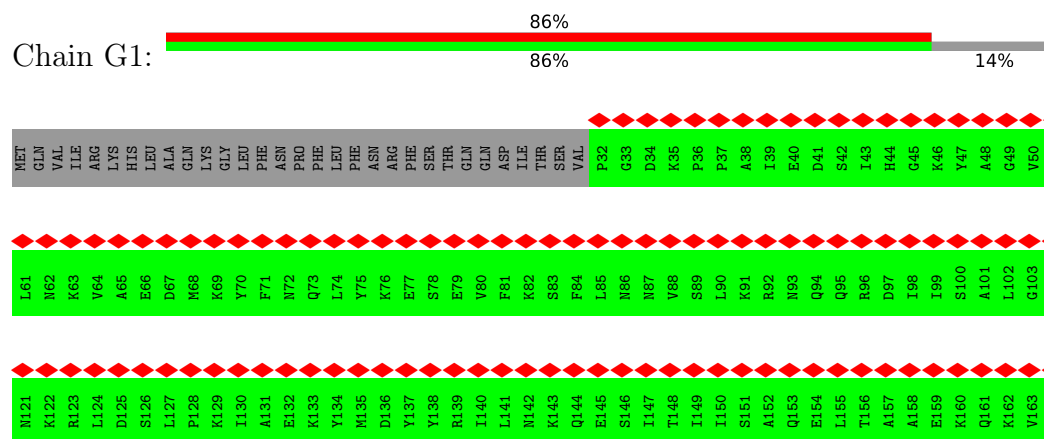
• Molecule 21: ATPPT2



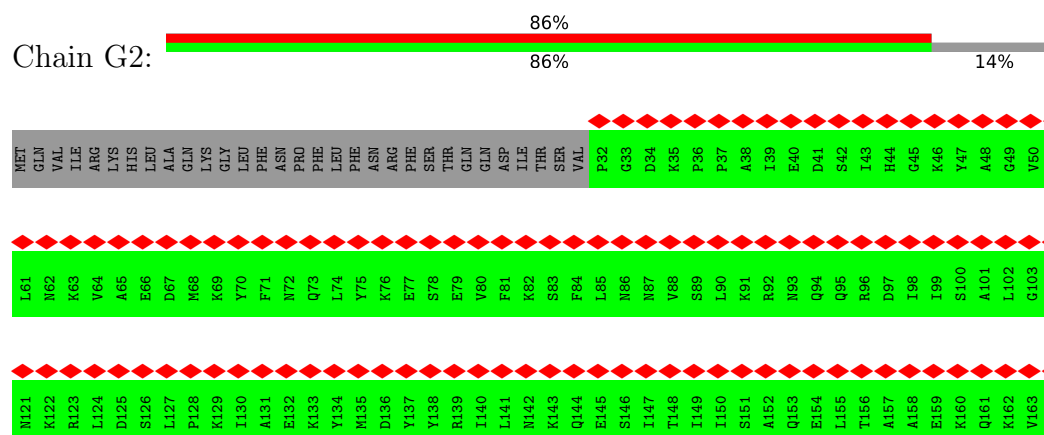
- Molecule 21: ATPTT2

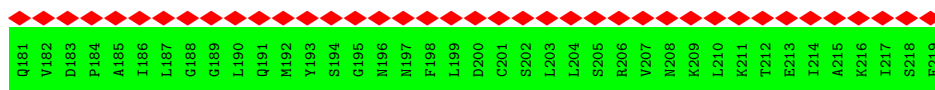


- Molecule 22: Oligomycin sensitivity-conferring protein (OSCP)

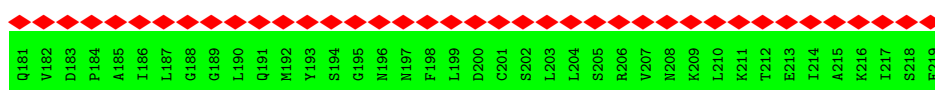
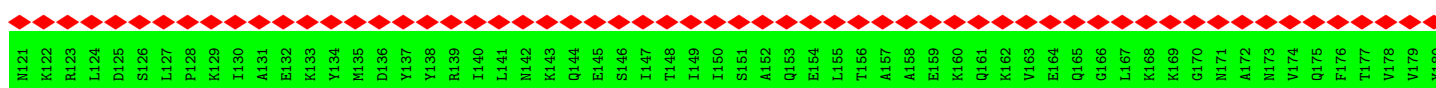
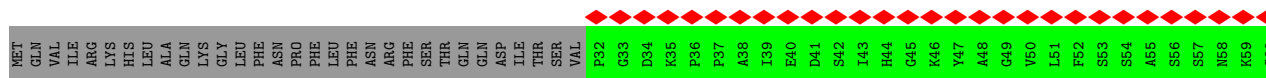
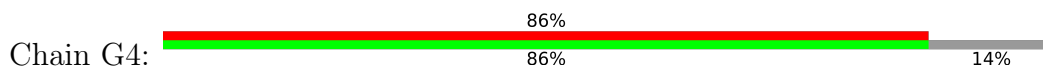


- Molecule 22: Oligomycin sensitivity-conferring protein (OSCP)

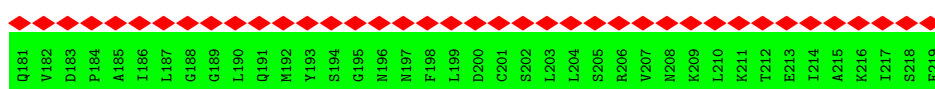
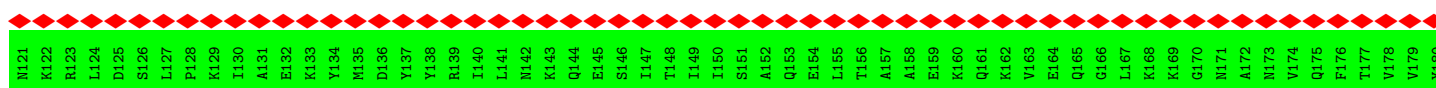
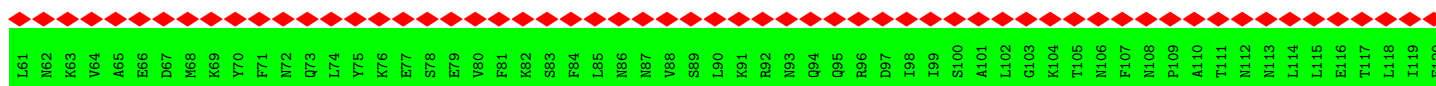
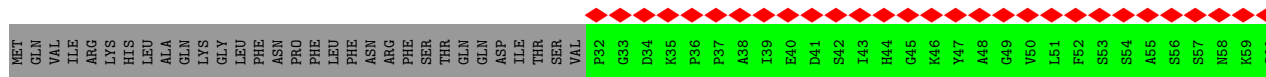
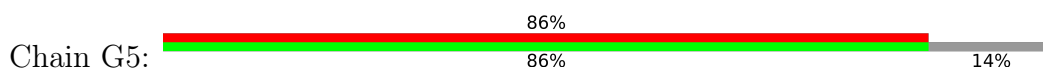




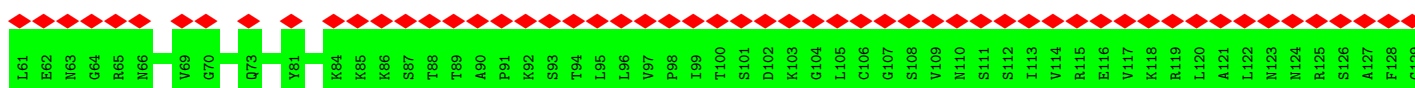
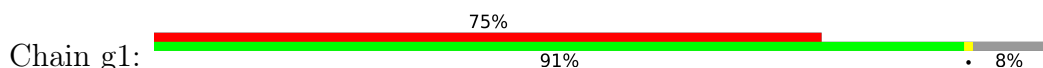
• Molecule 22: Oligomycin sensitivity-conferring protein (OSCP)

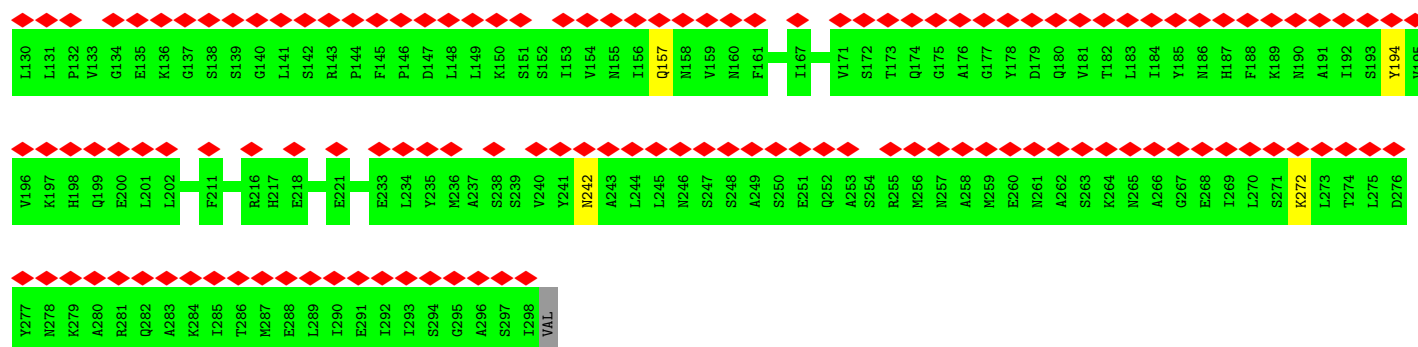


• Molecule 22: Oligomycin sensitivity-conferring protein (OSCP)

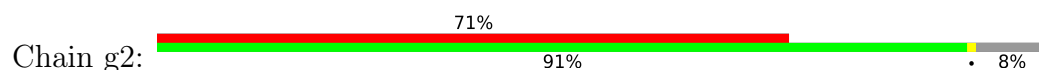


• Molecule 23: ATP synthase subunit gamma

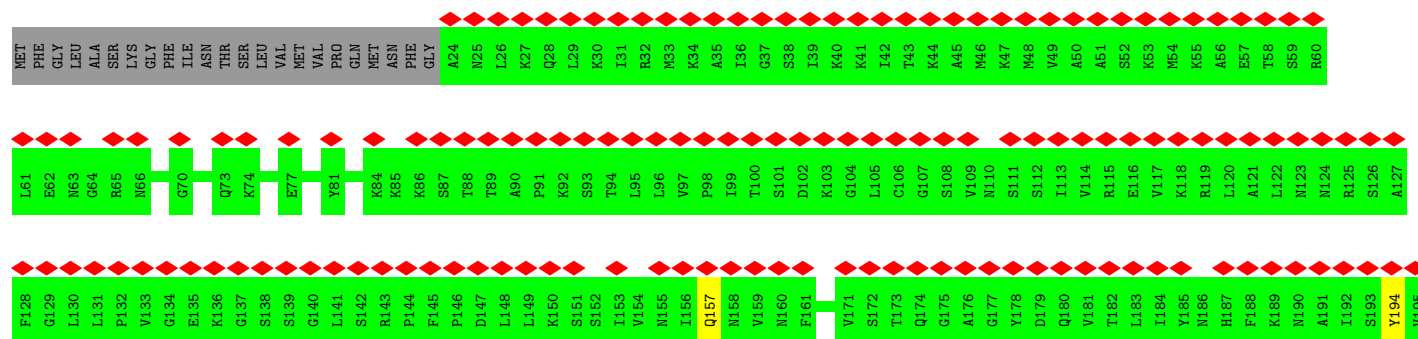
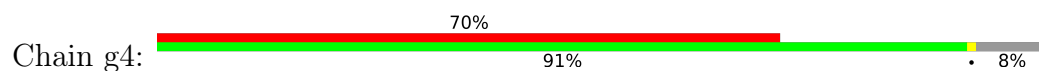




• Molecule 23: ATP synthase subunit gamma

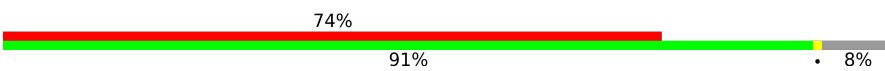


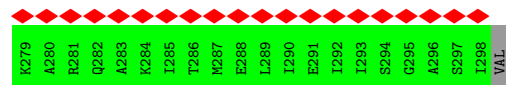
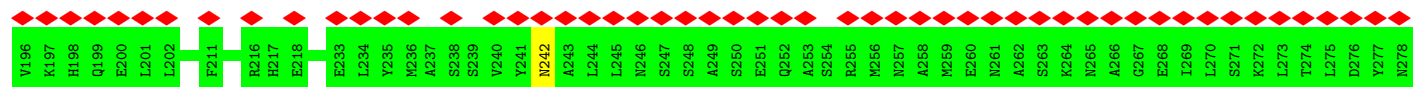
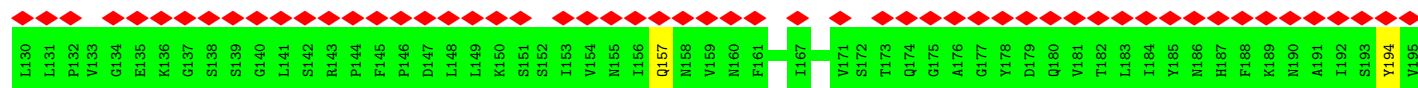
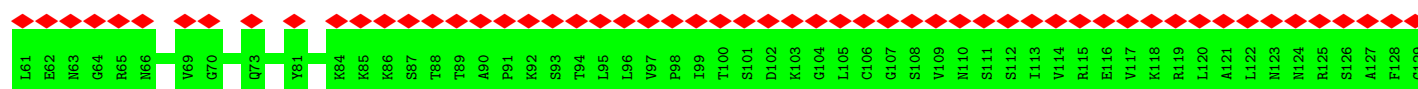
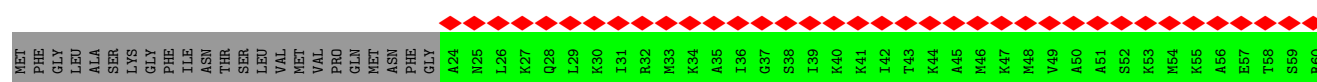
• Molecule 23: ATP synthase subunit gamma





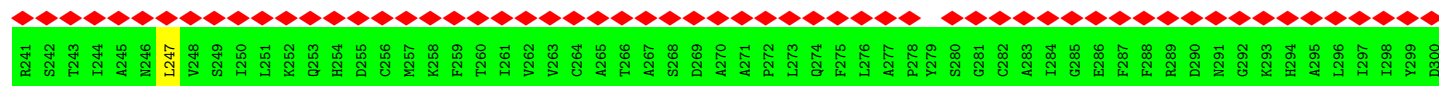
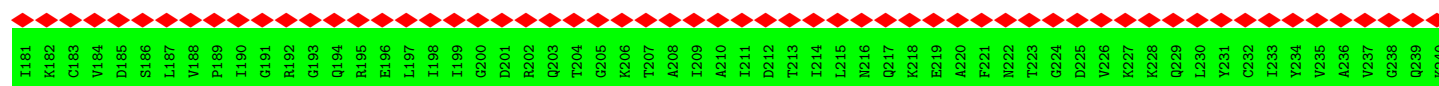
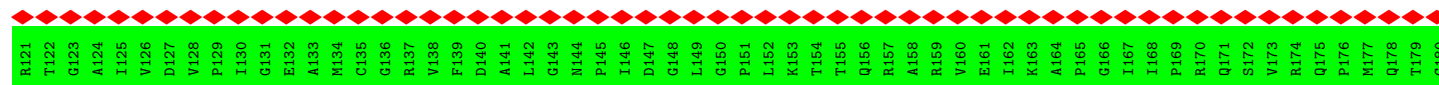
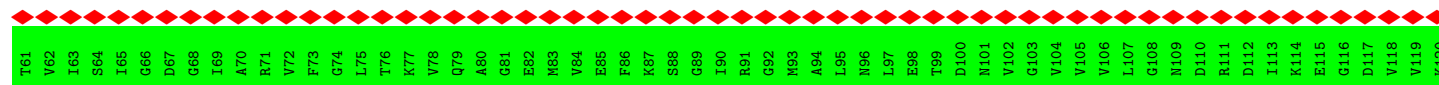
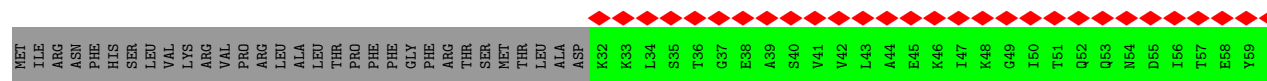
• Molecule 23: ATP synthase subunit gamma

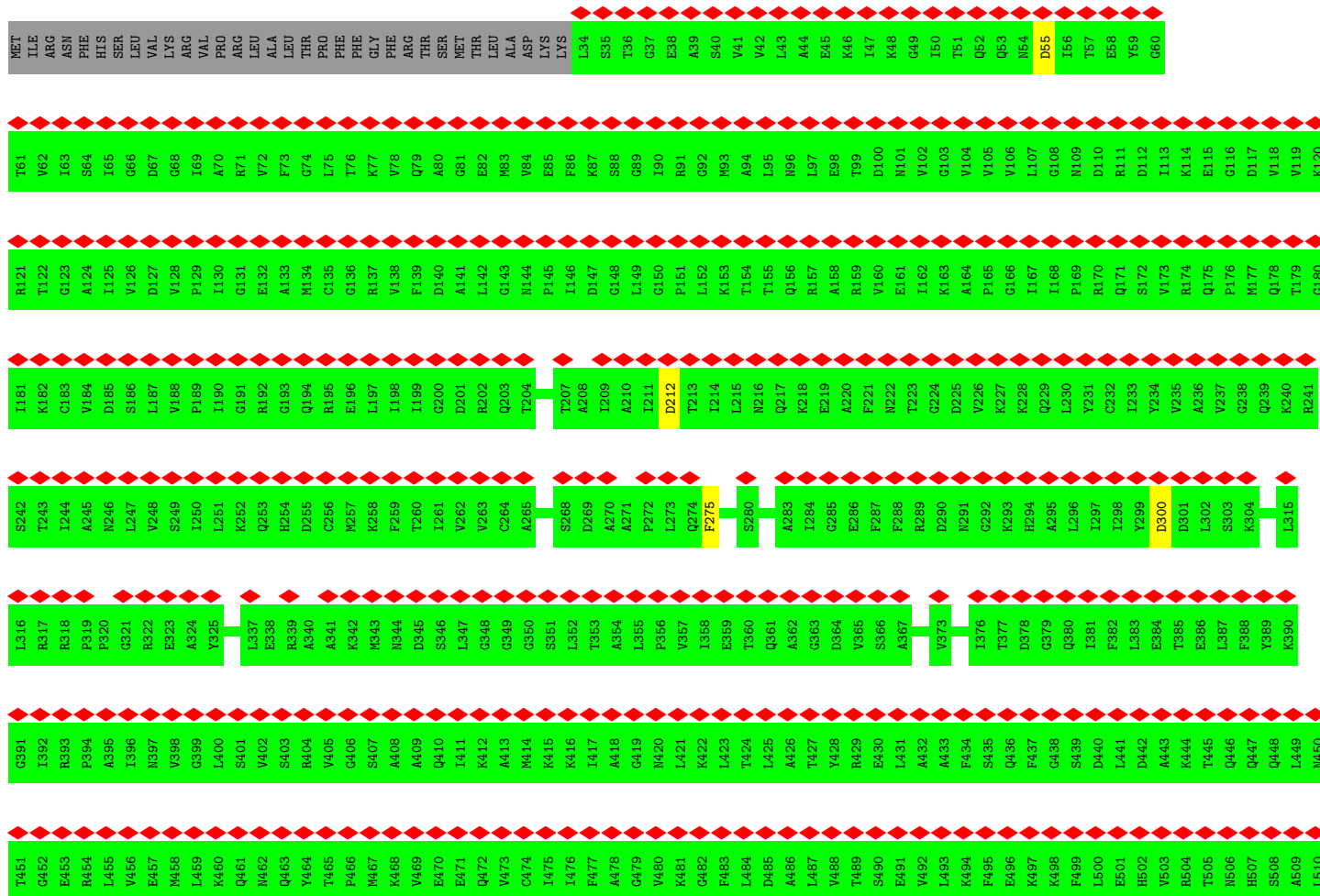
Chain g5:  74% 91% 8%

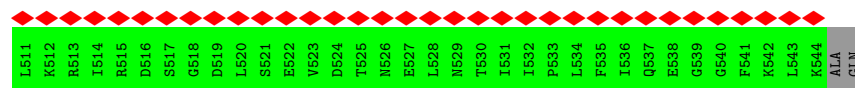


• Molecule 24: ATP synthase subunit alpha

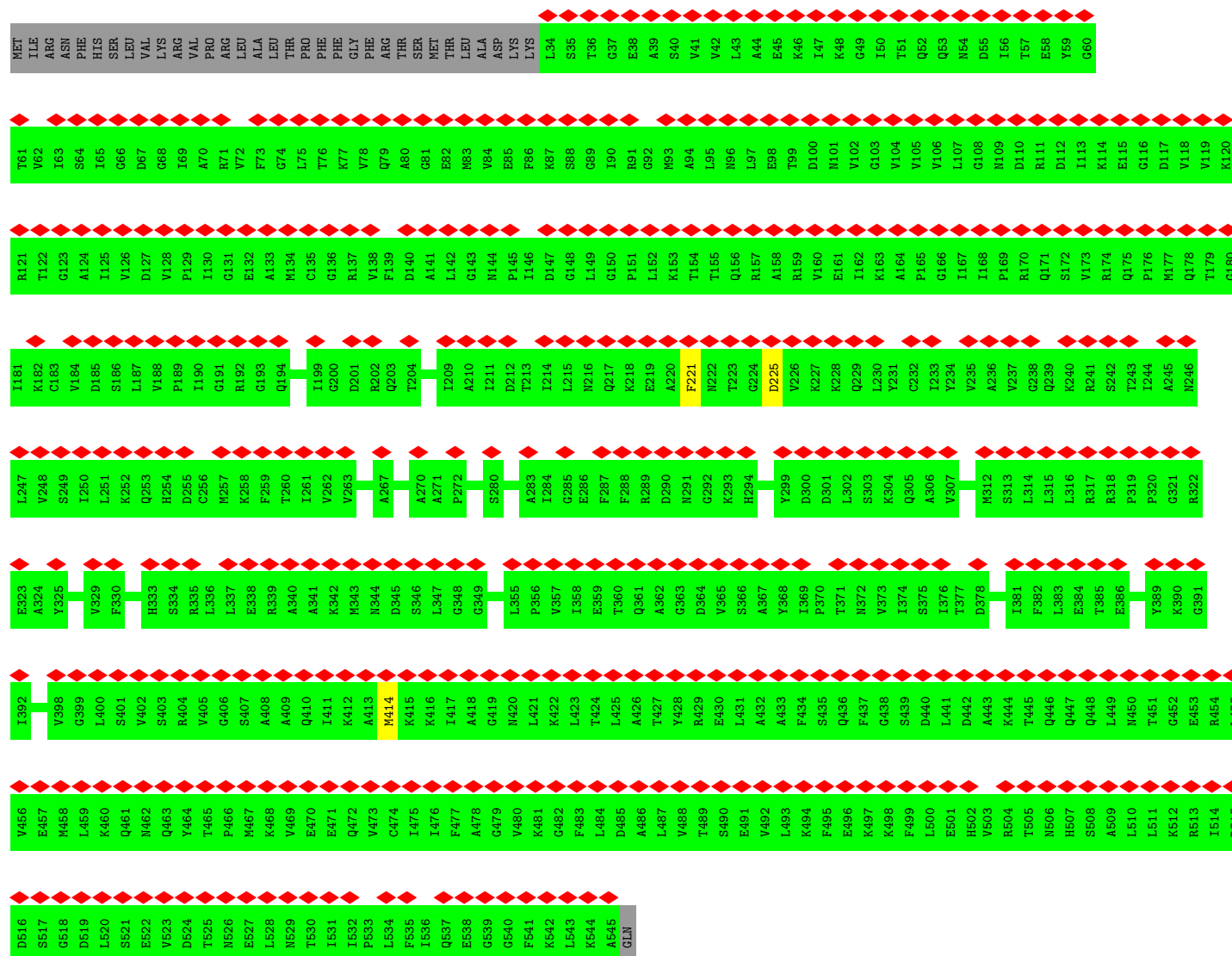
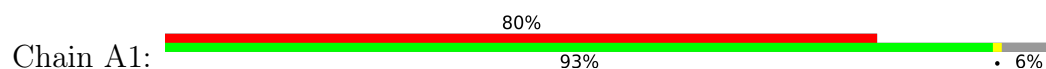
Chain C1:  93% 94% 6%





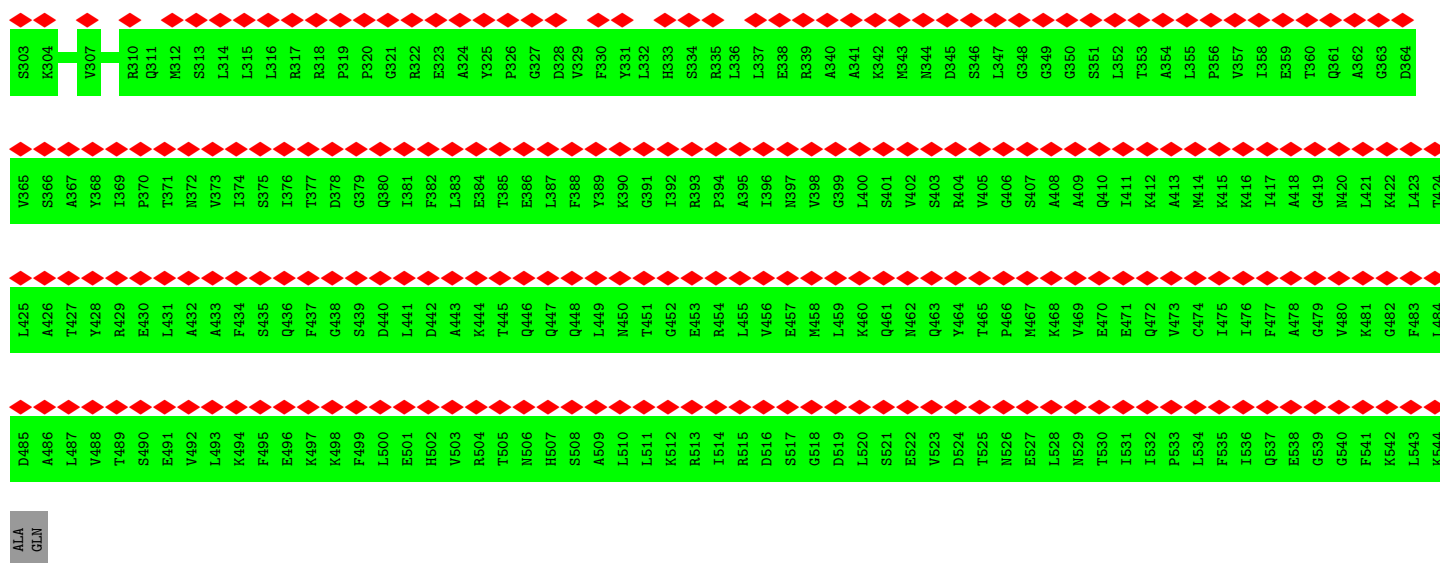


• Molecule 24: ATP synthase subunit alpha

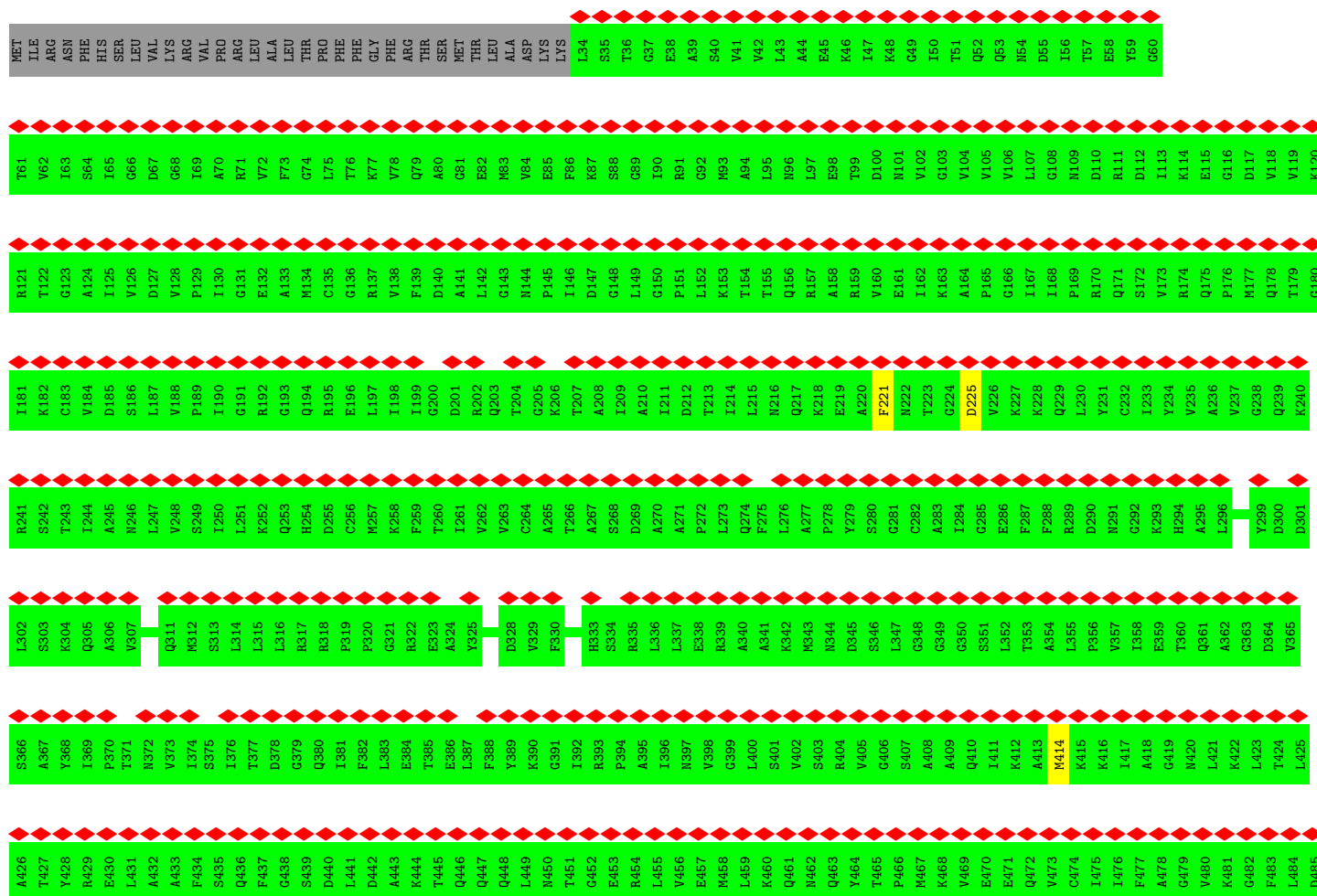


• Molecule 24: ATP synthase subunit alpha





• Molecule 24: ATP synthase subunit alpha



A486
L487
V488
T489
S490
E491
V492
L493
K494
F495
E496
K497
K498
F499
L500
E501
H502
V503
R504
T505
N506
H507
S508
A509
L510
L511
K512
R513
I514
R515
D516
S517
G518
D519
L520
S521
E522
V523
D524
T525
N526
E527
L528
N529
T530
I531
I532
P533
L534
F535
I536
Q537
E538
G539
G540
F541
K542
L543
K544
A545

GLN

• Molecule 24: ATP synthase subunit alpha

Chain C4: 

MET
ILE
ARG
ASN
PHE
HIS
SER
LEU
VAL
LYS
ARG
VAL
PRO
ARG
LEU
ALA
THR
PRO
PHE
PHE
GLY
PHE
ARG
THR
SER
MET
THR
LEU
ALA
ASP
K32
K33
L34
S35
T36
G37
E38
A39
S40
V41
V42
L43
A44
E45
K46
I47
K48
F49
I50
T51
Q52
Q53
N54
D55
I56
T57
E58
Y59
G60

T61
V62
I63
S64
I65
G66
D67
G68
I69
A70
R71
V72
F73
G74
L75
T76
K77
V78
Q79
A80
G81
E82
M83
V84
E85
F86
K87
S88
G89
I90
R91
Q92
M93
A94
L95
N96
L97
E98
T99
D100
M101
V102
G103
V104
V105
V106
L107
G108
M109
D110
R111
D112
I113
K114
E115
G116
D117
V118
V119
K120

R121
T122
C123
A124
I125
I126
D127
V128
P129
I130
G131
E132
A133
M134
C135
G136
V137
R138
F139
D140
A141
L142
G143
M144
P145
I146
D147
G148
L149
G150
P151
L152
K153
T154
T155
Q156
L157
A158
R159
V160
E161
I162
K163
A164
P165
P166
I167
I168
P169
R170
P171
Q171
S172
V173
R174
Q175
P176
M177
Q178
T179
G180

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C183
V184
D185
S186
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V188
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G191
R192
G193
Q194
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G200
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Q203
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G205
K206
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Q229
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V235
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P237
G238
Q239
K240

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S242
T243
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A245
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V248
S249
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L251
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D269
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A271
P272
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F275
L276
A277
P278
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S280
G281
C282
A283
I284
G285
E286
F287
F288
R289
D290
N291
G292
K293
H294
A295
L296
I297
I298
Y299
D300

D301
L302
S303
K304
Q305
A306
V307
A308
Y309
R310
Q311
M312
S313
L314
L315
L316
R317
R318
P319
P320
G321
R322
E323
A324
Y325
V329
F330
H333
L336
L337
E338
R339
A340
A341
K342
M343
N344
D345
D346
V405
S406
L347
G348
G349
G350
S351
L352
T353
A354
L355
P356
V357
I358
E359
T360
Q361
A362
G363
D364

V365
S366
A367
Y368
I369
P370
T371
N372
V373
I374
S375
I376
T377
D378
G379
Q380
I381
F382
L383
E384
T385
E386
L387
F388
Y389
K390
G391
I392
R393
P394
A395
I396
N397
V398
G399
L400
S401
V402
S403
R404
V405
G406
S407
A408
A409
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L423
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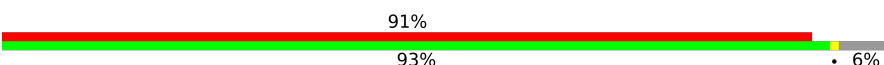
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F434
S435
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L441
D442
A443
K444
T445
Q446
Q447
Q448
L449
N450
T451
G452
E453
R454
L455
V456
A457
M458
L459
K460
Q461
N462
Q463
Y464
T465
P466
M467
K468
V469
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C474
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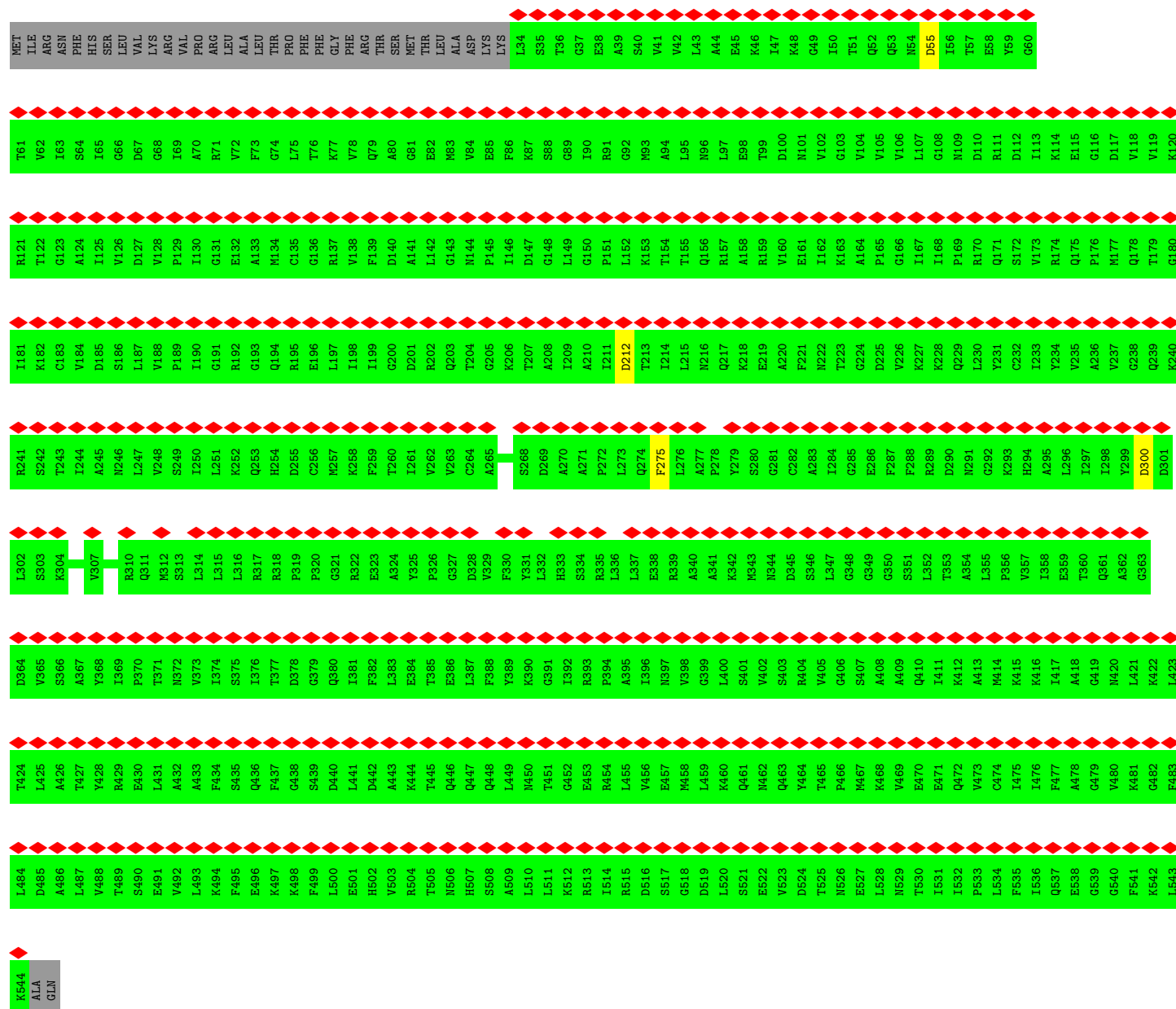
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E501
H502
V503
R504
T505
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H507
S508
A509
L510
L511
K512
R513
I514
R515
D516
S517
G518
D519
L520
S521
E522
V523
D524
T525
N526
E527
L528
N529
T530
I531
I532
P533
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Q537
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G540
F541
K542
L543
K544

ALA

GLN

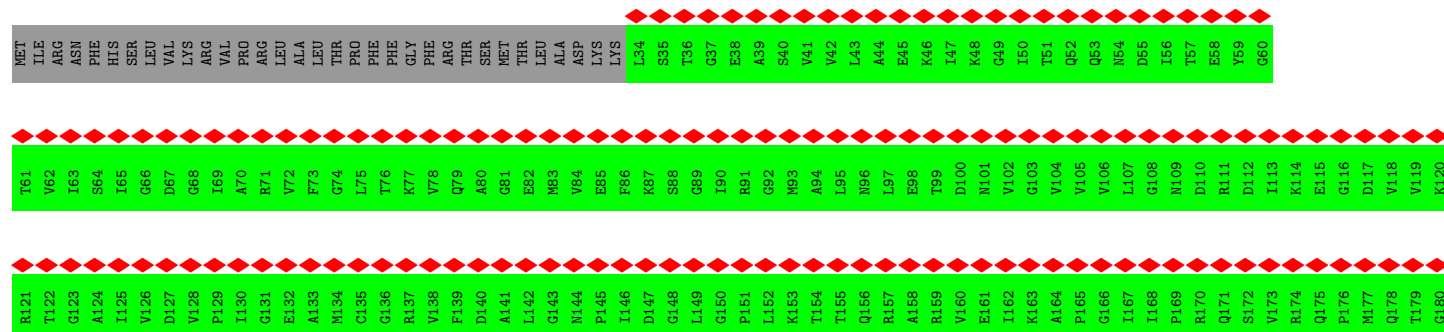
• Molecule 24: ATP synthase subunit alpha

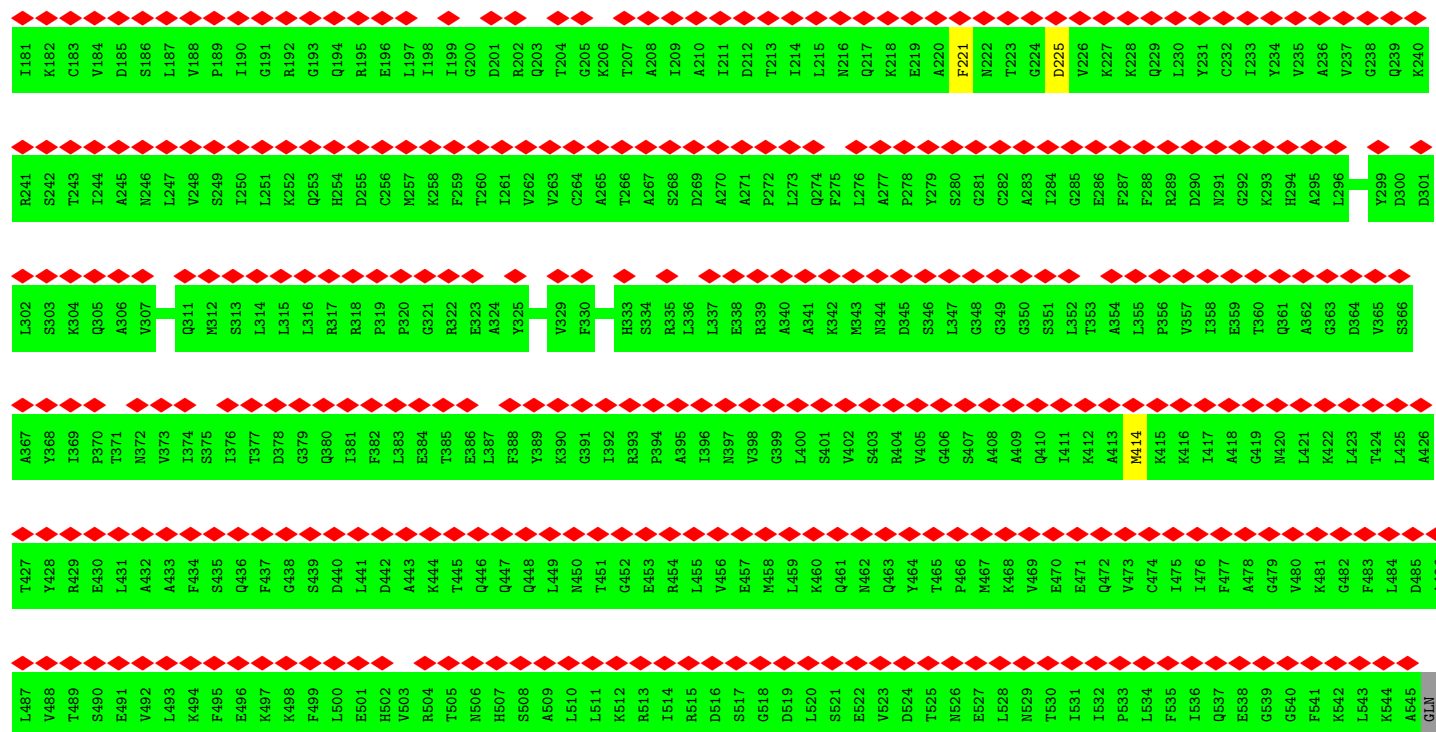
Chain B4: 



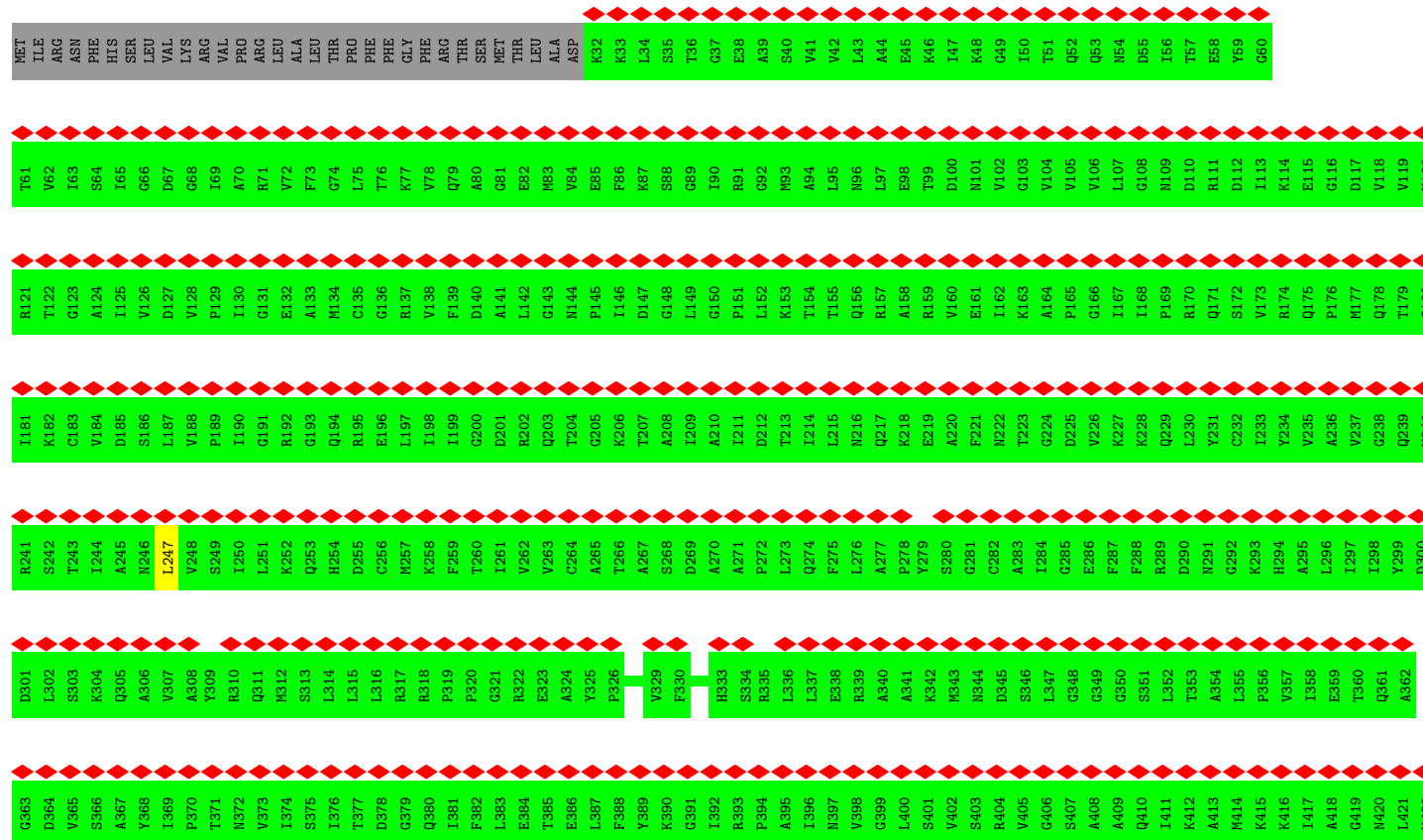
• Molecule 24: ATP synthase subunit alpha

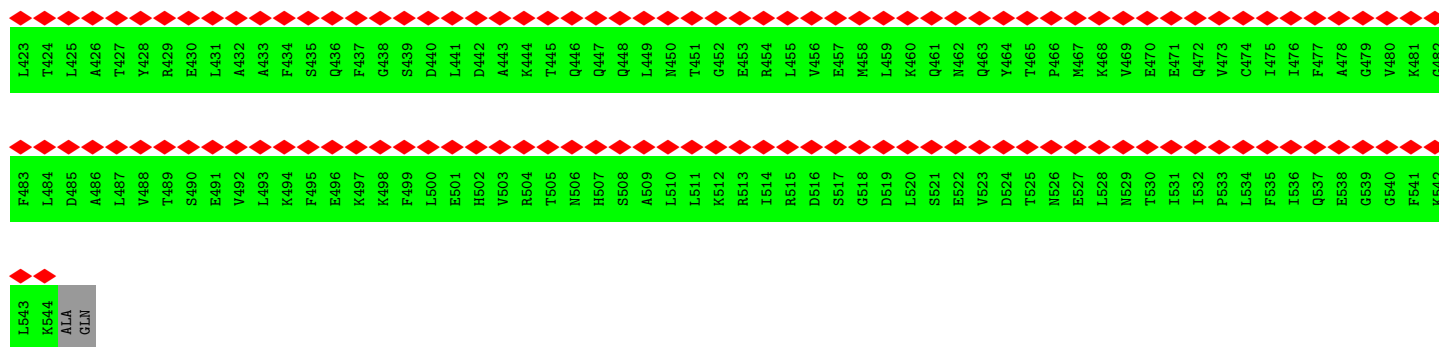
Chain A4: 89% 93% 6%



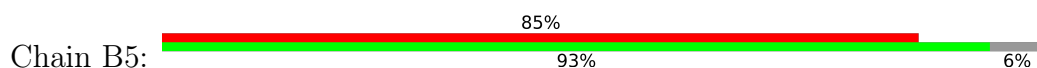


• Molecule 24: ATP synthase subunit alpha

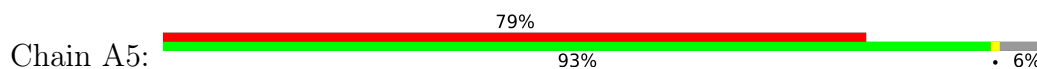


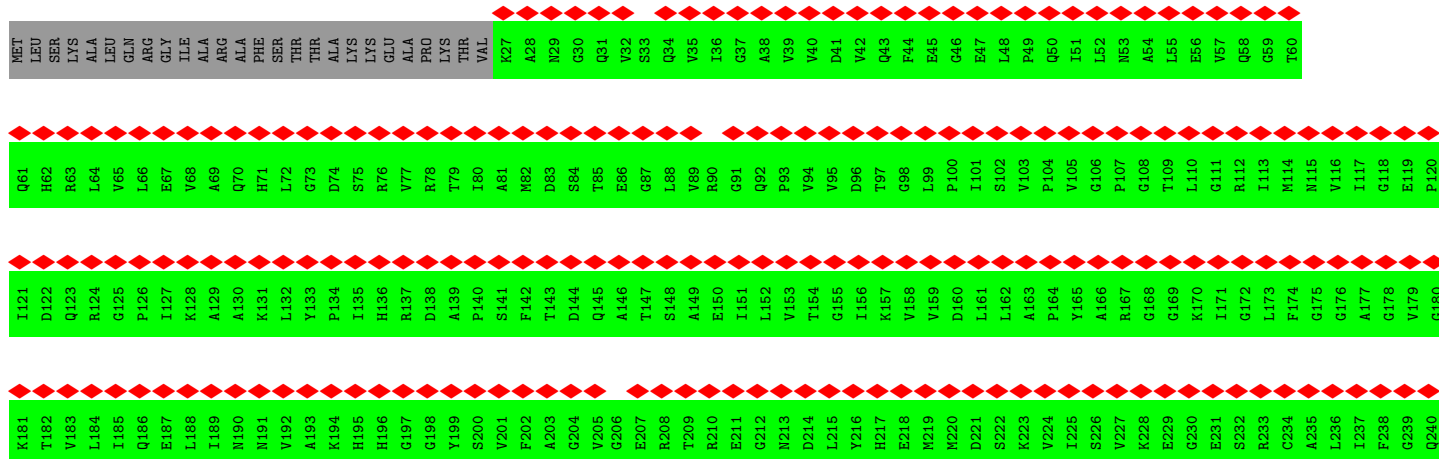


• Molecule 24: ATP synthase subunit alpha



• Molecule 24: ATP synthase subunit alpha



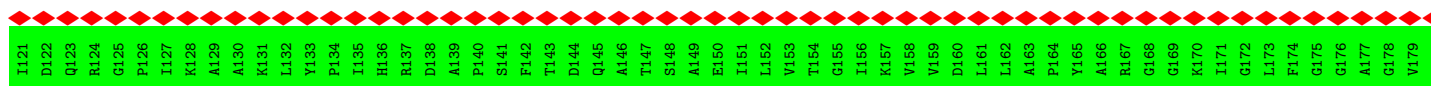


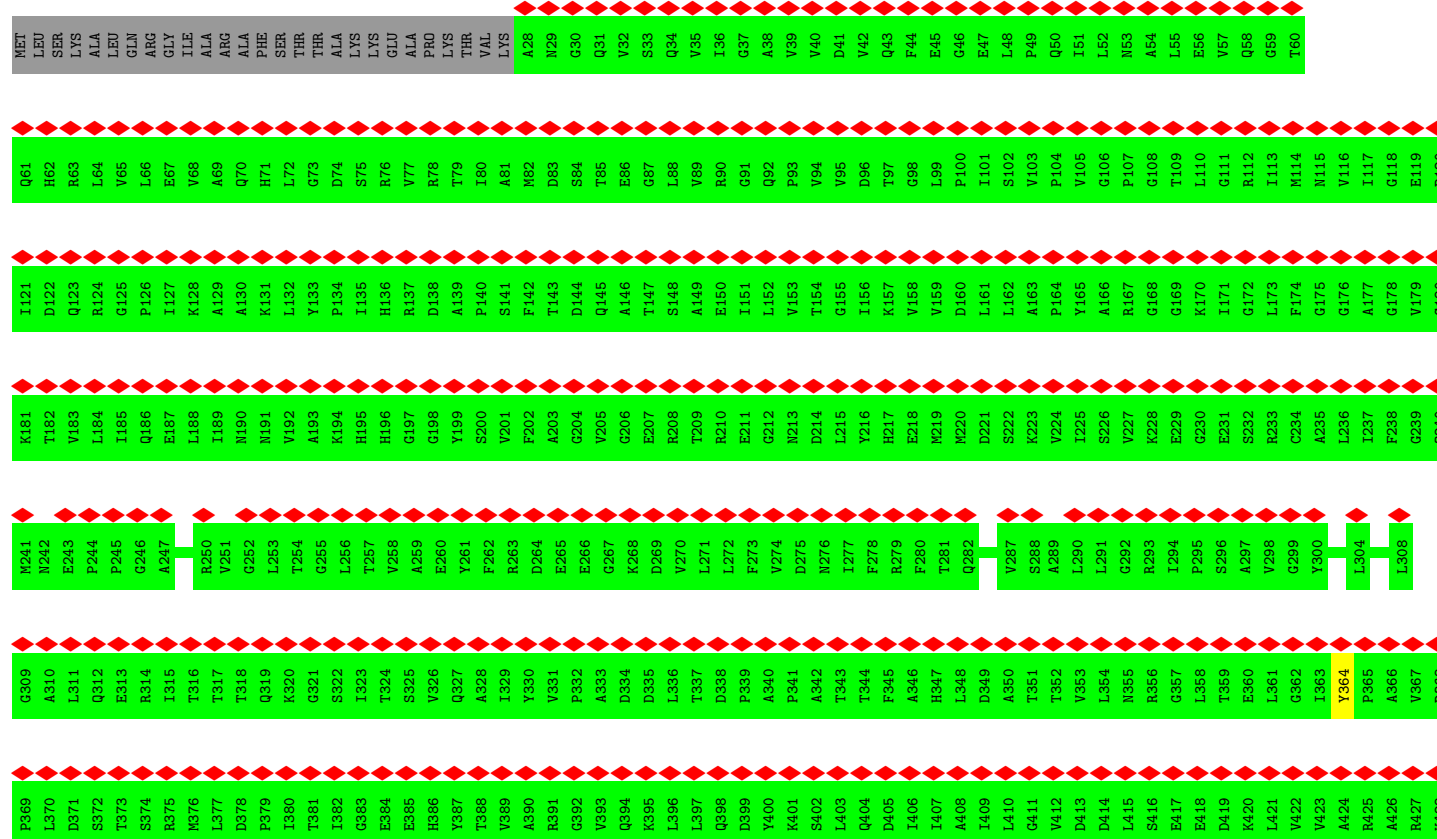
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|------|------|------|------|------|
| M241 | Q301 | L361 | L421 | D481 |
| N242 | P302 | G362 | V422 | L482 |
| E243 | T303 | I363 | V423 | L483 |
| P244 | L304 | Y364 | A424 | E484 |
| P245 | A305 | P365 | R425 | L485 |
| G246 | T306 | A366 | A426 | L486 |
| A247 | D307 | V367 | R427 | A487 |
| R248 | L308 | D368 | K428 | A488 |
| A249 | G309 | P369 | A429 | A489 |
| R250 | A310 | L370 | Q430 | R490 |
| V251 | L311 | D371 | K431 | A491 |
| G252 | Q312 | S372 | F432 | D492 |
| L253 | E313 | T373 | L433 | T493 |
| T254 | R314 | S374 | S434 | L494 |
| G255 | I315 | R375 | Q435 | K495 |
| L256 | T316 | M376 | P436 | S496 |
| T257 | T317 | L377 | F437 | LYS |
| V258 | T318 | D378 | F438 | |
| A259 | Q319 | P379 | M439 | |
| E260 | K320 | I380 | S440 | |
| Y261 | G321 | T381 | E441 | |
| F262 | S322 | I382 | V442 | |
| R263 | I323 | G383 | F443 | |
| D264 | T324 | E384 | S444 | |
| E265 | S325 | E385 | G445 | |
| E266 | V326 | H386 | I446 | |
| G267 | Q327 | Y387 | P447 | |
| K268 | A328 | T388 | G448 | |
| D269 | I329 | V389 | R449 | |
| V270 | Y330 | A390 | F450 | |
| L271 | V331 | R391 | V451 | |
| L272 | P332 | G392 | N452 | |
| F273 | A333 | V393 | L453 | |
| V274 | D334 | Q394 | K454 | |
| D275 | D335 | K395 | Q455 | |
| N276 | L336 | L396 | N456 | |
| I277 | T337 | L397 | I457 | |
| F278 | D338 | Q398 | A458 | |
| R279 | P339 | D399 | S459 | |
| F280 | A340 | Y400 | F460 | |
| T281 | P341 | K401 | K461 | |
| Q282 | A342 | S402 | A462 | |
| A283 | T343 | L403 | L463 | |
| C284 | T344 | Q404 | L464 | |
| S285 | F345 | D405 | E465 | |
| E286 | A346 | I406 | G466 | |
| V287 | H347 | I407 | A467 | |
| A289 | L348 | A408 | G468 | |
| L290 | A350 | I409 | D469 | |
| L291 | T351 | L410 | E470 | |
| G292 | T352 | G411 | Y471 | |
| R293 | V353 | V412 | P472 | |
| I294 | L354 | D413 | E473 | |
| P295 | N355 | D414 | S474 | |
| S296 | R356 | L415 | C475 | |
| A297 | G357 | S416 | F476 | |
| V298 | L358 | E417 | Y477 | |
| G299 | T359 | E418 | M478 | |
| Y300 | E360 | D419 | K479 | |
| | | K420 | G480 | |

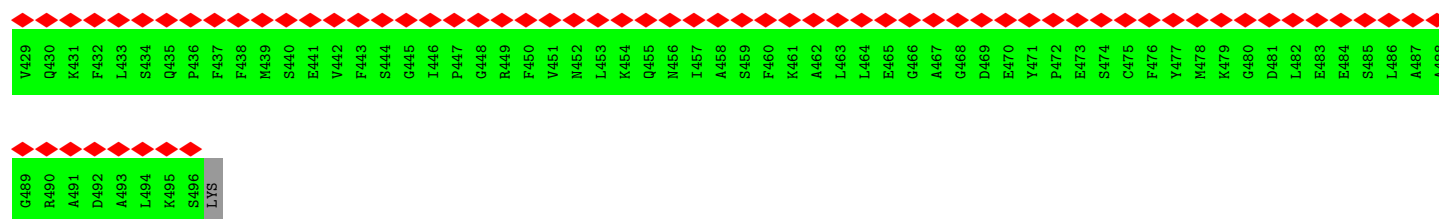
● Molecule 25: ATP synthase subunit beta



| | | | | | | | | |
|-----|-----|------|------|------|------|------|------|------|
| ME1 | A28 | Q61 | I121 | K181 | M241 | L311 | S372 | F432 |
| LEU | N29 | H62 | D122 | T182 | N242 | Q312 | T373 | L433 |
| SER | C30 | R63 | Q123 | V183 | E243 | E313 | S374 | S434 |
| ALA | Q31 | L64 | L184 | L184 | P244 | R314 | R375 | Q435 |
| LEU | V32 | V65 | G125 | T185 | P245 | L315 | M376 | P436 |
| GLN | S33 | L66 | P126 | Q186 | G246 | T316 | L377 | F437 |
| ARG | Q34 | E67 | I127 | E187 | A247 | T317 | D378 | F438 |
| GLY | T35 | V68 | K128 | L188 | | T318 | P379 | M439 |
| ILE | I36 | A69 | A129 | I189 | R250 | Q319 | I380 | S440 |
| ALA | V35 | T79 | A130 | N190 | V251 | K320 | T381 | E441 |
| ARG | R38 | T80 | A139 | M191 | G252 | G321 | I382 | V442 |
| ALA | F44 | A81 | K131 | V192 | L253 | S322 | G383 | F443 |
| PHE | T44 | D83 | L132 | A193 | T254 | I323 | E384 | S444 |
| SER | S33 | H85 | Y133 | K194 | G255 | T324 | E385 | Q445 |
| THR | Q34 | E86 | D144 | H195 | L256 | S325 | H386 | I446 |
| THR | V32 | G87 | Q145 | H196 | T257 | V326 | Y387 | P447 |
| ALA | I36 | T147 | A146 | G197 | V258 | Q327 | T388 | G448 |
| GLU | T36 | L88 | S148 | G198 | V259 | A328 | V389 | R449 |
| ALA | R90 | V89 | A149 | Y199 | E260 | I329 | A390 | F450 |
| PRO | G37 | T91 | E150 | T209 | Y261 | Y330 | R391 | V451 |
| LYS | A38 | G91 | I151 | E211 | F262 | V331 | G392 | N452 |
| THR | V39 | Q92 | L152 | Q212 | R263 | P332 | V393 | L453 |
| VAL | V40 | P93 | V153 | N213 | D264 | A333 | Q394 | K454 |
| LYS | D41 | V94 | T154 | D214 | E265 | D334 | K395 | N456 |
| | V42 | V95 | G155 | L215 | E266 | D335 | L396 | G455 |
| | Q43 | D96 | I156 | Y216 | G267 | L336 | L397 | I457 |
| | F44 | T97 | K157 | H217 | G268 | T337 | Q398 | A458 |
| | E45 | G98 | V158 | E218 | D269 | D338 | D399 | S459 |
| | O46 | L99 | V159 | M219 | V270 | Y400 | F460 | K461 |
| | E47 | P100 | D160 | M220 | L271 | K401 | S402 | A462 |
| | L48 | I101 | L161 | D221 | L272 | L403 | Q404 | L463 |
| | P49 | S102 | L162 | S222 | F273 | F345 | D405 | E465 |
| | O50 | V103 | A163 | K223 | V274 | A346 | I406 | G466 |
| | I51 | P104 | P164 | V224 | N276 | H347 | I407 | A467 |
| | L52 | V105 | Y165 | I225 | D275 | L348 | D349 | A468 |
| | N53 | G106 | A166 | S226 | F278 | A350 | R279 | F469 |
| | A54 | P107 | R167 | V227 | T281 | T351 | F280 | E470 |
| | L55 | G108 | G168 | K228 | Q282 | T352 | T281 | Y471 |
| | E56 | T109 | G169 | E229 | V287 | V353 | D287 | F472 |
| | V57 | L110 | K170 | E231 | A289 | L354 | S288 | A473 |
| | O58 | R112 | I171 | R233 | L291 | N355 | A289 | S474 |
| | T60 | I113 | L173 | C234 | G292 | G357 | L291 | C475 |
| | | M114 | F174 | A235 | L290 | L358 | G292 | F476 |
| | | N115 | G175 | G175 | L291 | T359 | L291 | Y477 |
| | | V116 | G176 | G176 | L361 | E360 | R293 | M478 |
| | | I117 | A177 | I177 | L362 | L361 | T294 | K479 |
| | | G118 | I177 | G178 | I363 | G362 | I294 | G480 |
| | | E119 | V179 | G180 | Y364 | I363 | G295 | D481 |
| | | P120 | | | P365 | P365 | P296 | L482 |
| | | | | | A366 | A366 | Y300 | E483 |
| | | | | | V367 | V367 | | E484 |
| | | | | | P369 | P369 | | S485 |
| | | | | | L370 | L370 | | L486 |
| | | | | | D371 | D371 | | A487 |
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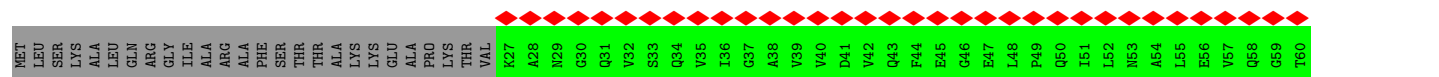


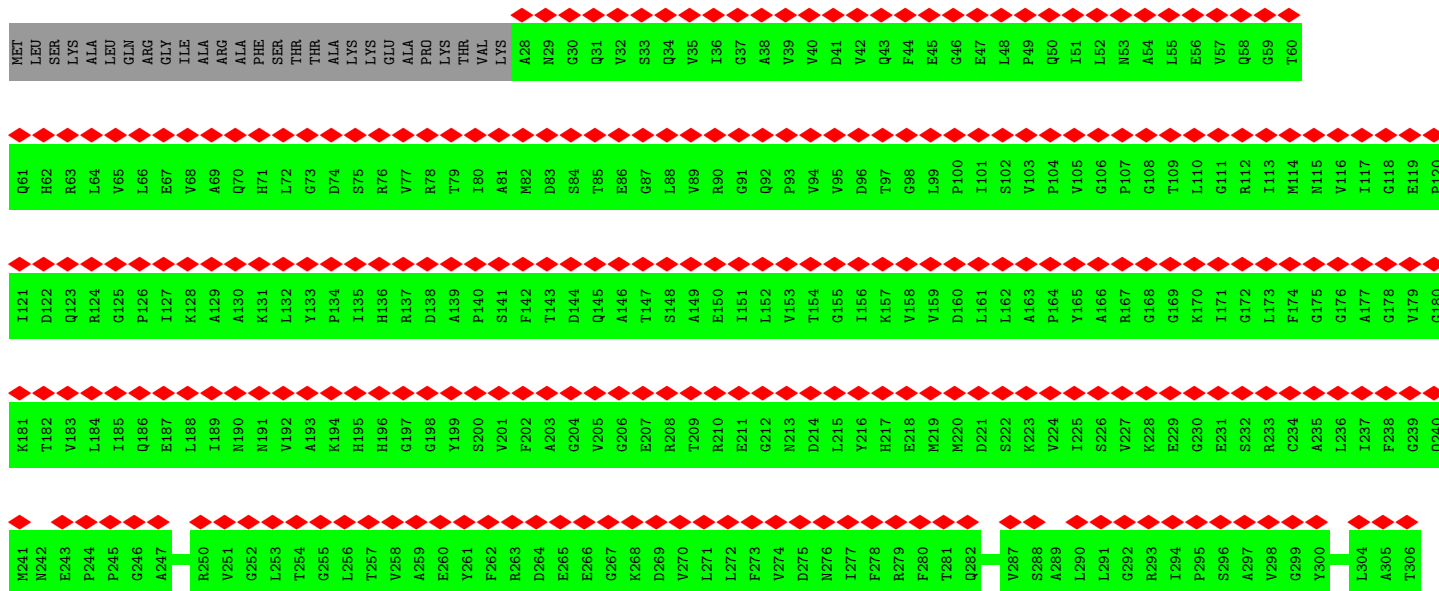


• Molecule 25: ATP synthase subunit beta



• Molecule 25: ATP synthase subunit beta





| | | | |
|------|------|------|------|
| D307 | V367 | R427 | A487 |
| L308 | D368 | K428 | A488 |
| G309 | P369 | V429 | G489 |
| A310 | L370 | Q430 | R490 |
| L311 | D371 | K431 | LEU |
| Q312 | S372 | F432 | GLN |
| E313 | T373 | L433 | ARG |
| R314 | S374 | S434 | GLY |
| I315 | R375 | Q435 | ILE |
| T316 | M376 | P436 | ALA |
| T317 | L377 | F437 | ALA |
| T318 | D378 | F438 | PHE |
| Q319 | P379 | M439 | SER |
| K320 | I380 | S440 | THR |
| G321 | T381 | E441 | ALA |
| S322 | I382 | V442 | LYS |
| I323 | G383 | F443 | LYS |
| T324 | E384 | S444 | GLU |
| S325 | E385 | G445 | ALA |
| V326 | H386 | I446 | PRO |
| Q327 | Y387 | P447 | LYS |
| A328 | T388 | G448 | THR |
| I329 | V389 | R449 | VAL |
| Y330 | A390 | F450 | K27 |
| V331 | R391 | V451 | A28 |
| P332 | G392 | N452 | N29 |
| A333 | V393 | L453 | G30 |
| D334 | Q394 | K454 | Q31 |
| D335 | K395 | Q455 | V32 |
| L336 | L396 | N456 | S33 |
| T337 | L397 | I457 | Q34 |
| D338 | Q398 | A458 | V35 |
| P339 | D399 | S459 | I36 |
| A340 | Y400 | F460 | G37 |
| P341 | K401 | K461 | A38 |
| A342 | S402 | A462 | V39 |
| T343 | L403 | L463 | D41 |
| T344 | Q404 | L464 | V42 |
| F345 | D405 | E465 | V42 |
| A346 | I406 | G466 | Q43 |
| H347 | I407 | A467 | F44 |
| L348 | A408 | G468 | E45 |
| D349 | I409 | D469 | G46 |
| A350 | L410 | E470 | E47 |
| T351 | G411 | Y471 | L101 |
| T352 | V412 | P472 | S102 |
| V353 | D413 | E473 | V103 |
| L354 | D414 | S474 | P104 |
| N355 | L415 | C475 | V105 |
| R356 | S416 | F476 | L106 |
| G357 | E417 | Y477 | P107 |
| L358 | E418 | M478 | G108 |
| T359 | D419 | K479 | T109 |
| E360 | K420 | G480 | L110 |
| L361 | L421 | D481 | G111 |
| G362 | V422 | L482 | R112 |
| I363 | V423 | E483 | I113 |
| Y364 | A424 | E484 | M14 |
| P365 | R425 | S485 | N15 |
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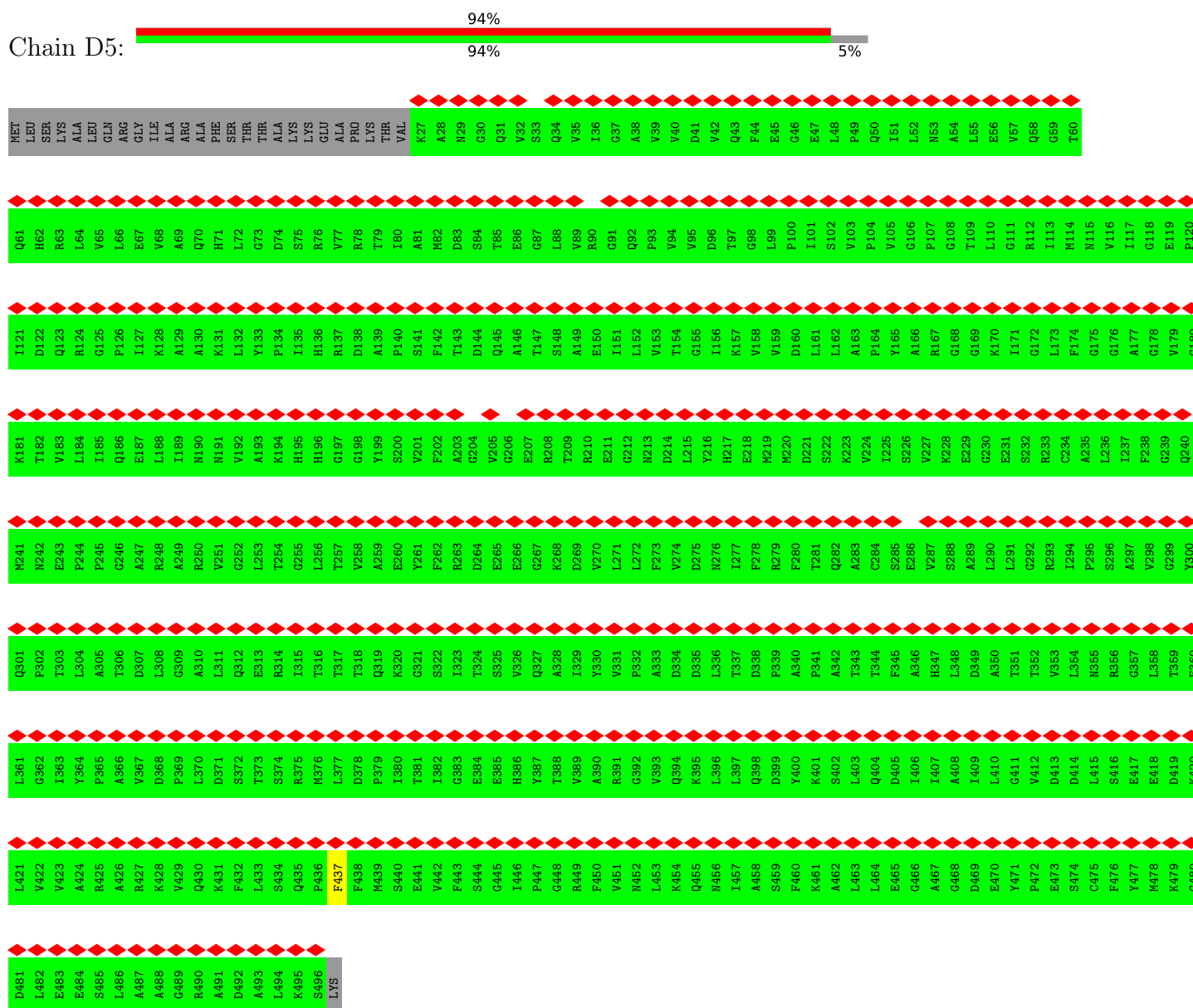
• Molecule 25: ATP synthase subunit beta



| | | | | | | | | |
|------|------|------|------|------|------|------|------|------|
| MET | Q61 | I121 | K181 | M241 | Q391 | L361 | L421 | D481 |
| LEU | H62 | D122 | T182 | N242 | P302 | G362 | V422 | I482 |
| SER | R63 | Q123 | V183 | E243 | T303 | I363 | V423 | E483 |
| ALA | L64 | R124 | L184 | P244 | L304 | Y364 | A424 | E484 |
| LEU | V65 | G125 | I185 | P245 | A305 | P365 | R425 | S485 |
| GLN | L66 | P126 | Q186 | G246 | T306 | A366 | A426 | I486 |
| ARG | E67 | I127 | E187 | A247 | D307 | V367 | R427 | A487 |
| GLY | V68 | K128 | L188 | R248 | L308 | D368 | K428 | A488 |
| ILE | A69 | A129 | I189 | A249 | G309 | P369 | V429 | G489 |
| ALA | Q70 | A130 | N190 | R250 | A310 | L370 | Q430 | R490 |
| ALA | H71 | K131 | M191 | V251 | L311 | D371 | K431 | A491 |
| PHE | L72 | I132 | V192 | G252 | Q312 | S372 | F432 | D492 |
| SER | G73 | V133 | A193 | L253 | E313 | T373 | L433 | A493 |
| THR | D74 | P134 | K194 | T254 | R314 | S374 | S434 | I494 |
| ALA | S75 | I135 | H195 | G255 | I315 | R375 | Q435 | K495 |
| LYS | R76 | H136 | H196 | L256 | T316 | M376 | P436 | S496 |
| GLU | V77 | R137 | G197 | T257 | T317 | L377 | F437 | LYS |
| ALA | R78 | D138 | G198 | V258 | T318 | D378 | F438 | |
| PRO | T79 | A139 | Y199 | A259 | Q319 | P379 | M439 | |
| LYS | T80 | P140 | S200 | E260 | K320 | I380 | S440 | |
| THR | A81 | S141 | V201 | F261 | G321 | T381 | E441 | |
| VAL | D82 | F142 | F202 | G262 | S322 | I382 | V442 | |
| K27 | D83 | T143 | A203 | R263 | I323 | G383 | F443 | |
| A28 | S84 | D144 | G204 | D264 | T324 | E384 | S444 | |
| N29 | T85 | Q145 | V205 | E265 | S325 | E385 | G445 | |
| G30 | E86 | A146 | G206 | E266 | V326 | H386 | I446 | |
| Q31 | G87 | T147 | E207 | G267 | Q327 | Y387 | P447 | |
| V32 | L88 | S148 | R208 | K268 | A328 | T388 | G448 | |
| S33 | W89 | A149 | T209 | D269 | I329 | V389 | R449 | |
| Q34 | R90 | E150 | V270 | K288 | Y330 | A390 | F450 | |
| V35 | G91 | I151 | L271 | L271 | V331 | R391 | V451 | |
| I36 | Q92 | D152 | G212 | L272 | P332 | G392 | N452 | |
| G37 | P93 | V153 | N213 | F273 | A333 | V393 | L453 | |
| A38 | V94 | T154 | D214 | V274 | D334 | Q394 | K454 | |
| V39 | V95 | G155 | L215 | D275 | D335 | K395 | Q455 | |
| D41 | D96 | I156 | V216 | N276 | L336 | K395 | Q455 | |
| V42 | T97 | K157 | H217 | L277 | T337 | L397 | I457 | |
| Q43 | G98 | V158 | E218 | F278 | L336 | L396 | N456 | |
| F44 | L99 | V159 | M219 | R279 | T337 | L397 | I457 | |
| E45 | P100 | D160 | M220 | F280 | D338 | Q398 | A458 | |
| G46 | I101 | L161 | D221 | T281 | P339 | D399 | S459 | |
| E47 | S102 | L162 | G222 | Q282 | A340 | Y400 | F460 | |
| L48 | V103 | A163 | K223 | A283 | P341 | K401 | K461 | |
| P49 | P104 | P164 | V224 | C284 | A342 | S402 | A462 | |
| Q50 | V105 | V165 | I225 | S285 | T343 | L403 | L463 | |
| I51 | L106 | A166 | G226 | E286 | T344 | Q404 | L464 | |
| L52 | P107 | R167 | V227 | V287 | F345 | D405 | E465 | |
| N53 | G108 | G168 | K228 | S288 | A346 | I406 | G466 | |
| A54 | T109 | G169 | E229 | A289 | H347 | I407 | A467 | |
| L55 | L110 | K170 | G230 | L290 | L348 | A408 | G468 | |
| E56 | G111 | I171 | E231 | L291 | D349 | I409 | D469 | |
| V57 | R112 | G172 | S232 | G292 | A350 | L410 | E470 | |
| Q58 | I113 | L173 | R233 | E233 | T351 | G411 | Y471 | |
| S59 | M14 | F174 | C234 | I294 | T352 | V412 | P472 | |
| N15 | V16 | G175 | A235 | P295 | V353 | D413 | E473 | |
| V16 | I117 | G176 | L236 | S296 | L354 | S474 | S474 | |
| I117 | G118 | A177 | I237 | G297 | N355 | C475 | C475 | |
| E119 | P120 | G178 | F238 | G299 | R356 | F476 | F476 | |
| | | V179 | V298 | | G357 | Y477 | Y477 | |
| | | G180 | V298 | | L358 | M478 | M478 | |
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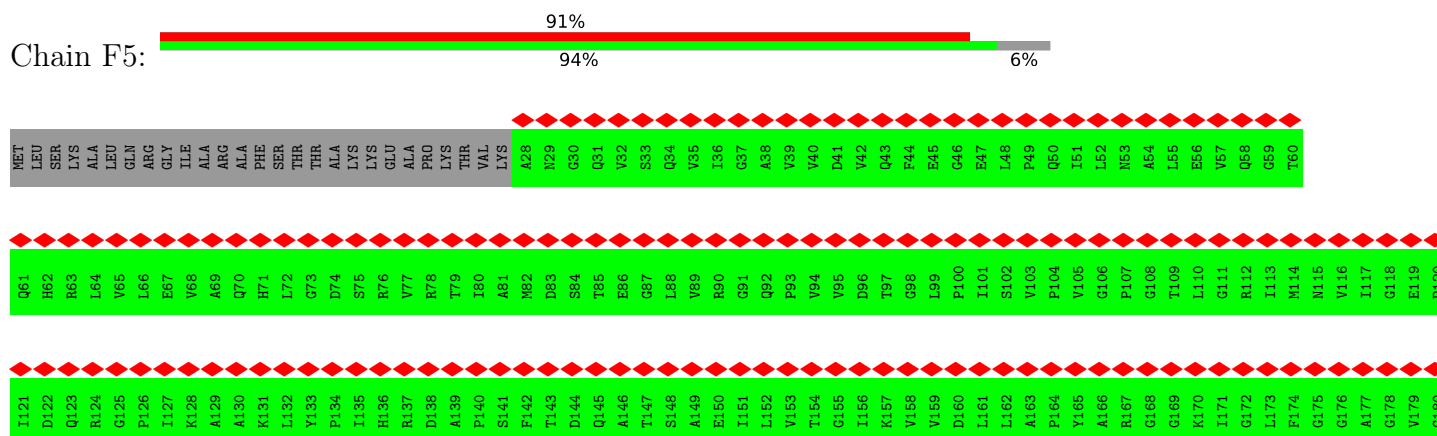
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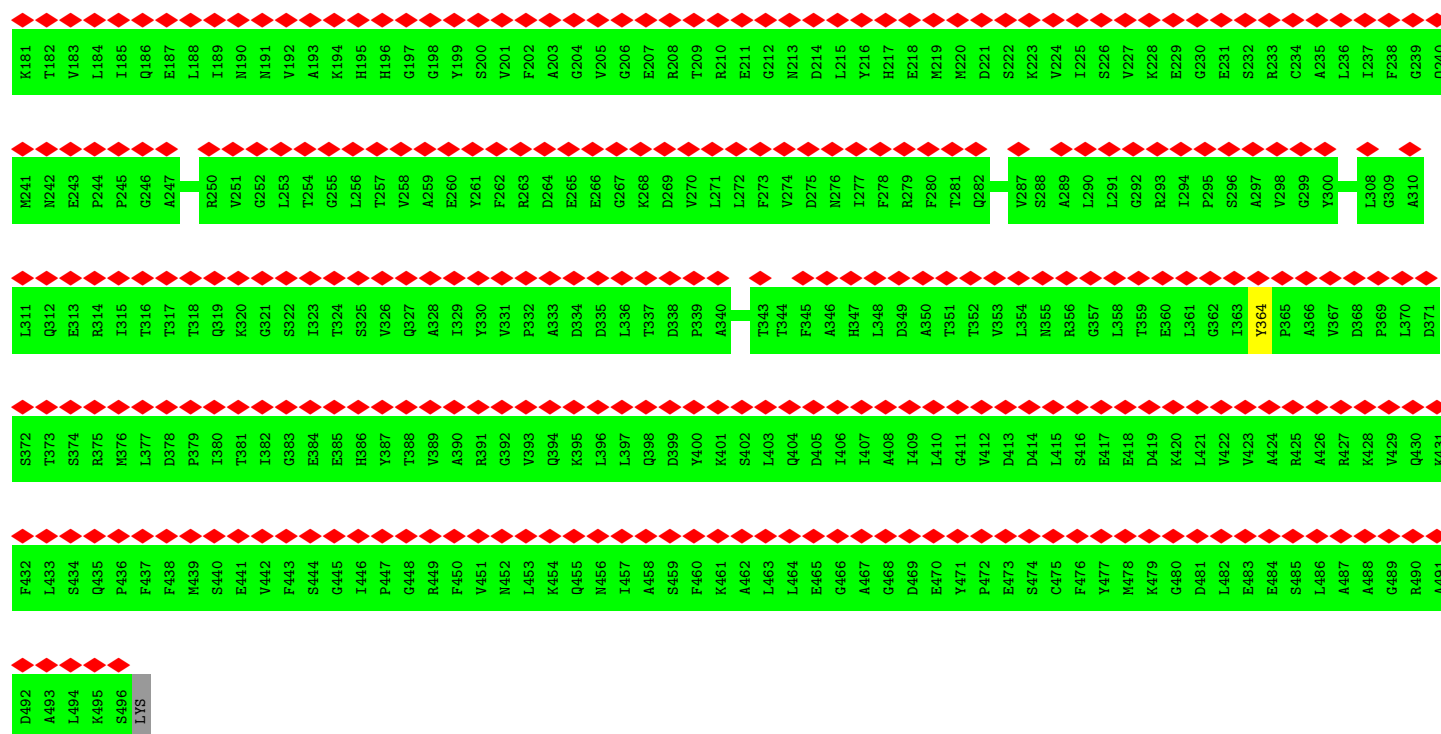
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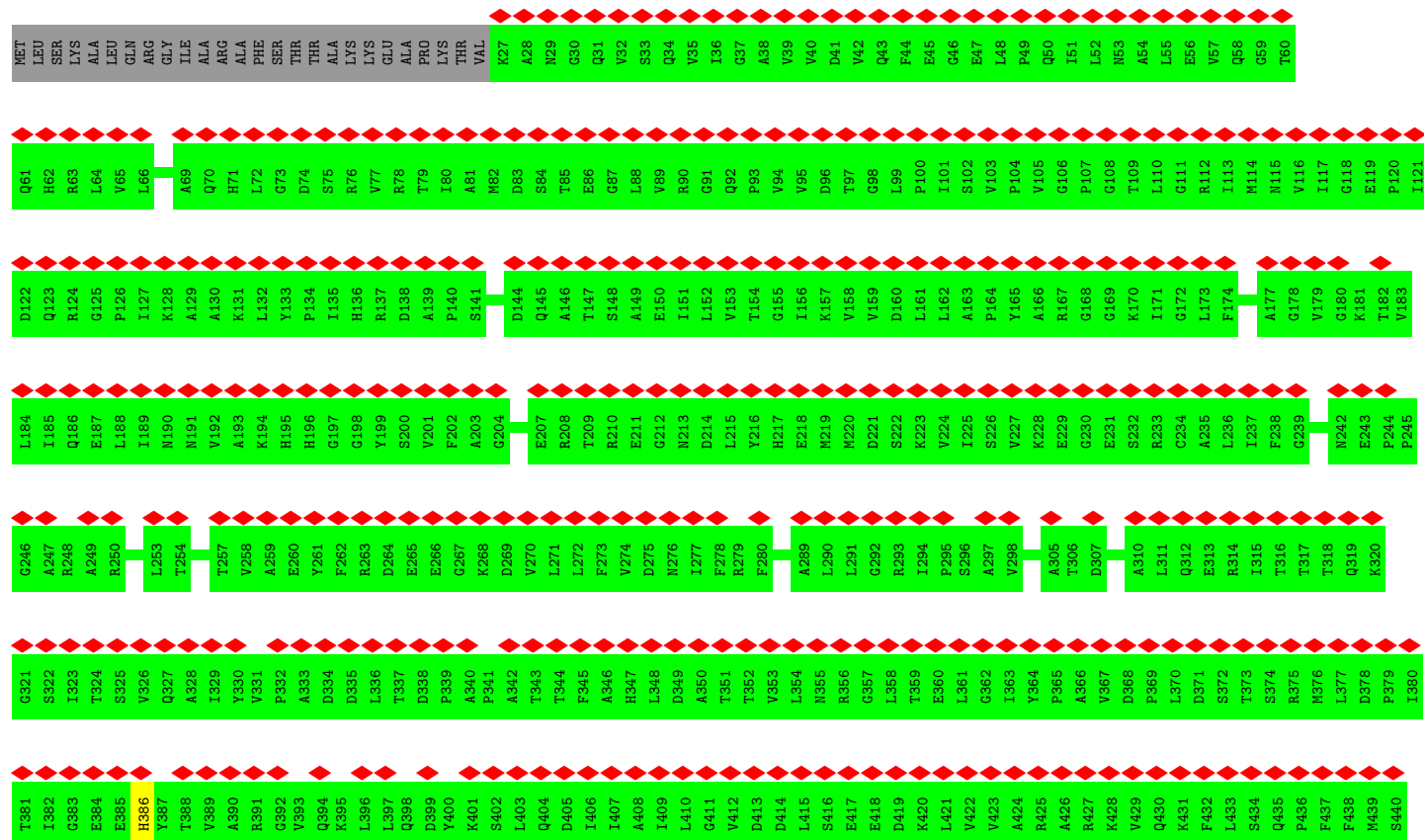
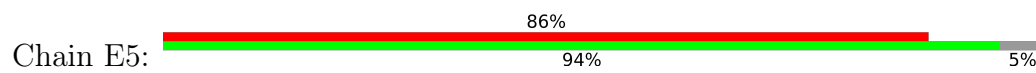
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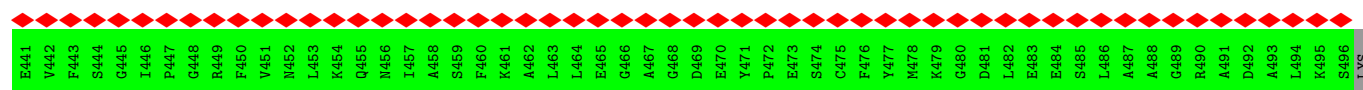
Chain F5:





● Molecule 25: ATP synthase subunit beta





- Molecule 26: ATP synthase F0 subunit 9



- Molecule 26: ATP synthase F0 subunit 9



- Molecule 26: ATP synthase F0 subunit 9



- Molecule 26: ATP synthase F0 subunit 9



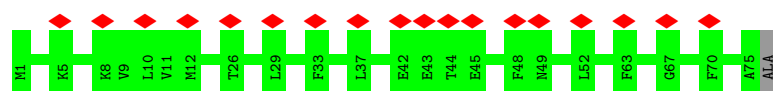
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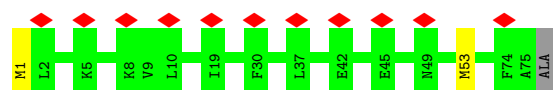
- Molecule 26: ATP synthase F0 subunit 9



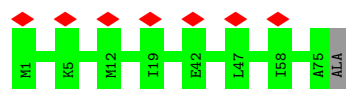
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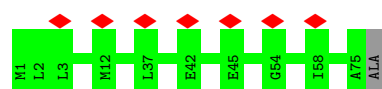
- Molecule 26: ATP synthase F0 subunit 9



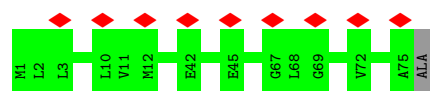
- Molecule 26: ATP synthase F0 subunit 9



- Molecule 26: ATP synthase F0 subunit 9



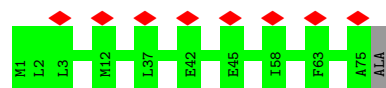
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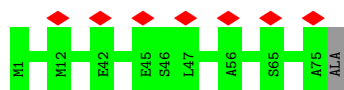
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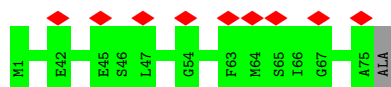
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- Molecule 26: ATP synthase F0 subunit 9



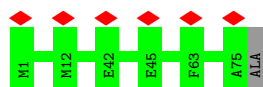
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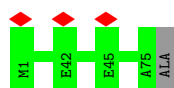
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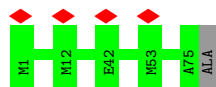
- Molecule 26: ATP synthase F0 subunit 9



- Molecule 26: ATP synthase F0 subunit 9

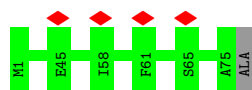


- Molecule 26: ATP synthase F0 subunit 9

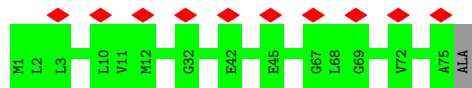


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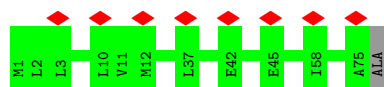




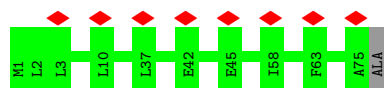
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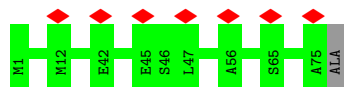
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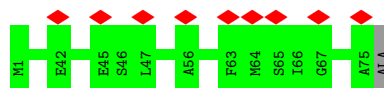
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- Molecule 26: ATP synthase F0 subunit 9



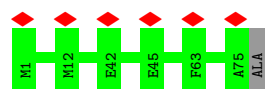
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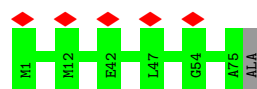
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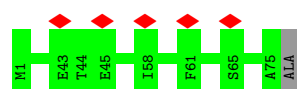
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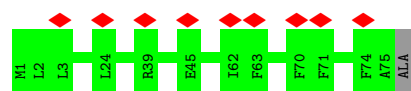
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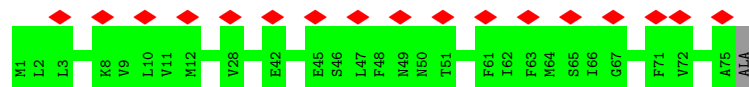
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- Molecule 26: ATP synthase F0 subunit 9



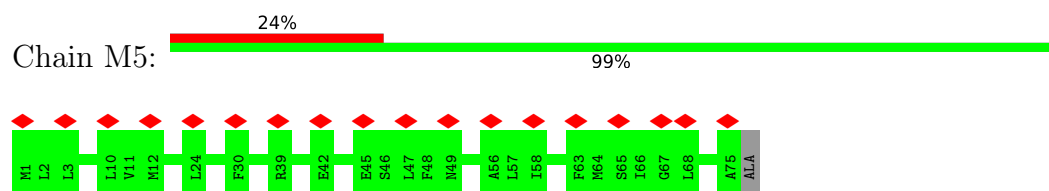
- Molecule 26: ATP synthase F0 subunit 9



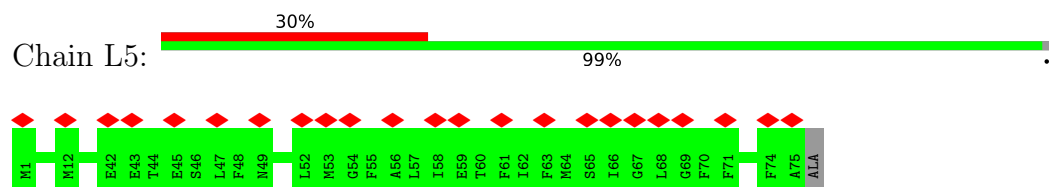
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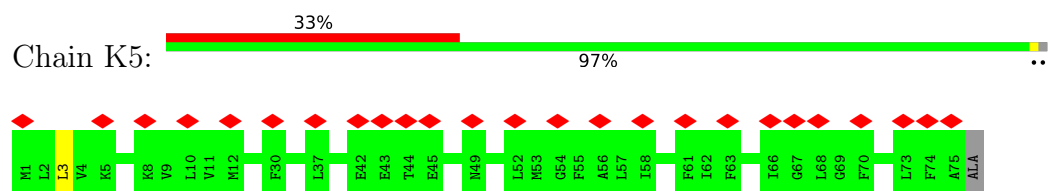
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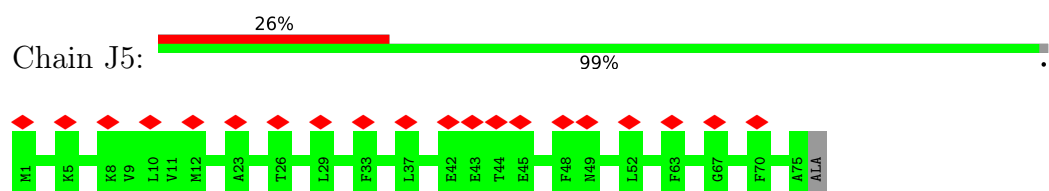
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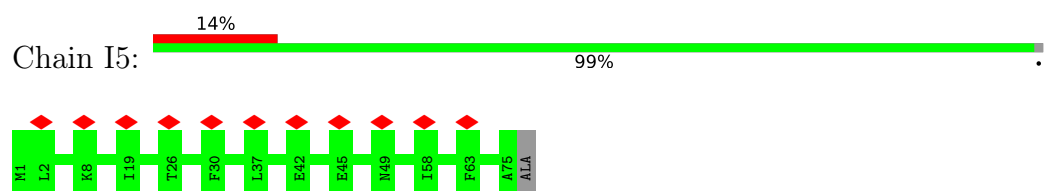
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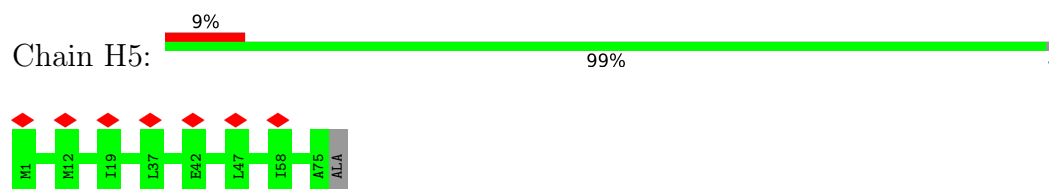
• Molecule 26: ATP synthase F0 subunit 9



• Molecule 26: ATP synthase F0 subunit 9



• Molecule 26: ATP synthase F0 subunit 9

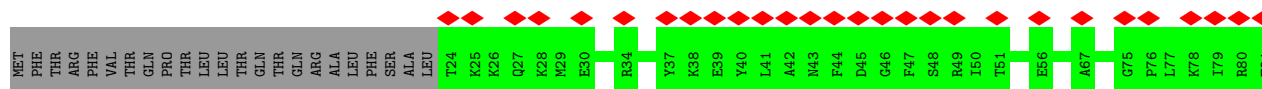
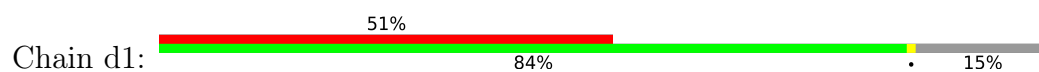


• Molecule 26: ATP synthase F0 subunit 9

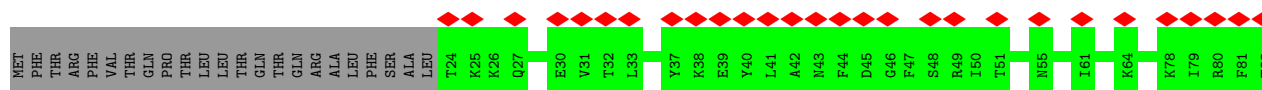
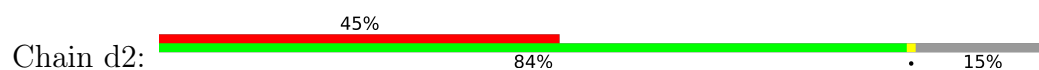




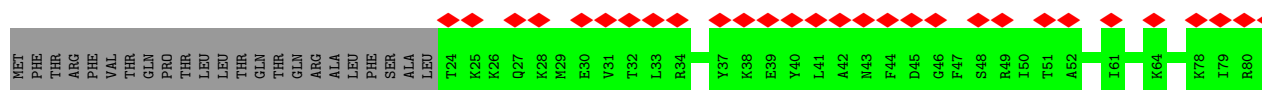
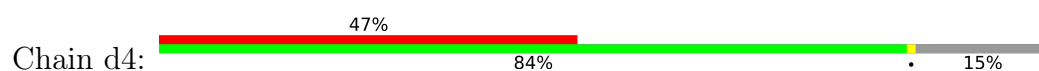
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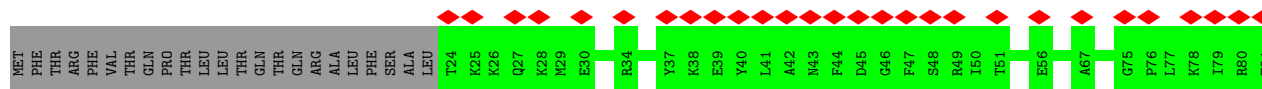
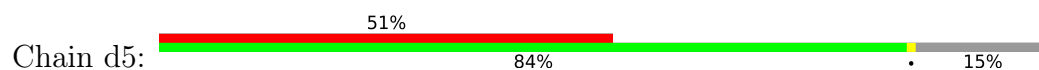
- Molecule 27: subunit delta



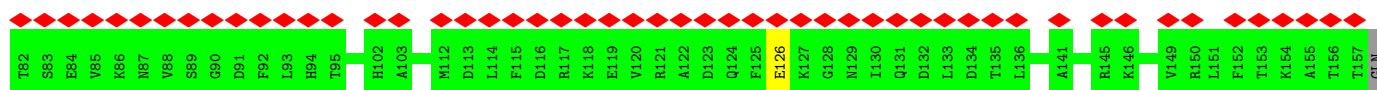
- Molecule 27: subunit delta

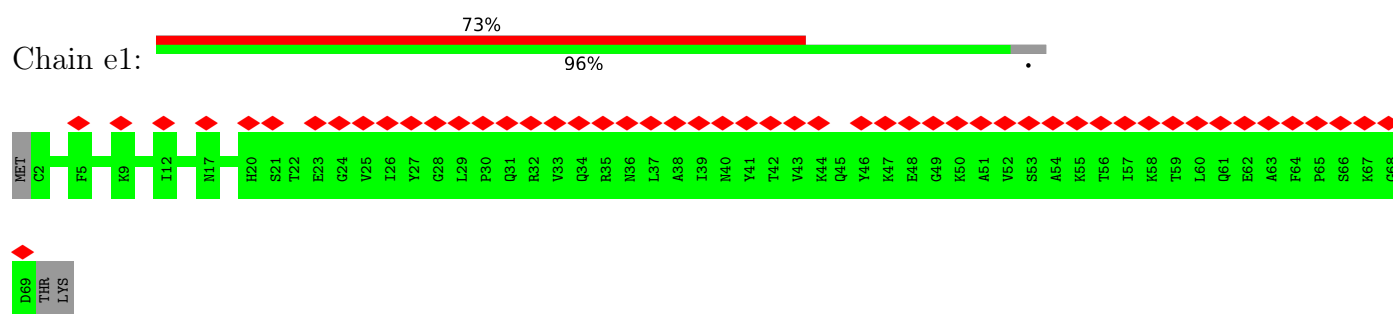


- Molecule 27: subunit delta

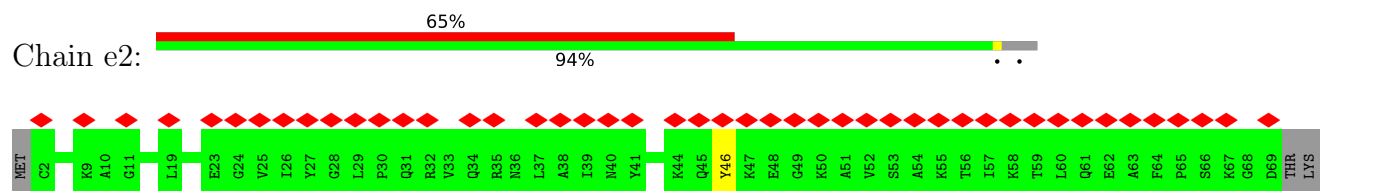


- Molecule 28: subunit epsilon

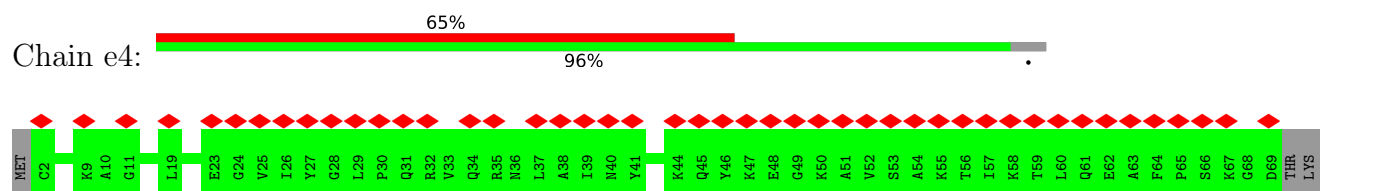




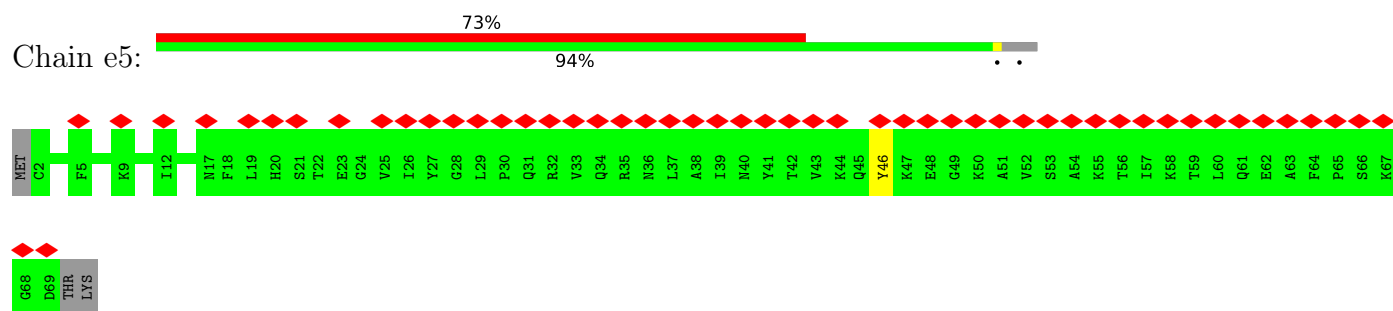
- Molecule 28: subunit epsilon



- Molecule 28: subunit epsilon



- Molecule 28: subunit epsilon



4 Experimental information

| Property | Value | Source |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C2 | Depositor |
| Number of particles used | 40691 | 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 ($e^-/\text{\AA}^2$) | 30.9 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | 165000 | Depositor |
| Image detector | GATAN K2 QUANTUM (4k x 4k) | Depositor |
| Maximum map value | 0.070 | Depositor |
| Minimum map value | -0.027 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.003 | Depositor |
| Recommended contour level | 0.012 | Depositor |
| Map size (Å) | 498.0, 498.0, 498.0 | wwPDB |
| Map dimensions | 600, 600, 600 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.83, 0.83, 0.83 | Depositor |

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, CDL, PO4, MG, PEE, PC1, UQ8, NAD, ATP

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------|-------------|-------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | A | 0.29 | 0/3752 | 0.38 | 0/5109 |
| 1 | A3 | 0.29 | 0/3752 | 0.38 | 0/5109 |
| 1 | a | 0.29 | 0/3752 | 0.38 | 0/5109 |
| 1 | a3 | 0.30 | 0/3752 | 0.38 | 0/5109 |
| 2 | B | 0.26 | 0/2940 | 0.36 | 0/3969 |
| 2 | B3 | 0.26 | 0/2940 | 0.36 | 0/3969 |
| 2 | b | 0.26 | 0/2940 | 0.36 | 0/3969 |
| 2 | b3 | 0.26 | 0/2940 | 0.36 | 0/3969 |
| 3 | D | 0.26 | 0/1715 | 0.37 | 0/2321 |
| 3 | D3 | 0.26 | 0/1715 | 0.37 | 0/2321 |
| 3 | d | 0.26 | 0/1715 | 0.37 | 0/2321 |
| 3 | d3 | 0.26 | 0/1715 | 0.37 | 0/2321 |
| 4 | F | 0.29 | 0/1733 | 0.40 | 0/2327 |
| 4 | F3 | 0.29 | 0/1733 | 0.39 | 0/2327 |
| 4 | f | 0.29 | 0/1733 | 0.39 | 0/2327 |
| 4 | f3 | 0.29 | 0/1733 | 0.39 | 0/2327 |
| 5 | I | 0.29 | 0/1771 | 0.38 | 0/2394 |
| 5 | I3 | 0.28 | 0/1771 | 0.38 | 0/2394 |
| 5 | i | 0.28 | 0/1771 | 0.39 | 0/2394 |
| 5 | i3 | 0.29 | 0/1771 | 0.38 | 0/2394 |
| 6 | K | 0.26 | 0/1508 | 0.37 | 0/2024 |
| 6 | K3 | 0.26 | 0/1508 | 0.37 | 0/2024 |
| 6 | k | 0.26 | 0/1508 | 0.38 | 0/2024 |
| 6 | k3 | 0.26 | 0/1508 | 0.38 | 0/2024 |
| 7 | C | 0.28 | 0/866 | 0.39 | 0/1176 |
| 7 | C3 | 0.27 | 0/866 | 0.39 | 0/1176 |
| 7 | c | 0.27 | 0/866 | 0.39 | 0/1176 |
| 7 | c3 | 0.28 | 0/866 | 0.38 | 0/1176 |
| 8 | G | 0.28 | 0/2302 | 0.40 | 0/3115 |
| 8 | G3 | 0.27 | 0/2302 | 0.40 | 0/3115 |
| 8 | g | 0.27 | 0/2302 | 0.40 | 0/3115 |
| 8 | g3 | 0.28 | 0/2302 | 0.40 | 0/3115 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 9 | H | 0.26 | 0/2006 | 0.39 | 0/2704 |
| 9 | H3 | 0.26 | 0/2006 | 0.39 | 0/2704 |
| 9 | h | 0.25 | 0/2006 | 0.39 | 0/2704 |
| 9 | h3 | 0.26 | 0/2006 | 0.38 | 0/2704 |
| 10 | J | 0.28 | 0/2256 | 0.40 | 0/3069 |
| 10 | J3 | 0.27 | 0/2256 | 0.40 | 0/3069 |
| 10 | j | 0.27 | 0/2256 | 0.40 | 0/3069 |
| 10 | j3 | 0.28 | 0/2256 | 0.40 | 0/3069 |
| 11 | L | 0.29 | 0/2140 | 0.39 | 0/2903 |
| 11 | L3 | 0.29 | 0/2140 | 0.39 | 0/2903 |
| 11 | l | 0.29 | 0/2140 | 0.39 | 0/2903 |
| 11 | l3 | 0.29 | 0/2140 | 0.38 | 0/2903 |
| 12 | M | 0.28 | 0/1912 | 0.37 | 0/2598 |
| 12 | M3 | 0.27 | 0/1912 | 0.37 | 0/2598 |
| 12 | m | 0.27 | 0/1912 | 0.37 | 0/2598 |
| 12 | m3 | 0.28 | 0/1912 | 0.37 | 0/2598 |
| 13 | N | 0.30 | 0/1030 | 0.39 | 0/1393 |
| 13 | N3 | 0.29 | 0/1030 | 0.39 | 0/1393 |
| 13 | n | 0.29 | 0/1030 | 0.40 | 0/1393 |
| 13 | n3 | 0.30 | 0/1030 | 0.40 | 0/1393 |
| 14 | O | 0.26 | 0/821 | 0.39 | 0/1104 |
| 14 | O3 | 0.26 | 0/821 | 0.40 | 0/1104 |
| 14 | o | 0.27 | 0/821 | 0.40 | 0/1104 |
| 14 | o3 | 0.26 | 0/821 | 0.40 | 0/1104 |
| 15 | P | 0.25 | 0/1249 | 0.37 | 0/1695 |
| 15 | P3 | 0.24 | 0/1249 | 0.37 | 0/1695 |
| 15 | p | 0.24 | 0/1249 | 0.38 | 0/1695 |
| 15 | p3 | 0.25 | 0/1249 | 0.38 | 0/1695 |
| 16 | Q | 0.26 | 0/888 | 0.39 | 0/1200 |
| 16 | Q3 | 0.25 | 0/888 | 0.39 | 0/1200 |
| 16 | q | 0.25 | 0/888 | 0.39 | 0/1200 |
| 16 | q3 | 0.26 | 0/888 | 0.39 | 0/1200 |
| 17 | R | 0.28 | 0/1185 | 0.38 | 0/1594 |
| 17 | R3 | 0.28 | 0/1185 | 0.38 | 0/1594 |
| 17 | r | 0.28 | 0/1225 | 0.38 | 0/1649 |
| 17 | r3 | 0.29 | 0/1225 | 0.38 | 0/1649 |
| 18 | S | 0.26 | 0/1044 | 0.41 | 0/1414 |
| 18 | S3 | 0.26 | 0/1044 | 0.41 | 0/1414 |
| 18 | s | 0.25 | 0/1037 | 0.41 | 0/1404 |
| 18 | s3 | 0.26 | 0/1037 | 0.41 | 0/1404 |
| 19 | E | 0.25 | 0/3492 | 0.40 | 0/4720 |
| 19 | E3 | 0.25 | 0/3492 | 0.40 | 0/4720 |
| 19 | e | 0.24 | 0/3492 | 0.40 | 0/4720 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 19 | e3 | 0.25 | 0/3492 | 0.40 | 0/4720 |
| 20 | i1 | 0.22 | 0/593 | 0.34 | 0/795 |
| 20 | i2 | 0.22 | 0/563 | 0.34 | 0/753 |
| 20 | i4 | 0.22 | 0/593 | 0.34 | 0/795 |
| 20 | i5 | 0.22 | 0/563 | 0.34 | 0/753 |
| 21 | t | 0.25 | 0/3103 | 0.39 | 0/4200 |
| 21 | t3 | 0.25 | 0/3103 | 0.39 | 0/4200 |
| 22 | G1 | 0.24 | 0/1507 | 0.37 | 0/2027 |
| 22 | G2 | 0.24 | 0/1507 | 0.37 | 0/2027 |
| 22 | G4 | 0.24 | 0/1507 | 0.37 | 0/2027 |
| 22 | G5 | 0.24 | 0/1507 | 0.37 | 0/2027 |
| 23 | g1 | 0.24 | 0/2156 | 0.38 | 0/2900 |
| 23 | g2 | 0.24 | 0/2156 | 0.38 | 0/2900 |
| 23 | g4 | 0.24 | 0/2156 | 0.38 | 0/2900 |
| 23 | g5 | 0.24 | 0/2156 | 0.38 | 0/2900 |
| 24 | A1 | 0.24 | 0/3961 | 0.40 | 0/5346 |
| 24 | A2 | 0.24 | 0/3961 | 0.40 | 0/5346 |
| 24 | A4 | 0.24 | 0/3961 | 0.40 | 0/5346 |
| 24 | A5 | 0.24 | 0/3961 | 0.40 | 0/5346 |
| 24 | B1 | 0.24 | 0/3956 | 0.40 | 0/5339 |
| 24 | B2 | 0.24 | 0/3956 | 0.40 | 0/5339 |
| 24 | B4 | 0.23 | 0/3956 | 0.40 | 0/5339 |
| 24 | B5 | 0.24 | 0/3956 | 0.40 | 0/5339 |
| 24 | C1 | 0.24 | 0/3974 | 0.40 | 0/5361 |
| 24 | C2 | 0.24 | 0/3974 | 0.40 | 0/5361 |
| 24 | C4 | 0.24 | 0/3974 | 0.40 | 0/5361 |
| 24 | C5 | 0.24 | 0/3974 | 0.40 | 0/5361 |
| 25 | D1 | 0.24 | 0/3613 | 0.39 | 0/4900 |
| 25 | D2 | 0.24 | 0/3613 | 0.40 | 0/4900 |
| 25 | D4 | 0.24 | 0/3613 | 0.39 | 0/4900 |
| 25 | D5 | 0.24 | 0/3613 | 0.39 | 0/4900 |
| 25 | E1 | 0.24 | 0/3613 | 0.40 | 0/4900 |
| 25 | E2 | 0.24 | 0/3613 | 0.40 | 0/4900 |
| 25 | E4 | 0.24 | 0/3613 | 0.40 | 0/4900 |
| 25 | E5 | 0.24 | 0/3613 | 0.40 | 0/4900 |
| 25 | F1 | 0.24 | 0/3604 | 0.40 | 0/4889 |
| 25 | F2 | 0.24 | 0/3604 | 0.40 | 0/4889 |
| 25 | F4 | 0.24 | 0/3604 | 0.40 | 0/4889 |
| 25 | F5 | 0.24 | 0/3604 | 0.40 | 0/4889 |
| 26 | H1 | 0.27 | 0/572 | 0.35 | 0/771 |
| 26 | H2 | 0.27 | 0/572 | 0.37 | 0/771 |
| 26 | H4 | 0.27 | 0/572 | 0.35 | 0/771 |
| 26 | H5 | 0.27 | 0/572 | 0.36 | 0/771 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 26 | I1 | 0.27 | 0/572 | 0.36 | 0/771 |
| 26 | I2 | 0.27 | 0/572 | 0.37 | 0/771 |
| 26 | I4 | 0.27 | 0/572 | 0.36 | 0/771 |
| 26 | I5 | 0.27 | 0/572 | 0.37 | 0/771 |
| 26 | J1 | 0.27 | 0/572 | 0.35 | 0/771 |
| 26 | J2 | 0.26 | 0/572 | 0.35 | 0/771 |
| 26 | J4 | 0.27 | 0/572 | 0.35 | 0/771 |
| 26 | J5 | 0.27 | 0/572 | 0.35 | 0/771 |
| 26 | K1 | 0.27 | 0/572 | 0.35 | 0/771 |
| 26 | K2 | 0.26 | 0/572 | 0.36 | 0/771 |
| 26 | K4 | 0.26 | 0/572 | 0.35 | 0/771 |
| 26 | K5 | 0.26 | 0/572 | 0.36 | 0/771 |
| 26 | L1 | 0.26 | 0/572 | 0.35 | 0/771 |
| 26 | L2 | 0.26 | 0/572 | 0.35 | 0/771 |
| 26 | L4 | 0.26 | 0/572 | 0.35 | 0/771 |
| 26 | L5 | 0.26 | 0/572 | 0.35 | 0/771 |
| 26 | M1 | 0.26 | 0/572 | 0.35 | 0/771 |
| 26 | M2 | 0.26 | 0/572 | 0.35 | 0/771 |
| 26 | M4 | 0.26 | 0/572 | 0.35 | 0/771 |
| 26 | M5 | 0.26 | 0/572 | 0.35 | 0/771 |
| 26 | N1 | 0.26 | 0/572 | 0.35 | 0/771 |
| 26 | N2 | 0.26 | 0/572 | 0.35 | 0/771 |
| 26 | N4 | 0.26 | 0/572 | 0.35 | 0/771 |
| 26 | N5 | 0.26 | 0/572 | 0.35 | 0/771 |
| 26 | O1 | 0.26 | 0/572 | 0.35 | 0/771 |
| 26 | O2 | 0.27 | 0/572 | 0.35 | 0/771 |
| 26 | O4 | 0.26 | 0/572 | 0.35 | 0/771 |
| 26 | O5 | 0.26 | 0/572 | 0.35 | 0/771 |
| 26 | P1 | 0.26 | 0/572 | 0.36 | 0/771 |
| 26 | P2 | 0.26 | 0/572 | 0.35 | 0/771 |
| 26 | P4 | 0.26 | 0/572 | 0.36 | 0/771 |
| 26 | P5 | 0.26 | 0/572 | 0.35 | 0/771 |
| 26 | Q1 | 0.27 | 0/572 | 0.35 | 0/771 |
| 26 | Q2 | 0.26 | 0/572 | 0.34 | 0/771 |
| 26 | Q4 | 0.27 | 0/572 | 0.35 | 0/771 |
| 26 | Q5 | 0.26 | 0/572 | 0.35 | 0/771 |
| 27 | d1 | 0.25 | 0/1081 | 0.45 | 0/1459 |
| 27 | d2 | 0.25 | 0/1081 | 0.45 | 0/1459 |
| 27 | d4 | 0.25 | 0/1081 | 0.44 | 0/1459 |
| 27 | d5 | 0.25 | 0/1081 | 0.45 | 0/1459 |
| 28 | e1 | 0.24 | 0/547 | 0.41 | 0/735 |
| 28 | e2 | 0.24 | 0/547 | 0.42 | 0/735 |
| 28 | e4 | 0.24 | 0/547 | 0.41 | 0/735 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------|-------------|-------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 28 | e5 | 0.24 | 0/547 | 0.41 | 0/735 |
| All | All | 0.26 | 0/281952 | 0.39 | 0/381166 |

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 |
|-----|-------|---------------------|---------------------|
| 25 | F1 | 0 | 1 |
| 25 | F2 | 0 | 1 |
| 25 | F4 | 0 | 1 |
| 25 | F5 | 0 | 1 |
| 28 | e2 | 0 | 1 |
| 28 | e5 | 0 | 1 |
| All | All | 0 | 6 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 25 | F1 | 364 | TYR | Peptide |
| 25 | F2 | 364 | TYR | Peptide |
| 25 | F4 | 364 | TYR | Peptide |
| 25 | F5 | 364 | TYR | Peptide |
| 28 | e2 | 46 | TYR | 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 | A | 431/446 (97%) | 426 (99%) | 5 (1%) | 0 | 100 | 100 |
| 1 | A3 | 431/446 (97%) | 426 (99%) | 5 (1%) | 0 | 100 | 100 |
| 1 | a | 431/446 (97%) | 423 (98%) | 8 (2%) | 0 | 100 | 100 |
| 1 | a3 | 431/446 (97%) | 421 (98%) | 10 (2%) | 0 | 100 | 100 |
| 2 | B | 352/381 (92%) | 341 (97%) | 11 (3%) | 0 | 100 | 100 |
| 2 | B3 | 352/381 (92%) | 341 (97%) | 11 (3%) | 0 | 100 | 100 |
| 2 | b | 352/381 (92%) | 340 (97%) | 12 (3%) | 0 | 100 | 100 |
| 2 | b3 | 352/381 (92%) | 339 (96%) | 13 (4%) | 0 | 100 | 100 |
| 3 | D | 204/234 (87%) | 199 (98%) | 5 (2%) | 0 | 100 | 100 |
| 3 | D3 | 204/234 (87%) | 198 (97%) | 6 (3%) | 0 | 100 | 100 |
| 3 | d | 204/234 (87%) | 198 (97%) | 6 (3%) | 0 | 100 | 100 |
| 3 | d3 | 204/234 (87%) | 198 (97%) | 6 (3%) | 0 | 100 | 100 |
| 4 | F | 198/204 (97%) | 197 (100%) | 1 (0%) | 0 | 100 | 100 |
| 4 | F3 | 198/204 (97%) | 197 (100%) | 1 (0%) | 0 | 100 | 100 |
| 4 | f | 198/204 (97%) | 197 (100%) | 1 (0%) | 0 | 100 | 100 |
| 4 | f3 | 198/204 (97%) | 196 (99%) | 2 (1%) | 0 | 100 | 100 |
| 5 | I | 207/209 (99%) | 199 (96%) | 8 (4%) | 0 | 100 | 100 |
| 5 | I3 | 207/209 (99%) | 199 (96%) | 8 (4%) | 0 | 100 | 100 |
| 5 | i | 207/209 (99%) | 202 (98%) | 5 (2%) | 0 | 100 | 100 |
| 5 | i3 | 207/209 (99%) | 202 (98%) | 5 (2%) | 0 | 100 | 100 |
| 6 | K | 177/179 (99%) | 166 (94%) | 11 (6%) | 0 | 100 | 100 |
| 6 | K3 | 177/179 (99%) | 166 (94%) | 11 (6%) | 0 | 100 | 100 |
| 6 | k | 177/179 (99%) | 169 (96%) | 8 (4%) | 0 | 100 | 100 |
| 6 | k3 | 177/179 (99%) | 169 (96%) | 8 (4%) | 0 | 100 | 100 |
| 7 | C | 94/100 (94%) | 90 (96%) | 4 (4%) | 0 | 100 | 100 |
| 7 | C3 | 94/100 (94%) | 90 (96%) | 4 (4%) | 0 | 100 | 100 |
| 7 | c | 94/100 (94%) | 90 (96%) | 4 (4%) | 0 | 100 | 100 |
| 7 | c3 | 94/100 (94%) | 90 (96%) | 4 (4%) | 0 | 100 | 100 |
| 8 | G | 254/286 (89%) | 245 (96%) | 9 (4%) | 0 | 100 | 100 |
| 8 | G3 | 254/286 (89%) | 246 (97%) | 8 (3%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 8 | g | 254/286 (89%) | 243 (96%) | 11 (4%) | 0 | 100 | 100 |
| 8 | g3 | 254/286 (89%) | 244 (96%) | 10 (4%) | 0 | 100 | 100 |
| 9 | H | 229/268 (85%) | 226 (99%) | 3 (1%) | 0 | 100 | 100 |
| 9 | H3 | 229/268 (85%) | 225 (98%) | 4 (2%) | 0 | 100 | 100 |
| 9 | h | 229/268 (85%) | 225 (98%) | 4 (2%) | 0 | 100 | 100 |
| 9 | h3 | 229/268 (85%) | 226 (99%) | 3 (1%) | 0 | 100 | 100 |
| 10 | J | 267/273 (98%) | 261 (98%) | 6 (2%) | 0 | 100 | 100 |
| 10 | J3 | 267/273 (98%) | 261 (98%) | 6 (2%) | 0 | 100 | 100 |
| 10 | j | 267/273 (98%) | 263 (98%) | 4 (2%) | 0 | 100 | 100 |
| 10 | j3 | 267/273 (98%) | 262 (98%) | 5 (2%) | 0 | 100 | 100 |
| 11 | L | 244/247 (99%) | 239 (98%) | 5 (2%) | 0 | 100 | 100 |
| 11 | L3 | 244/247 (99%) | 239 (98%) | 5 (2%) | 0 | 100 | 100 |
| 11 | l | 244/247 (99%) | 241 (99%) | 3 (1%) | 0 | 100 | 100 |
| 11 | l3 | 244/247 (99%) | 241 (99%) | 3 (1%) | 0 | 100 | 100 |
| 12 | M | 219/221 (99%) | 219 (100%) | 0 | 0 | 100 | 100 |
| 12 | M3 | 219/221 (99%) | 219 (100%) | 0 | 0 | 100 | 100 |
| 12 | m | 219/221 (99%) | 218 (100%) | 1 (0%) | 0 | 100 | 100 |
| 12 | m3 | 219/221 (99%) | 217 (99%) | 2 (1%) | 0 | 100 | 100 |
| 13 | N | 117/179 (65%) | 114 (97%) | 3 (3%) | 0 | 100 | 100 |
| 13 | N3 | 117/179 (65%) | 114 (97%) | 3 (3%) | 0 | 100 | 100 |
| 13 | n | 117/179 (65%) | 115 (98%) | 2 (2%) | 0 | 100 | 100 |
| 13 | n3 | 117/179 (65%) | 115 (98%) | 2 (2%) | 0 | 100 | 100 |
| 14 | O | 97/154 (63%) | 95 (98%) | 2 (2%) | 0 | 100 | 100 |
| 14 | O3 | 97/154 (63%) | 95 (98%) | 2 (2%) | 0 | 100 | 100 |
| 14 | o | 97/154 (63%) | 96 (99%) | 1 (1%) | 0 | 100 | 100 |
| 14 | o3 | 97/154 (63%) | 96 (99%) | 1 (1%) | 0 | 100 | 100 |
| 15 | P | 148/152 (97%) | 140 (95%) | 8 (5%) | 0 | 100 | 100 |
| 15 | P3 | 148/152 (97%) | 140 (95%) | 8 (5%) | 0 | 100 | 100 |
| 15 | p | 148/152 (97%) | 139 (94%) | 9 (6%) | 0 | 100 | 100 |
| 15 | p3 | 148/152 (97%) | 138 (93%) | 10 (7%) | 0 | 100 | 100 |
| 16 | Q | 106/152 (70%) | 105 (99%) | 1 (1%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 16 | Q3 | 106/152 (70%) | 105 (99%) | 1 (1%) | 0 | 100 | 100 |
| 16 | q | 106/152 (70%) | 105 (99%) | 1 (1%) | 0 | 100 | 100 |
| 16 | q3 | 106/152 (70%) | 105 (99%) | 1 (1%) | 0 | 100 | 100 |
| 17 | R | 138/149 (93%) | 136 (99%) | 2 (1%) | 0 | 100 | 100 |
| 17 | R3 | 138/149 (93%) | 136 (99%) | 2 (1%) | 0 | 100 | 100 |
| 17 | r | 143/149 (96%) | 142 (99%) | 1 (1%) | 0 | 100 | 100 |
| 17 | r3 | 143/149 (96%) | 142 (99%) | 1 (1%) | 0 | 100 | 100 |
| 18 | S | 123/145 (85%) | 118 (96%) | 5 (4%) | 0 | 100 | 100 |
| 18 | S3 | 123/145 (85%) | 121 (98%) | 2 (2%) | 0 | 100 | 100 |
| 18 | s | 122/145 (84%) | 122 (100%) | 0 | 0 | 100 | 100 |
| 18 | s3 | 122/145 (84%) | 122 (100%) | 0 | 0 | 100 | 100 |
| 19 | E | 415/480 (86%) | 407 (98%) | 8 (2%) | 0 | 100 | 100 |
| 19 | E3 | 415/480 (86%) | 406 (98%) | 9 (2%) | 0 | 100 | 100 |
| 19 | e | 415/480 (86%) | 405 (98%) | 10 (2%) | 0 | 100 | 100 |
| 19 | e3 | 415/480 (86%) | 403 (97%) | 12 (3%) | 0 | 100 | 100 |
| 20 | i1 | 64/108 (59%) | 64 (100%) | 0 | 0 | 100 | 100 |
| 20 | i2 | 60/108 (56%) | 60 (100%) | 0 | 0 | 100 | 100 |
| 20 | i4 | 64/108 (59%) | 64 (100%) | 0 | 0 | 100 | 100 |
| 20 | i5 | 60/108 (56%) | 60 (100%) | 0 | 0 | 100 | 100 |
| 21 | t | 363/460 (79%) | 360 (99%) | 3 (1%) | 0 | 100 | 100 |
| 21 | t3 | 363/460 (79%) | 360 (99%) | 3 (1%) | 0 | 100 | 100 |
| 22 | G1 | 186/219 (85%) | 176 (95%) | 10 (5%) | 0 | 100 | 100 |
| 22 | G2 | 186/219 (85%) | 176 (95%) | 10 (5%) | 0 | 100 | 100 |
| 22 | G4 | 186/219 (85%) | 176 (95%) | 10 (5%) | 0 | 100 | 100 |
| 22 | G5 | 186/219 (85%) | 176 (95%) | 10 (5%) | 0 | 100 | 100 |
| 23 | g1 | 273/299 (91%) | 265 (97%) | 8 (3%) | 0 | 100 | 100 |
| 23 | g2 | 273/299 (91%) | 265 (97%) | 8 (3%) | 0 | 100 | 100 |
| 23 | g4 | 273/299 (91%) | 265 (97%) | 8 (3%) | 0 | 100 | 100 |
| 23 | g5 | 273/299 (91%) | 264 (97%) | 9 (3%) | 0 | 100 | 100 |
| 24 | A1 | 510/546 (93%) | 504 (99%) | 6 (1%) | 0 | 100 | 100 |
| 24 | A2 | 510/546 (93%) | 502 (98%) | 8 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 24 | A4 | 510/546 (93%) | 503 (99%) | 7 (1%) | 0 | 100 | 100 |
| 24 | A5 | 510/546 (93%) | 502 (98%) | 8 (2%) | 0 | 100 | 100 |
| 24 | B1 | 509/546 (93%) | 498 (98%) | 10 (2%) | 1 (0%) | 44 | 74 |
| 24 | B2 | 509/546 (93%) | 500 (98%) | 9 (2%) | 0 | 100 | 100 |
| 24 | B4 | 509/546 (93%) | 498 (98%) | 10 (2%) | 1 (0%) | 44 | 74 |
| 24 | B5 | 509/546 (93%) | 499 (98%) | 10 (2%) | 0 | 100 | 100 |
| 24 | C1 | 511/546 (94%) | 509 (100%) | 2 (0%) | 0 | 100 | 100 |
| 24 | C2 | 511/546 (94%) | 508 (99%) | 3 (1%) | 0 | 100 | 100 |
| 24 | C4 | 511/546 (94%) | 509 (100%) | 2 (0%) | 0 | 100 | 100 |
| 24 | C5 | 511/546 (94%) | 507 (99%) | 4 (1%) | 0 | 100 | 100 |
| 25 | D1 | 468/497 (94%) | 461 (98%) | 7 (2%) | 0 | 100 | 100 |
| 25 | D2 | 468/497 (94%) | 463 (99%) | 5 (1%) | 0 | 100 | 100 |
| 25 | D4 | 468/497 (94%) | 461 (98%) | 7 (2%) | 0 | 100 | 100 |
| 25 | D5 | 468/497 (94%) | 462 (99%) | 6 (1%) | 0 | 100 | 100 |
| 25 | E1 | 468/497 (94%) | 458 (98%) | 10 (2%) | 0 | 100 | 100 |
| 25 | E2 | 468/497 (94%) | 459 (98%) | 9 (2%) | 0 | 100 | 100 |
| 25 | E4 | 468/497 (94%) | 458 (98%) | 10 (2%) | 0 | 100 | 100 |
| 25 | E5 | 468/497 (94%) | 459 (98%) | 9 (2%) | 0 | 100 | 100 |
| 25 | F1 | 467/497 (94%) | 454 (97%) | 13 (3%) | 0 | 100 | 100 |
| 25 | F2 | 467/497 (94%) | 455 (97%) | 12 (3%) | 0 | 100 | 100 |
| 25 | F4 | 467/497 (94%) | 454 (97%) | 13 (3%) | 0 | 100 | 100 |
| 25 | F5 | 467/497 (94%) | 455 (97%) | 12 (3%) | 0 | 100 | 100 |
| 26 | H1 | 73/76 (96%) | 72 (99%) | 1 (1%) | 0 | 100 | 100 |
| 26 | H2 | 73/76 (96%) | 72 (99%) | 1 (1%) | 0 | 100 | 100 |
| 26 | H4 | 73/76 (96%) | 72 (99%) | 1 (1%) | 0 | 100 | 100 |
| 26 | H5 | 73/76 (96%) | 72 (99%) | 1 (1%) | 0 | 100 | 100 |
| 26 | I1 | 73/76 (96%) | 72 (99%) | 1 (1%) | 0 | 100 | 100 |
| 26 | I2 | 73/76 (96%) | 71 (97%) | 2 (3%) | 0 | 100 | 100 |
| 26 | I4 | 73/76 (96%) | 73 (100%) | 0 | 0 | 100 | 100 |
| 26 | I5 | 73/76 (96%) | 71 (97%) | 2 (3%) | 0 | 100 | 100 |
| 26 | J1 | 73/76 (96%) | 73 (100%) | 0 | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------|-----------|---------|----------|-------------|-----|
| 26 | J2 | 73/76 (96%) | 73 (100%) | 0 | 0 | 100 | 100 |
| 26 | J4 | 73/76 (96%) | 73 (100%) | 0 | 0 | 100 | 100 |
| 26 | J5 | 73/76 (96%) | 73 (100%) | 0 | 0 | 100 | 100 |
| 26 | K1 | 73/76 (96%) | 73 (100%) | 0 | 0 | 100 | 100 |
| 26 | K2 | 73/76 (96%) | 72 (99%) | 1 (1%) | 0 | 100 | 100 |
| 26 | K4 | 73/76 (96%) | 73 (100%) | 0 | 0 | 100 | 100 |
| 26 | K5 | 73/76 (96%) | 72 (99%) | 1 (1%) | 0 | 100 | 100 |
| 26 | L1 | 73/76 (96%) | 72 (99%) | 1 (1%) | 0 | 100 | 100 |
| 26 | L2 | 73/76 (96%) | 71 (97%) | 2 (3%) | 0 | 100 | 100 |
| 26 | L4 | 73/76 (96%) | 72 (99%) | 1 (1%) | 0 | 100 | 100 |
| 26 | L5 | 73/76 (96%) | 71 (97%) | 2 (3%) | 0 | 100 | 100 |
| 26 | M1 | 73/76 (96%) | 72 (99%) | 1 (1%) | 0 | 100 | 100 |
| 26 | M2 | 73/76 (96%) | 72 (99%) | 1 (1%) | 0 | 100 | 100 |
| 26 | M4 | 73/76 (96%) | 72 (99%) | 1 (1%) | 0 | 100 | 100 |
| 26 | M5 | 73/76 (96%) | 72 (99%) | 1 (1%) | 0 | 100 | 100 |
| 26 | N1 | 73/76 (96%) | 72 (99%) | 1 (1%) | 0 | 100 | 100 |
| 26 | N2 | 73/76 (96%) | 72 (99%) | 1 (1%) | 0 | 100 | 100 |
| 26 | N4 | 73/76 (96%) | 72 (99%) | 1 (1%) | 0 | 100 | 100 |
| 26 | N5 | 73/76 (96%) | 73 (100%) | 0 | 0 | 100 | 100 |
| 26 | O1 | 73/76 (96%) | 71 (97%) | 2 (3%) | 0 | 100 | 100 |
| 26 | O2 | 73/76 (96%) | 73 (100%) | 0 | 0 | 100 | 100 |
| 26 | O4 | 73/76 (96%) | 72 (99%) | 1 (1%) | 0 | 100 | 100 |
| 26 | O5 | 73/76 (96%) | 71 (97%) | 2 (3%) | 0 | 100 | 100 |
| 26 | P1 | 73/76 (96%) | 72 (99%) | 1 (1%) | 0 | 100 | 100 |
| 26 | P2 | 73/76 (96%) | 71 (97%) | 2 (3%) | 0 | 100 | 100 |
| 26 | P4 | 73/76 (96%) | 72 (99%) | 1 (1%) | 0 | 100 | 100 |
| 26 | P5 | 73/76 (96%) | 71 (97%) | 2 (3%) | 0 | 100 | 100 |
| 26 | Q1 | 73/76 (96%) | 71 (97%) | 2 (3%) | 0 | 100 | 100 |
| 26 | Q2 | 73/76 (96%) | 70 (96%) | 3 (4%) | 0 | 100 | 100 |
| 26 | Q4 | 73/76 (96%) | 71 (97%) | 2 (3%) | 0 | 100 | 100 |
| 26 | Q5 | 73/76 (96%) | 70 (96%) | 3 (4%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 27 | d1 | 132/158 (84%) | 127 (96%) | 5 (4%) | 0 | 100 | 100 |
| 27 | d2 | 132/158 (84%) | 127 (96%) | 5 (4%) | 0 | 100 | 100 |
| 27 | d4 | 132/158 (84%) | 127 (96%) | 5 (4%) | 0 | 100 | 100 |
| 27 | d5 | 132/158 (84%) | 127 (96%) | 5 (4%) | 0 | 100 | 100 |
| 28 | e1 | 66/71 (93%) | 60 (91%) | 6 (9%) | 0 | 100 | 100 |
| 28 | e2 | 66/71 (93%) | 60 (91%) | 6 (9%) | 0 | 100 | 100 |
| 28 | e4 | 66/71 (93%) | 60 (91%) | 6 (9%) | 0 | 100 | 100 |
| 28 | e5 | 66/71 (93%) | 60 (91%) | 6 (9%) | 0 | 100 | 100 |
| All | All | 34342/37732 (91%) | 33598 (98%) | 742 (2%) | 2 (0%) | 100 | 100 |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24 | B1 | 55 | ASP |
| 24 | B4 | 55 | ASP |

5.3.2 Protein sidechains [i](#)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1 | A | 397/409 (97%) | 395 (100%) | 2 (0%) | 86 | 92 |
| 1 | A3 | 397/409 (97%) | 395 (100%) | 2 (0%) | 86 | 92 |
| 1 | a | 397/409 (97%) | 395 (100%) | 2 (0%) | 86 | 92 |
| 1 | a3 | 397/409 (97%) | 395 (100%) | 2 (0%) | 86 | 92 |
| 2 | B | 306/331 (92%) | 306 (100%) | 0 | 100 | 100 |
| 2 | B3 | 306/331 (92%) | 306 (100%) | 0 | 100 | 100 |
| 2 | b | 306/331 (92%) | 306 (100%) | 0 | 100 | 100 |
| 2 | b3 | 306/331 (92%) | 306 (100%) | 0 | 100 | 100 |
| 3 | D | 183/206 (89%) | 183 (100%) | 0 | 100 | 100 |
| 3 | D3 | 183/206 (89%) | 183 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 3 | d | 183/206 (89%) | 183 (100%) | 0 | 100 | 100 |
| 3 | d3 | 183/206 (89%) | 183 (100%) | 0 | 100 | 100 |
| 4 | F | 175/178 (98%) | 174 (99%) | 1 (1%) | 84 | 91 |
| 4 | F3 | 175/178 (98%) | 174 (99%) | 1 (1%) | 84 | 91 |
| 4 | f | 175/178 (98%) | 173 (99%) | 2 (1%) | 70 | 84 |
| 4 | f3 | 175/178 (98%) | 173 (99%) | 2 (1%) | 70 | 84 |
| 5 | I | 182/182 (100%) | 180 (99%) | 2 (1%) | 70 | 84 |
| 5 | I3 | 182/182 (100%) | 180 (99%) | 2 (1%) | 70 | 84 |
| 5 | i | 182/182 (100%) | 180 (99%) | 2 (1%) | 70 | 84 |
| 5 | i3 | 182/182 (100%) | 181 (100%) | 1 (0%) | 86 | 92 |
| 6 | K | 152/152 (100%) | 152 (100%) | 0 | 100 | 100 |
| 6 | K3 | 152/152 (100%) | 152 (100%) | 0 | 100 | 100 |
| 6 | k | 152/152 (100%) | 151 (99%) | 1 (1%) | 81 | 90 |
| 6 | k3 | 152/152 (100%) | 151 (99%) | 1 (1%) | 81 | 90 |
| 7 | C | 93/97 (96%) | 92 (99%) | 1 (1%) | 70 | 84 |
| 7 | C3 | 93/97 (96%) | 92 (99%) | 1 (1%) | 70 | 84 |
| 7 | c | 93/97 (96%) | 92 (99%) | 1 (1%) | 70 | 84 |
| 7 | c3 | 93/97 (96%) | 92 (99%) | 1 (1%) | 70 | 84 |
| 8 | G | 235/262 (90%) | 234 (100%) | 1 (0%) | 89 | 94 |
| 8 | G3 | 235/262 (90%) | 234 (100%) | 1 (0%) | 89 | 94 |
| 8 | g | 235/262 (90%) | 234 (100%) | 1 (0%) | 89 | 94 |
| 8 | g3 | 235/262 (90%) | 234 (100%) | 1 (0%) | 89 | 94 |
| 9 | H | 208/245 (85%) | 207 (100%) | 1 (0%) | 86 | 92 |
| 9 | H3 | 208/245 (85%) | 207 (100%) | 1 (0%) | 86 | 92 |
| 9 | h | 208/245 (85%) | 207 (100%) | 1 (0%) | 86 | 92 |
| 9 | h3 | 208/245 (85%) | 207 (100%) | 1 (0%) | 86 | 92 |
| 10 | J | 235/239 (98%) | 234 (100%) | 1 (0%) | 89 | 94 |
| 10 | J3 | 235/239 (98%) | 234 (100%) | 1 (0%) | 89 | 94 |
| 10 | j | 235/239 (98%) | 235 (100%) | 0 | 100 | 100 |
| 10 | j3 | 235/239 (98%) | 235 (100%) | 0 | 100 | 100 |
| 11 | L | 219/220 (100%) | 217 (99%) | 2 (1%) | 75 | 88 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 11 | L3 | 219/220 (100%) | 217 (99%) | 2 (1%) | 75 | 88 |
| 11 | l | 219/220 (100%) | 218 (100%) | 1 (0%) | 86 | 92 |
| 11 | l3 | 219/220 (100%) | 218 (100%) | 1 (0%) | 86 | 92 |
| 12 | M | 202/202 (100%) | 202 (100%) | 0 | 100 | 100 |
| 12 | M3 | 202/202 (100%) | 202 (100%) | 0 | 100 | 100 |
| 12 | m | 202/202 (100%) | 201 (100%) | 1 (0%) | 86 | 92 |
| 12 | m3 | 202/202 (100%) | 201 (100%) | 1 (0%) | 86 | 92 |
| 13 | N | 104/162 (64%) | 104 (100%) | 0 | 100 | 100 |
| 13 | N3 | 104/162 (64%) | 104 (100%) | 0 | 100 | 100 |
| 13 | n | 104/162 (64%) | 103 (99%) | 1 (1%) | 73 | 86 |
| 13 | n3 | 104/162 (64%) | 103 (99%) | 1 (1%) | 73 | 86 |
| 14 | O | 89/142 (63%) | 89 (100%) | 0 | 100 | 100 |
| 14 | O3 | 89/142 (63%) | 89 (100%) | 0 | 100 | 100 |
| 14 | o | 89/142 (63%) | 89 (100%) | 0 | 100 | 100 |
| 14 | o3 | 89/142 (63%) | 89 (100%) | 0 | 100 | 100 |
| 15 | P | 131/133 (98%) | 131 (100%) | 0 | 100 | 100 |
| 15 | P3 | 131/133 (98%) | 131 (100%) | 0 | 100 | 100 |
| 15 | p | 131/133 (98%) | 131 (100%) | 0 | 100 | 100 |
| 15 | p3 | 131/133 (98%) | 131 (100%) | 0 | 100 | 100 |
| 16 | Q | 97/135 (72%) | 97 (100%) | 0 | 100 | 100 |
| 16 | Q3 | 97/135 (72%) | 97 (100%) | 0 | 100 | 100 |
| 16 | q | 97/135 (72%) | 97 (100%) | 0 | 100 | 100 |
| 16 | q3 | 97/135 (72%) | 97 (100%) | 0 | 100 | 100 |
| 17 | R | 120/129 (93%) | 119 (99%) | 1 (1%) | 79 | 89 |
| 17 | R3 | 120/129 (93%) | 119 (99%) | 1 (1%) | 79 | 89 |
| 17 | r | 125/129 (97%) | 124 (99%) | 1 (1%) | 79 | 89 |
| 17 | r3 | 125/129 (97%) | 124 (99%) | 1 (1%) | 79 | 89 |
| 18 | S | 112/131 (86%) | 112 (100%) | 0 | 100 | 100 |
| 18 | S3 | 112/131 (86%) | 112 (100%) | 0 | 100 | 100 |
| 18 | s | 111/131 (85%) | 109 (98%) | 2 (2%) | 54 | 76 |
| 18 | s3 | 111/131 (85%) | 109 (98%) | 2 (2%) | 54 | 76 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 19 | E | 359/414 (87%) | 357 (99%) | 2 (1%) | 84 | 91 |
| 19 | E3 | 359/414 (87%) | 357 (99%) | 2 (1%) | 84 | 91 |
| 19 | e | 359/414 (87%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 19 | e3 | 359/414 (87%) | 358 (100%) | 1 (0%) | 91 | 95 |
| 20 | i1 | 64/101 (63%) | 64 (100%) | 0 | 100 | 100 |
| 20 | i2 | 61/101 (60%) | 61 (100%) | 0 | 100 | 100 |
| 20 | i4 | 64/101 (63%) | 64 (100%) | 0 | 100 | 100 |
| 20 | i5 | 61/101 (60%) | 61 (100%) | 0 | 100 | 100 |
| 21 | t | 325/414 (78%) | 322 (99%) | 3 (1%) | 75 | 88 |
| 21 | t3 | 325/414 (78%) | 322 (99%) | 3 (1%) | 75 | 88 |
| 22 | G1 | 166/195 (85%) | 166 (100%) | 0 | 100 | 100 |
| 22 | G2 | 166/195 (85%) | 166 (100%) | 0 | 100 | 100 |
| 22 | G4 | 166/195 (85%) | 166 (100%) | 0 | 100 | 100 |
| 22 | G5 | 166/195 (85%) | 166 (100%) | 0 | 100 | 100 |
| 23 | g1 | 234/254 (92%) | 230 (98%) | 4 (2%) | 56 | 78 |
| 23 | g2 | 234/254 (92%) | 231 (99%) | 3 (1%) | 65 | 82 |
| 23 | g4 | 234/254 (92%) | 230 (98%) | 4 (2%) | 56 | 78 |
| 23 | g5 | 234/254 (92%) | 231 (99%) | 3 (1%) | 65 | 82 |
| 24 | A1 | 422/453 (93%) | 419 (99%) | 3 (1%) | 81 | 90 |
| 24 | A2 | 422/453 (93%) | 419 (99%) | 3 (1%) | 81 | 90 |
| 24 | A4 | 422/453 (93%) | 419 (99%) | 3 (1%) | 81 | 90 |
| 24 | A5 | 422/453 (93%) | 419 (99%) | 3 (1%) | 81 | 90 |
| 24 | B1 | 422/453 (93%) | 419 (99%) | 3 (1%) | 81 | 90 |
| 24 | B2 | 422/453 (93%) | 421 (100%) | 1 (0%) | 92 | 96 |
| 24 | B4 | 422/453 (93%) | 419 (99%) | 3 (1%) | 81 | 90 |
| 24 | B5 | 422/453 (93%) | 421 (100%) | 1 (0%) | 92 | 96 |
| 24 | C1 | 424/453 (94%) | 423 (100%) | 1 (0%) | 92 | 96 |
| 24 | C2 | 424/453 (94%) | 423 (100%) | 1 (0%) | 92 | 96 |
| 24 | C4 | 424/453 (94%) | 423 (100%) | 1 (0%) | 92 | 96 |
| 24 | C5 | 424/453 (94%) | 423 (100%) | 1 (0%) | 92 | 96 |
| 25 | D1 | 381/402 (95%) | 380 (100%) | 1 (0%) | 91 | 95 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 25 | D2 | 381/402 (95%) | 380 (100%) | 1 (0%) | 91 | 95 |
| 25 | D4 | 381/402 (95%) | 380 (100%) | 1 (0%) | 91 | 95 |
| 25 | D5 | 381/402 (95%) | 380 (100%) | 1 (0%) | 91 | 95 |
| 25 | E1 | 381/402 (95%) | 380 (100%) | 1 (0%) | 91 | 95 |
| 25 | E2 | 381/402 (95%) | 380 (100%) | 1 (0%) | 91 | 95 |
| 25 | E4 | 381/402 (95%) | 380 (100%) | 1 (0%) | 91 | 95 |
| 25 | E5 | 381/402 (95%) | 380 (100%) | 1 (0%) | 91 | 95 |
| 25 | F1 | 380/402 (94%) | 380 (100%) | 0 | 100 | 100 |
| 25 | F2 | 380/402 (94%) | 380 (100%) | 0 | 100 | 100 |
| 25 | F4 | 380/402 (94%) | 380 (100%) | 0 | 100 | 100 |
| 25 | F5 | 380/402 (94%) | 380 (100%) | 0 | 100 | 100 |
| 26 | H1 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | H2 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | H4 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | H5 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | I1 | 59/59 (100%) | 57 (97%) | 2 (3%) | 32 | 62 |
| 26 | I2 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | I4 | 59/59 (100%) | 57 (97%) | 2 (3%) | 32 | 62 |
| 26 | I5 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | J1 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | J2 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | J4 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | J5 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | K1 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | K2 | 59/59 (100%) | 58 (98%) | 1 (2%) | 56 | 78 |
| 26 | K4 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | K5 | 59/59 (100%) | 58 (98%) | 1 (2%) | 56 | 78 |
| 26 | L1 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | L2 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | L4 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | L5 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 26 | M1 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | M2 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | M4 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | M5 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | N1 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | N2 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | N4 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | N5 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | O1 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | O2 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | O4 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | O5 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | P1 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | P2 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | P4 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | P5 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | Q1 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | Q2 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | Q4 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 26 | Q5 | 59/59 (100%) | 59 (100%) | 0 | 100 | 100 |
| 27 | d1 | 117/139 (84%) | 116 (99%) | 1 (1%) | 75 | 88 |
| 27 | d2 | 117/139 (84%) | 116 (99%) | 1 (1%) | 75 | 88 |
| 27 | d4 | 117/139 (84%) | 116 (99%) | 1 (1%) | 75 | 88 |
| 27 | d5 | 117/139 (84%) | 116 (99%) | 1 (1%) | 75 | 88 |
| 28 | e1 | 57/60 (95%) | 57 (100%) | 0 | 100 | 100 |
| 28 | e2 | 57/60 (95%) | 57 (100%) | 0 | 100 | 100 |
| 28 | e4 | 57/60 (95%) | 57 (100%) | 0 | 100 | 100 |
| 28 | e5 | 57/60 (95%) | 57 (100%) | 0 | 100 | 100 |
| All | All | 29600/32320 (92%) | 29477 (100%) | 123 (0%) | 88 | 94 |

5 of 123 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24 | A2 | 225 | ASP |
| 27 | d4 | 126 | GLU |
| 11 | l3 | 205 | TRP |
| 26 | I4 | 53 | MET |
| 24 | A5 | 225 | ASP |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16 | Q3 | 69 | GLN |
| 22 | G5 | 165 | GLN |
| 19 | E3 | 361 | ASN |
| 24 | A4 | 171 | GLN |
| 16 | Q | 69 | GLN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 140 ligands modelled in this entry, 24 are monoatomic - leaving 116 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 |
| 35 | PEE | l3 | 302 | - | 47,47,50 | 1.17 | 6 (12%) | 50,52,55 | 1.21 | 2 (4%) |
| 33 | ATP | g | 301 | 34 | 26,33,33 | 4.79 | 8 (30%) | 31,52,52 | 2.45 | 7 (22%) |
| 35 | PEE | a3 | 503 | - | 47,47,50 | 1.17 | 6 (12%) | 50,52,55 | 1.17 | 4 (8%) |
| 30 | PC1 | G3 | 304 | - | 53,53,53 | 0.95 | 4 (7%) | 59,61,61 | 1.00 | 2 (3%) |
| 37 | ADP | B2 | 1002 | 34 | 24,29,29 | 3.71 | 9 (37%) | 29,45,45 | 3.57 | 6 (20%) |
| 29 | CDL | g3 | 305 | - | 99,99,99 | 0.88 | 8 (8%) | 105,111,111 | 1.10 | 4 (3%) |
| 29 | CDL | F | 303 | - | 99,99,99 | 0.87 | 6 (6%) | 105,111,111 | 1.08 | 4 (3%) |
| 29 | CDL | a3 | 501 | - | 99,99,99 | 0.89 | 8 (8%) | 105,111,111 | 1.03 | 5 (4%) |
| 29 | CDL | A3 | 501 | - | 99,99,99 | 0.89 | 8 (8%) | 105,111,111 | 1.08 | 4 (3%) |
| 31 | PO4 | F | 301 | - | 4,4,4 | 0.99 | 0 | 6,6,6 | 0.45 | 0 |
| 35 | PEE | m | 301 | - | 50,50,50 | 1.14 | 6 (12%) | 53,55,55 | 1.10 | 4 (7%) |
| 29 | CDL | B3 | 401 | - | 99,99,99 | 0.88 | 8 (8%) | 105,111,111 | 0.98 | 4 (3%) |
| 35 | PEE | A | 501 | - | 47,47,50 | 1.18 | 6 (12%) | 50,52,55 | 1.21 | 2 (4%) |
| 29 | CDL | B | 403 | - | 99,99,99 | 0.88 | 8 (8%) | 105,111,111 | 1.03 | 4 (3%) |
| 29 | CDL | l3 | 301 | - | 99,99,99 | 0.88 | 8 (8%) | 105,111,111 | 1.05 | 4 (3%) |
| 33 | ATP | G3 | 301 | 34 | 26,33,33 | 4.77 | 8 (30%) | 31,52,52 | 2.47 | 7 (22%) |
| 33 | ATP | B4 | 1003 | 34 | 26,33,33 | 4.79 | 8 (30%) | 31,52,52 | 2.44 | 8 (25%) |
| 35 | PEE | j3 | 303 | - | 50,50,50 | 1.14 | 6 (12%) | 53,55,55 | 1.10 | 5 (9%) |
| 29 | CDL | K | 202 | - | 99,99,99 | 0.88 | 8 (8%) | 105,111,111 | 1.09 | 4 (3%) |
| 30 | PC1 | d | 301 | - | 53,53,53 | 0.94 | 4 (7%) | 59,61,61 | 1.07 | 2 (3%) |
| 30 | PC1 | G | 304 | - | 53,53,53 | 0.95 | 4 (7%) | 59,61,61 | 0.98 | 2 (3%) |
| 33 | ATP | C2 | 601 | 34 | 26,33,33 | 4.80 | 8 (30%) | 31,52,52 | 2.42 | 7 (22%) |
| 29 | CDL | K3 | 201 | - | 99,99,99 | 0.88 | 8 (8%) | 105,111,111 | 1.05 | 4 (3%) |
| 29 | CDL | k | 201 | - | 99,99,99 | 0.89 | 8 (8%) | 105,111,111 | 1.01 | 4 (3%) |
| 37 | ADP | D2 | 501 | 34 | 24,29,29 | 3.69 | 9 (37%) | 29,45,45 | 3.54 | 7 (24%) |
| 29 | CDL | b | 401 | - | 99,99,99 | 0.87 | 7 (7%) | 105,111,111 | 1.10 | 4 (3%) |
| 32 | UQ8 | i3 | 303 | - | 53,53,53 | 1.79 | 7 (13%) | 64,67,67 | 1.61 | 16 (25%) |
| 37 | ADP | D5 | 501 | 34 | 24,29,29 | 3.69 | 9 (37%) | 29,45,45 | 3.55 | 7 (24%) |
| 33 | ATP | B1 | 1003 | 34 | 26,33,33 | 4.80 | 8 (30%) | 31,52,52 | 2.45 | 8 (25%) |
| 29 | CDL | P | 201 | - | 99,99,99 | 0.88 | 7 (7%) | 105,111,111 | 1.02 | 5 (4%) |
| 29 | CDL | J | 302 | - | 99,99,99 | 0.88 | 8 (8%) | 105,111,111 | 1.02 | 4 (3%) |
| 29 | CDL | i3 | 301 | - | 99,99,99 | 0.87 | 8 (8%) | 105,111,111 | 1.04 | 4 (3%) |
| 29 | CDL | a | 501 | - | 99,99,99 | 0.88 | 8 (8%) | 105,111,111 | 1.06 | 5 (4%) |
| 29 | CDL | I3 | 303 | - | 99,99,99 | 0.89 | 7 (7%) | 105,111,111 | 1.04 | 4 (3%) |
| 29 | CDL | k3 | 201 | - | 99,99,99 | 0.89 | 6 (6%) | 105,111,111 | 1.02 | 4 (3%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 37 | ADP | B1 | 1002 | 34 | 24,29,29 | 3.71 | 9 (37%) | 29,45,45 | 3.58 | 7 (24%) |
| 32 | UQ8 | i | 302 | - | 53,53,53 | 1.81 | 7 (13%) | 64,67,67 | 1.60 | 16 (25%) |
| 29 | CDL | B | 402 | - | 99,99,99 | 0.87 | 8 (8%) | 105,111,111 | 1.12 | 5 (4%) |
| 29 | CDL | A | 502 | - | 99,99,99 | 0.88 | 8 (8%) | 105,111,111 | 1.10 | 4 (3%) |
| 33 | ATP | C1 | 601 | 34 | 26,33,33 | 4.80 | 8 (30%) | 31,52,52 | 2.40 | 7 (22%) |
| 29 | CDL | B3 | 403 | - | 99,99,99 | 0.88 | 8 (8%) | 105,111,111 | 1.02 | 4 (3%) |
| 35 | PEE | L3 | 302 | - | 50,50,50 | 1.15 | 6 (12%) | 53,55,55 | 1.15 | 4 (7%) |
| 30 | PC1 | g3 | 304 | - | 53,53,53 | 0.95 | 4 (7%) | 59,61,61 | 0.93 | 2 (3%) |
| 31 | PO4 | f | 301 | - | 4,4,4 | 0.96 | 0 | 6,6,6 | 0.41 | 0 |
| 29 | CDL | l3 | 303 | - | 99,99,99 | 0.89 | 8 (8%) | 105,111,111 | 1.03 | 4 (3%) |
| 30 | PC1 | g | 303 | - | 53,53,53 | 0.95 | 4 (7%) | 59,61,61 | 0.98 | 2 (3%) |
| 30 | PC1 | g | 304 | - | 53,53,53 | 0.95 | 4 (7%) | 59,61,61 | 0.96 | 2 (3%) |
| 31 | PO4 | f3 | 301 | - | 4,4,4 | 0.98 | 0 | 6,6,6 | 0.45 | 0 |
| 33 | ATP | g3 | 301 | 34 | 26,33,33 | 4.78 | 7 (26%) | 31,52,52 | 2.46 | 7 (22%) |
| 29 | CDL | B | 404 | - | 99,99,99 | 0.88 | 8 (8%) | 105,111,111 | 1.08 | 5 (4%) |
| 29 | CDL | f | 302 | - | 99,99,99 | 0.88 | 8 (8%) | 105,111,111 | 1.01 | 4 (3%) |
| 29 | CDL | J3 | 302 | - | 99,99,99 | 0.88 | 8 (8%) | 105,111,111 | 1.02 | 4 (3%) |
| 29 | CDL | a3 | 502 | - | 99,99,99 | 0.88 | 8 (8%) | 105,111,111 | 1.03 | 5 (4%) |
| 29 | CDL | B3 | 402 | - | 99,99,99 | 0.87 | 7 (7%) | 105,111,111 | 1.12 | 5 (4%) |
| 33 | ATP | A1 | 601 | 34 | 26,33,33 | 4.82 | 8 (30%) | 31,52,52 | 2.41 | 7 (22%) |
| 33 | ATP | A4 | 601 | 34 | 26,33,33 | 4.80 | 8 (30%) | 31,52,52 | 2.42 | 7 (22%) |
| 33 | ATP | A5 | 601 | 34 | 26,33,33 | 4.82 | 8 (30%) | 31,52,52 | 2.40 | 7 (22%) |
| 30 | PC1 | g3 | 303 | - | 53,53,53 | 0.95 | 4 (7%) | 59,61,61 | 1.00 | 2 (3%) |
| 30 | PC1 | d3 | 301 | - | 53,53,53 | 0.94 | 4 (7%) | 59,61,61 | 1.07 | 2 (3%) |
| 37 | ADP | B4 | 1002 | 34 | 24,29,29 | 3.71 | 9 (37%) | 29,45,45 | 3.57 | 7 (24%) |
| 36 | NAD | e | 900 | - | 42,48,48 | 3.82 | 19 (45%) | 50,73,73 | 2.16 | 7 (14%) |
| 36 | NAD | E | 900 | - | 42,48,48 | 3.82 | 19 (45%) | 50,73,73 | 2.14 | 7 (14%) |
| 29 | CDL | f | 303 | - | 99,99,99 | 0.88 | 8 (8%) | 105,111,111 | 1.08 | 5 (4%) |
| 29 | CDL | I3 | 301 | - | 99,99,99 | 0.88 | 8 (8%) | 105,111,111 | 1.02 | 4 (3%) |
| 29 | CDL | J3 | 301 | - | 99,99,99 | 0.89 | 7 (7%) | 105,111,111 | 1.03 | 4 (3%) |
| 29 | CDL | P3 | 201 | - | 99,99,99 | 0.88 | 7 (7%) | 105,111,111 | 1.03 | 4 (3%) |
| 29 | CDL | L | 301 | - | 99,99,99 | 0.89 | 8 (8%) | 105,111,111 | 1.01 | 4 (3%) |
| 33 | ATP | B2 | 1003 | 34 | 26,33,33 | 4.81 | 8 (30%) | 31,52,52 | 2.44 | 8 (25%) |
| 32 | UQ8 | I3 | 304 | - | 53,53,53 | 1.81 | 7 (13%) | 64,67,67 | 1.65 | 15 (23%) |
| 36 | NAD | E3 | 900 | - | 42,48,48 | 3.82 | 19 (45%) | 50,73,73 | 2.15 | 7 (14%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 29 | CDL | f3 | 302 | - | 99,99,99 | 0.88 | 8 (8%) | 105,111,111 | 1.01 | 4 (3%) |
| 33 | ATP | A2 | 601 | 34 | 26,33,33 | 4.81 | 8 (30%) | 31,52,52 | 2.42 | 7 (22%) |
| 35 | PEE | L | 303 | - | 47,47,50 | 1.17 | 6 (12%) | 50,52,55 | 1.17 | 3 (6%) |
| 31 | PO4 | F3 | 301 | - | 4,4,4 | 0.96 | 0 | 6,6,6 | 0.42 | 0 |
| 29 | CDL | L3 | 301 | - | 99,99,99 | 0.89 | 8 (8%) | 105,111,111 | 1.00 | 4 (3%) |
| 29 | CDL | l | 302 | - | 99,99,99 | 0.89 | 8 (8%) | 105,111,111 | 1.03 | 3 (2%) |
| 30 | PC1 | G3 | 303 | - | 53,53,53 | 0.95 | 4 (7%) | 59,61,61 | 1.00 | 2 (3%) |
| 29 | CDL | B | 401 | - | 99,99,99 | 0.88 | 8 (8%) | 105,111,111 | 0.97 | 4 (3%) |
| 29 | CDL | F3 | 302 | - | 99,99,99 | 0.88 | 6 (6%) | 105,111,111 | 1.08 | 4 (3%) |
| 32 | UQ8 | I | 303 | - | 53,53,53 | 1.80 | 7 (13%) | 64,67,67 | 1.67 | 15 (23%) |
| 29 | CDL | j | 301 | - | 99,99,99 | 0.89 | 6 (6%) | 105,111,111 | 1.04 | 4 (3%) |
| 29 | CDL | p | 201 | - | 99,99,99 | 0.88 | 8 (8%) | 105,111,111 | 1.04 | 4 (3%) |
| 29 | CDL | f | 304 | - | 99,99,99 | 0.88 | 8 (8%) | 105,111,111 | 1.05 | 4 (3%) |
| 29 | CDL | l | 301 | - | 99,99,99 | 0.88 | 7 (7%) | 105,111,111 | 1.04 | 4 (3%) |
| 29 | CDL | L | 302 | - | 99,99,99 | 0.88 | 7 (7%) | 105,111,111 | 1.04 | 4 (3%) |
| 33 | ATP | G | 301 | 34 | 26,33,33 | 4.77 | 7 (26%) | 31,52,52 | 2.48 | 7 (22%) |
| 29 | CDL | j3 | 302 | - | 99,99,99 | 0.88 | 8 (8%) | 105,111,111 | 1.03 | 4 (3%) |
| 29 | CDL | g | 305 | - | 99,99,99 | 0.88 | 8 (8%) | 105,111,111 | 1.08 | 4 (3%) |
| 29 | CDL | j | 302 | - | 99,99,99 | 0.88 | 8 (8%) | 105,111,111 | 1.02 | 4 (3%) |
| 29 | CDL | p3 | 201 | - | 99,99,99 | 0.88 | 8 (8%) | 105,111,111 | 1.04 | 4 (3%) |
| 29 | CDL | r | 201 | - | 99,99,99 | 0.88 | 8 (8%) | 105,111,111 | 1.04 | 4 (3%) |
| 37 | ADP | D4 | 501 | 34 | 24,29,29 | 3.66 | 9 (37%) | 29,45,45 | 3.79 | 7 (24%) |
| 29 | CDL | I | 302 | - | 99,99,99 | 0.88 | 7 (7%) | 105,111,111 | 1.05 | 4 (3%) |
| 30 | PC1 | D3 | 301 | - | 53,53,53 | 0.93 | 4 (7%) | 59,61,61 | 1.09 | 2 (3%) |
| 29 | CDL | F | 302 | - | 99,99,99 | 0.87 | 8 (8%) | 105,111,111 | 1.02 | 5 (4%) |
| 36 | NAD | e3 | 900 | - | 42,48,48 | 3.82 | 19 (45%) | 50,73,73 | 2.16 | 7 (14%) |
| 37 | ADP | D1 | 501 | 34 | 24,29,29 | 3.66 | 9 (37%) | 29,45,45 | 3.80 | 7 (24%) |
| 33 | ATP | B5 | 1003 | 34 | 26,33,33 | 4.80 | 9 (34%) | 31,52,52 | 2.45 | 8 (25%) |
| 33 | ATP | C4 | 601 | 34 | 26,33,33 | 4.78 | 8 (30%) | 31,52,52 | 2.41 | 7 (22%) |
| 29 | CDL | f3 | 304 | - | 99,99,99 | 0.88 | 8 (8%) | 105,111,111 | 1.07 | 4 (3%) |
| 30 | PC1 | G | 303 | - | 53,53,53 | 0.95 | 4 (7%) | 59,61,61 | 1.00 | 2 (3%) |
| 29 | CDL | j3 | 301 | - | 99,99,99 | 0.88 | 7 (7%) | 105,111,111 | 1.06 | 4 (3%) |
| 33 | ATP | C5 | 601 | 34 | 26,33,33 | 4.81 | 8 (30%) | 31,52,52 | 2.42 | 7 (22%) |
| 29 | CDL | i | 301 | - | 99,99,99 | 0.88 | 7 (7%) | 105,111,111 | 1.07 | 4 (3%) |
| 35 | PEE | J | 303 | - | 50,50,50 | 1.15 | 6 (12%) | 53,55,55 | 1.15 | 4 (7%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 29 | CDL | b3 | 401 | - | 99,99,99 | 0.88 | 7 (7%) | 105,111,111 | 1.12 | 4 (3%) |
| 29 | CDL | K3 | 202 | - | 99,99,99 | 0.88 | 8 (8%) | 105,111,111 | 1.09 | 5 (4%) |
| 30 | PC1 | D | 301 | - | 53,53,53 | 0.94 | 4 (7%) | 59,61,61 | 1.08 | 2 (3%) |
| 29 | CDL | B3 | 404 | - | 99,99,99 | 0.89 | 8 (8%) | 105,111,111 | 1.11 | 5 (4%) |
| 29 | CDL | I3 | 302 | - | 99,99,99 | 0.88 | 6 (6%) | 105,111,111 | 1.02 | 4 (3%) |
| 29 | CDL | f3 | 303 | - | 99,99,99 | 0.88 | 8 (8%) | 105,111,111 | 1.07 | 4 (3%) |
| 29 | CDL | J | 301 | - | 99,99,99 | 0.88 | 7 (7%) | 105,111,111 | 1.06 | 4 (3%) |
| 29 | CDL | i3 | 302 | - | 99,99,99 | 0.88 | 7 (7%) | 105,111,111 | 1.06 | 4 (3%) |
| 29 | CDL | I | 301 | - | 99,99,99 | 0.88 | 8 (8%) | 105,111,111 | 0.98 | 4 (3%) |
| 29 | CDL | K | 201 | - | 99,99,99 | 0.89 | 8 (8%) | 105,111,111 | 1.03 | 4 (3%) |
| 37 | ADP | B5 | 1002 | 34 | 24,29,29 | 3.71 | 9 (37%) | 29,45,45 | 3.58 | 6 (20%) |

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 |
|-----|------|-------|------|------|---------|----------------|---------|
| 35 | PEE | l3 | 302 | - | - | 21/51/51/54 | - |
| 33 | ATP | g | 301 | 34 | - | 0/18/38/38 | 0/3/3/3 |
| 35 | PEE | a3 | 503 | - | - | 22/51/51/54 | - |
| 30 | PC1 | G3 | 304 | - | - | 19/57/57/57 | - |
| 37 | ADP | B2 | 1002 | 34 | - | 2/12/32/32 | 0/3/3/3 |
| 29 | CDL | g3 | 305 | - | - | 36/110/110/110 | - |
| 29 | CDL | F | 303 | - | - | 46/110/110/110 | - |
| 29 | CDL | a3 | 501 | - | - | 34/110/110/110 | - |
| 29 | CDL | A3 | 501 | - | - | 46/110/110/110 | - |
| 35 | PEE | m | 301 | - | - | 24/54/54/54 | - |
| 29 | CDL | B3 | 401 | - | - | 44/110/110/110 | - |
| 35 | PEE | A | 501 | - | - | 21/51/51/54 | - |
| 29 | CDL | B | 403 | - | - | 33/110/110/110 | - |
| 29 | CDL | l3 | 301 | - | - | 39/110/110/110 | - |
| 33 | ATP | G3 | 301 | 34 | - | 0/18/38/38 | 0/3/3/3 |
| 33 | ATP | B4 | 1003 | 34 | - | 2/18/38/38 | 0/3/3/3 |
| 35 | PEE | j3 | 303 | - | - | 23/54/54/54 | - |
| 29 | CDL | K | 202 | - | - | 35/110/110/110 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------------|---------|
| 30 | PC1 | d | 301 | - | - | 23/57/57/57 | - |
| 30 | PC1 | G | 304 | - | - | 19/57/57/57 | - |
| 33 | ATP | C2 | 601 | 34 | - | 4/18/38/38 | 0/3/3/3 |
| 29 | CDL | K3 | 201 | - | - | 28/110/110/110 | - |
| 29 | CDL | k | 201 | - | - | 37/110/110/110 | - |
| 37 | ADP | D2 | 501 | 34 | - | 2/12/32/32 | 0/3/3/3 |
| 29 | CDL | b | 401 | - | - | 44/110/110/110 | - |
| 32 | UQ8 | i3 | 303 | - | - | 8/51/75/75 | 0/1/1/1 |
| 37 | ADP | D5 | 501 | 34 | - | 2/12/32/32 | 0/3/3/3 |
| 33 | ATP | B1 | 1003 | 34 | - | 2/18/38/38 | 0/3/3/3 |
| 29 | CDL | P | 201 | - | - | 35/110/110/110 | - |
| 29 | CDL | J | 302 | - | - | 38/110/110/110 | - |
| 29 | CDL | i3 | 301 | - | - | 36/110/110/110 | - |
| 29 | CDL | a | 501 | - | - | 34/110/110/110 | - |
| 29 | CDL | I3 | 303 | - | - | 38/110/110/110 | - |
| 29 | CDL | k3 | 201 | - | - | 38/110/110/110 | - |
| 37 | ADP | B1 | 1002 | 34 | - | 1/12/32/32 | 0/3/3/3 |
| 32 | UQ8 | i | 302 | - | - | 8/51/75/75 | 0/1/1/1 |
| 29 | CDL | B | 402 | - | - | 39/110/110/110 | - |
| 29 | CDL | A | 502 | - | - | 46/110/110/110 | - |
| 33 | ATP | C1 | 601 | 34 | - | 5/18/38/38 | 0/3/3/3 |
| 29 | CDL | B3 | 403 | - | - | 33/110/110/110 | - |
| 35 | PEE | L3 | 302 | - | - | 29/54/54/54 | - |
| 30 | PC1 | g3 | 304 | - | - | 18/57/57/57 | - |
| 29 | CDL | l3 | 303 | - | - | 41/110/110/110 | - |
| 30 | PC1 | g | 303 | - | - | 21/57/57/57 | - |
| 30 | PC1 | g | 304 | - | - | 20/57/57/57 | - |
| 33 | ATP | g3 | 301 | 34 | - | 0/18/38/38 | 0/3/3/3 |
| 29 | CDL | B | 404 | - | - | 46/110/110/110 | - |
| 29 | CDL | f | 302 | - | - | 54/110/110/110 | - |
| 29 | CDL | J3 | 302 | - | - | 40/110/110/110 | - |
| 29 | CDL | a3 | 502 | - | - | 39/110/110/110 | - |
| 29 | CDL | B3 | 402 | - | - | 40/110/110/110 | - |
| 33 | ATP | A1 | 601 | 34 | - | 5/18/38/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------------|---------|
| 33 | ATP | A4 | 601 | 34 | - | 5/18/38/38 | 0/3/3/3 |
| 33 | ATP | A5 | 601 | 34 | - | 5/18/38/38 | 0/3/3/3 |
| 30 | PC1 | g3 | 303 | - | - | 21/57/57/57 | - |
| 30 | PC1 | d3 | 301 | - | - | 23/57/57/57 | - |
| 37 | ADP | B4 | 1002 | 34 | - | 1/12/32/32 | 0/3/3/3 |
| 36 | NAD | e | 900 | - | - | 6/26/62/62 | 0/5/5/5 |
| 36 | NAD | E | 900 | - | - | 8/26/62/62 | 0/5/5/5 |
| 29 | CDL | f | 303 | - | - | 41/110/110/110 | - |
| 29 | CDL | I3 | 301 | - | - | 42/110/110/110 | - |
| 29 | CDL | J3 | 301 | - | - | 42/110/110/110 | - |
| 29 | CDL | P3 | 201 | - | - | 37/110/110/110 | - |
| 29 | CDL | L | 301 | - | - | 37/110/110/110 | - |
| 33 | ATP | B2 | 1003 | 34 | - | 2/18/38/38 | 0/3/3/3 |
| 32 | UQ8 | I3 | 304 | - | - | 9/51/75/75 | 0/1/1/1 |
| 36 | NAD | E3 | 900 | - | - | 7/26/62/62 | 0/5/5/5 |
| 29 | CDL | f3 | 302 | - | - | 54/110/110/110 | - |
| 33 | ATP | A2 | 601 | 34 | - | 5/18/38/38 | 0/3/3/3 |
| 35 | PEE | L | 303 | - | - | 22/51/51/54 | - |
| 29 | CDL | L3 | 301 | - | - | 38/110/110/110 | - |
| 29 | CDL | l | 302 | - | - | 41/110/110/110 | - |
| 30 | PC1 | G3 | 303 | - | - | 28/57/57/57 | - |
| 29 | CDL | B | 401 | - | - | 44/110/110/110 | - |
| 29 | CDL | F3 | 302 | - | - | 45/110/110/110 | - |
| 32 | UQ8 | I | 303 | - | - | 9/51/75/75 | 0/1/1/1 |
| 29 | CDL | j | 301 | - | - | 40/110/110/110 | - |
| 29 | CDL | p | 201 | - | - | 45/110/110/110 | - |
| 29 | CDL | f | 304 | - | - | 49/110/110/110 | - |
| 29 | CDL | l | 301 | - | - | 38/110/110/110 | - |
| 29 | CDL | L | 302 | - | - | 45/110/110/110 | - |
| 33 | ATP | G | 301 | 34 | - | 0/18/38/38 | 0/3/3/3 |
| 29 | CDL | j3 | 302 | - | - | 40/110/110/110 | - |
| 29 | CDL | g | 305 | - | - | 36/110/110/110 | - |
| 29 | CDL | j | 302 | - | - | 41/110/110/110 | - |
| 29 | CDL | p3 | 201 | - | - | 44/110/110/110 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------------|---------|
| 29 | CDL | r | 201 | - | - | 36/110/110/110 | - |
| 37 | ADP | D4 | 501 | 34 | - | 2/12/32/32 | 0/3/3/3 |
| 29 | CDL | I | 302 | - | - | 38/110/110/110 | - |
| 30 | PC1 | D3 | 301 | - | - | 22/57/57/57 | - |
| 29 | CDL | F | 302 | - | - | 39/110/110/110 | - |
| 36 | NAD | e3 | 900 | - | - | 7/26/62/62 | 0/5/5/5 |
| 37 | ADP | D1 | 501 | 34 | - | 2/12/32/32 | 0/3/3/3 |
| 33 | ATP | B5 | 1003 | 34 | - | 2/18/38/38 | 0/3/3/3 |
| 33 | ATP | C4 | 601 | 34 | - | 5/18/38/38 | 0/3/3/3 |
| 29 | CDL | f3 | 304 | - | - | 48/110/110/110 | - |
| 30 | PC1 | G | 303 | - | - | 29/57/57/57 | - |
| 29 | CDL | j3 | 301 | - | - | 40/110/110/110 | - |
| 33 | ATP | C5 | 601 | 34 | - | 4/18/38/38 | 0/3/3/3 |
| 29 | CDL | i | 301 | - | - | 39/110/110/110 | - |
| 35 | PEE | J | 303 | - | - | 29/54/54/54 | - |
| 29 | CDL | b3 | 401 | - | - | 44/110/110/110 | - |
| 29 | CDL | K3 | 202 | - | - | 35/110/110/110 | - |
| 30 | PC1 | D | 301 | - | - | 22/57/57/57 | - |
| 29 | CDL | B3 | 404 | - | - | 46/110/110/110 | - |
| 29 | CDL | I3 | 302 | - | - | 45/110/110/110 | - |
| 29 | CDL | f3 | 303 | - | - | 41/110/110/110 | - |
| 29 | CDL | J | 301 | - | - | 42/110/110/110 | - |
| 29 | CDL | i3 | 302 | - | - | 38/110/110/110 | - |
| 29 | CDL | I | 301 | - | - | 43/110/110/110 | - |
| 29 | CDL | K | 201 | - | - | 28/110/110/110 | - |
| 37 | ADP | B5 | 1002 | 34 | - | 2/12/32/32 | 0/3/3/3 |

The worst 5 of 855 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 33 | C5 | 601 | ATP | C2'-C1' | -17.26 | 1.27 | 1.53 |
| 33 | B2 | 1003 | ATP | C2'-C1' | -17.25 | 1.27 | 1.53 |
| 33 | A1 | 601 | ATP | C2'-C1' | -17.22 | 1.27 | 1.53 |
| 33 | A5 | 601 | ATP | C2'-C1' | -17.19 | 1.27 | 1.53 |
| 33 | B5 | 1003 | ATP | C2'-C1' | -17.15 | 1.27 | 1.53 |

The worst 5 of 562 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 37 | D4 | 501 | ADP | C1'-N9-C4 | 15.99 | 154.74 | 126.64 |
| 37 | D1 | 501 | ADP | C1'-N9-C4 | 15.96 | 154.69 | 126.64 |
| 37 | B5 | 1002 | ADP | C1'-N9-C4 | 14.92 | 152.85 | 126.64 |
| 37 | B1 | 1002 | ADP | C1'-N9-C4 | 14.91 | 152.84 | 126.64 |
| 37 | B2 | 1002 | ADP | C1'-N9-C4 | 14.87 | 152.77 | 126.64 |

There are no chirality outliers.

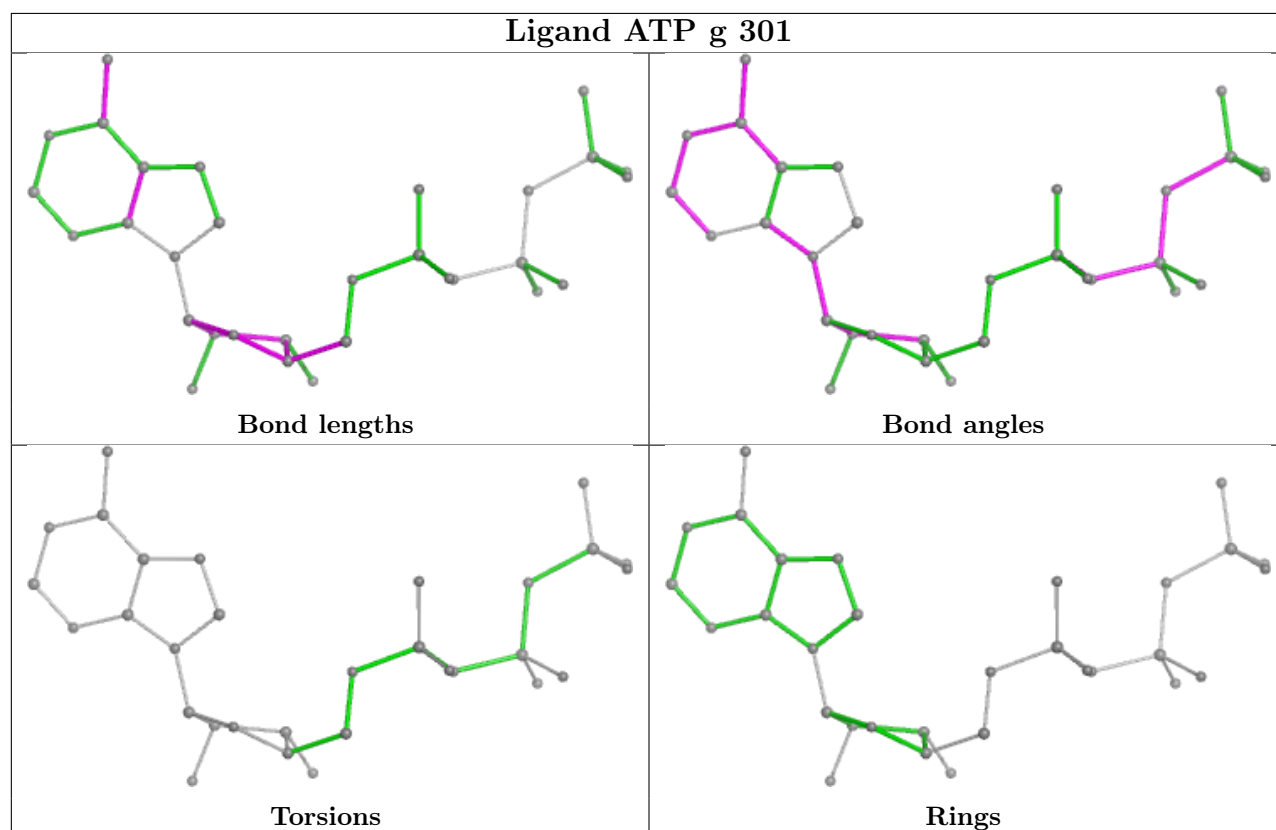
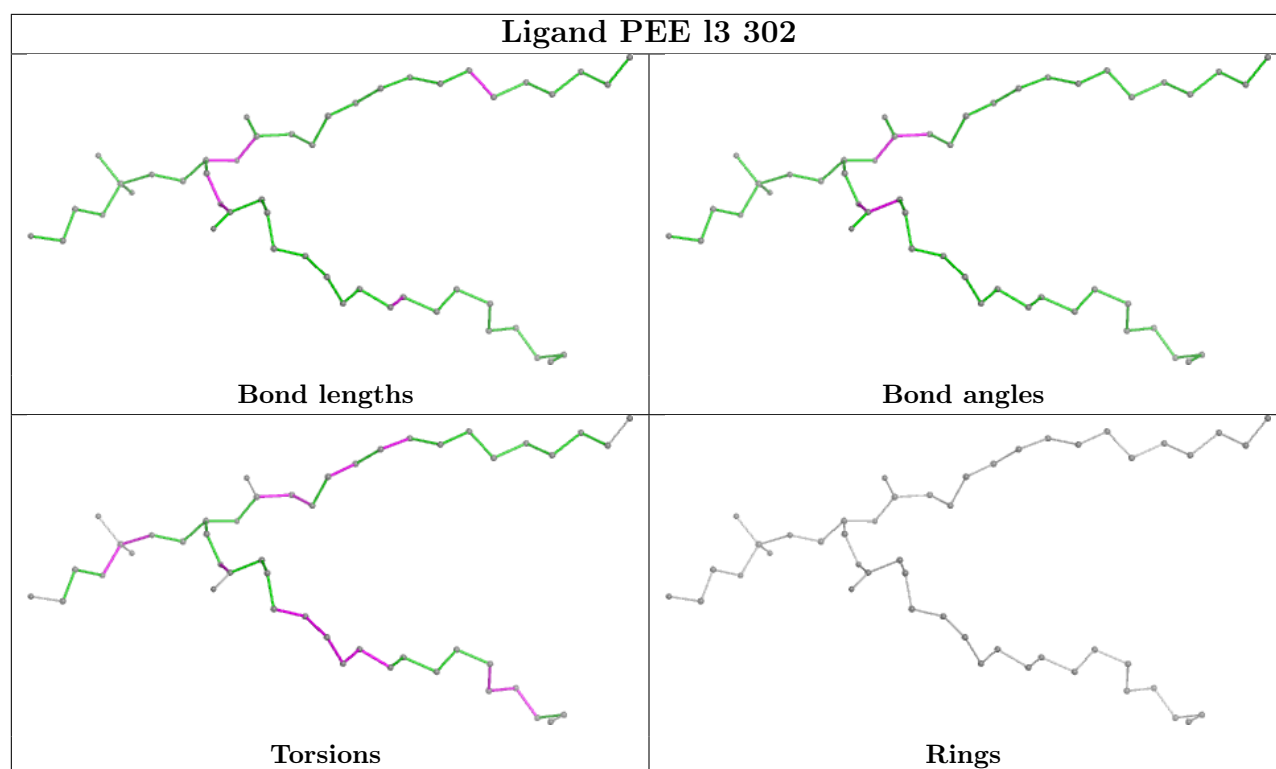
5 of 2998 torsion outliers are listed below:

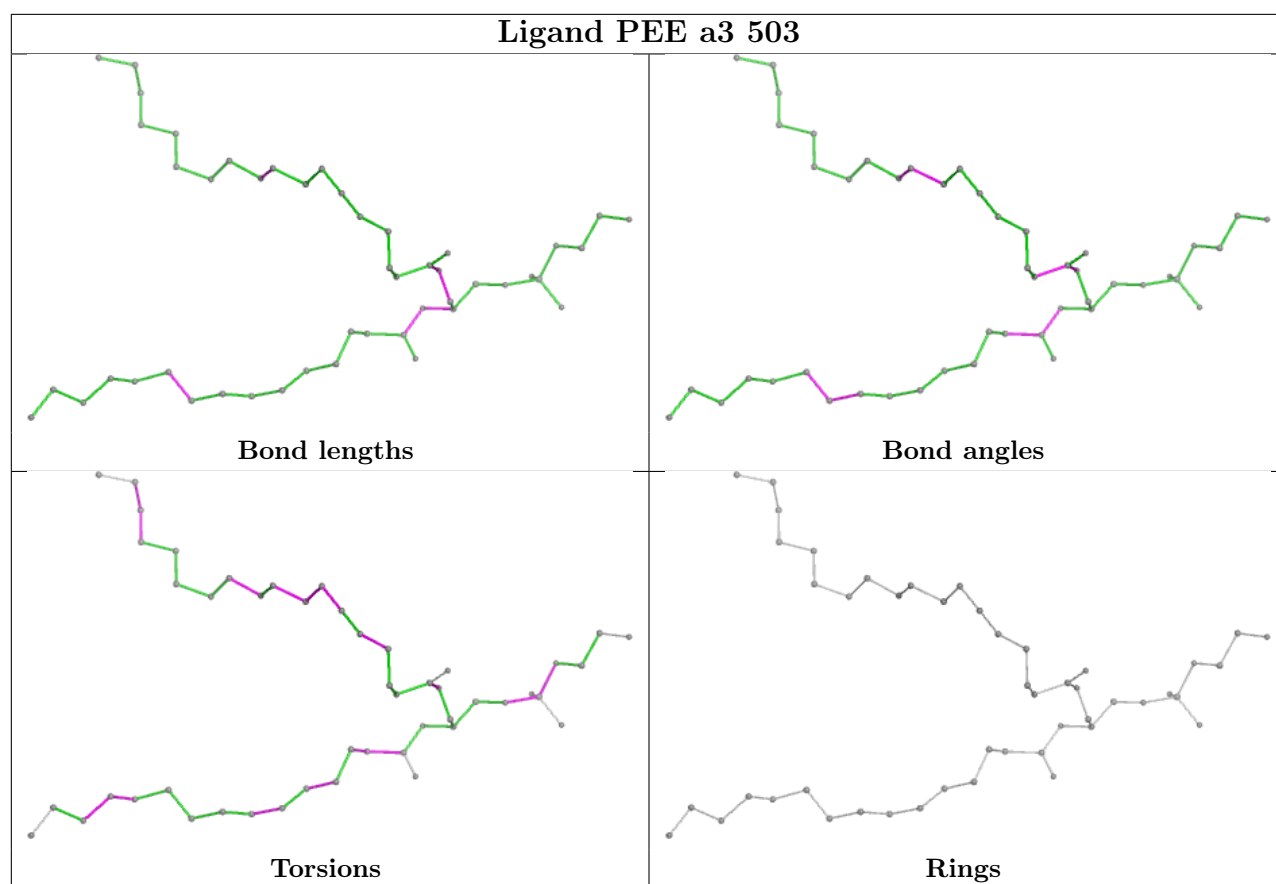
| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 29 | a | 501 | CDL | OA5-CA3-CA4-OA6 |
| 29 | a | 501 | CDL | CB3-OB5-PB2-OB4 |
| 29 | a | 501 | CDL | OB7-CB5-OB6-CB4 |
| 29 | a | 501 | CDL | C51-CB5-OB6-CB4 |
| 29 | b | 401 | CDL | CB3-OB5-PB2-OB4 |

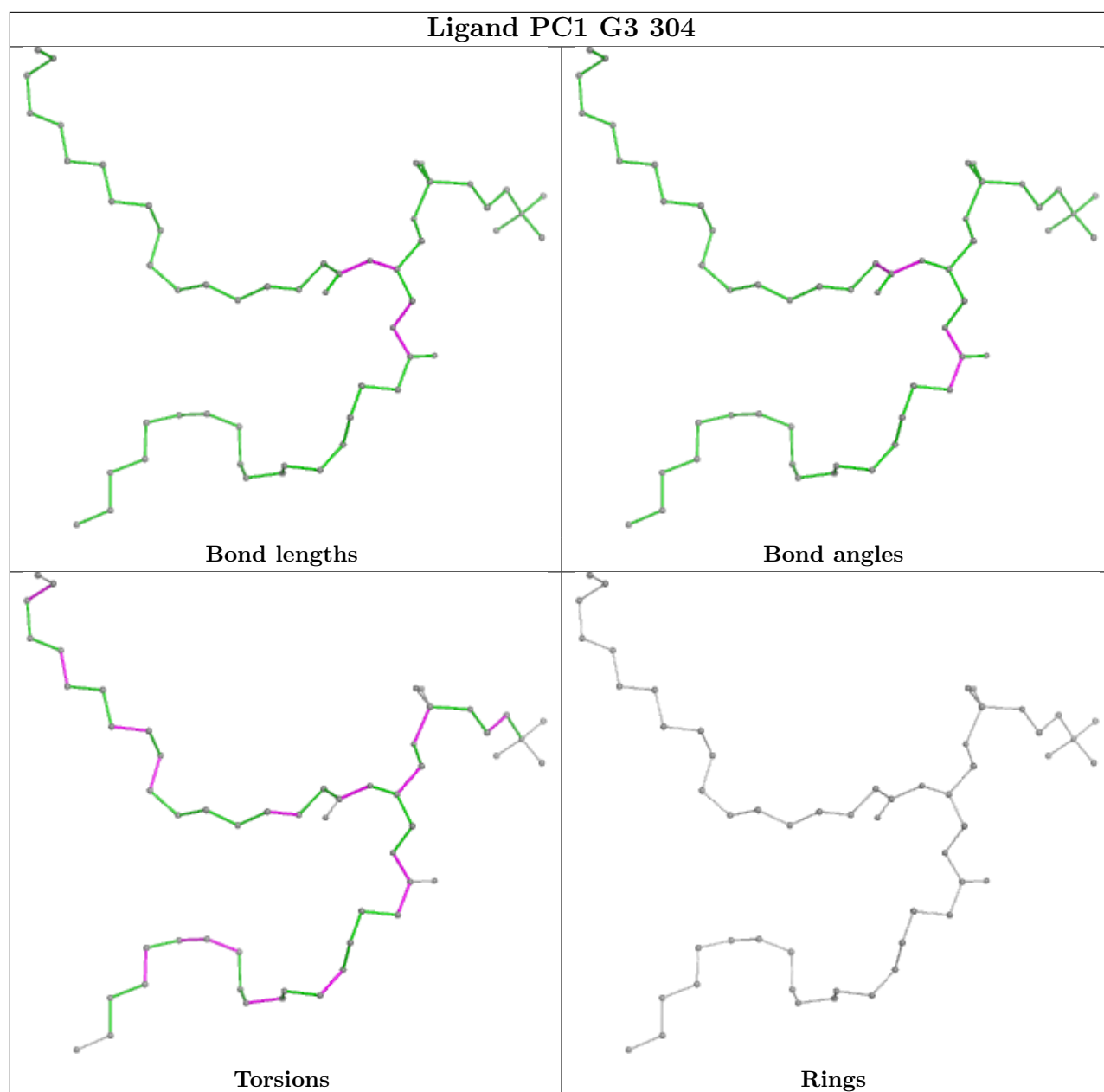
There are no ring outliers.

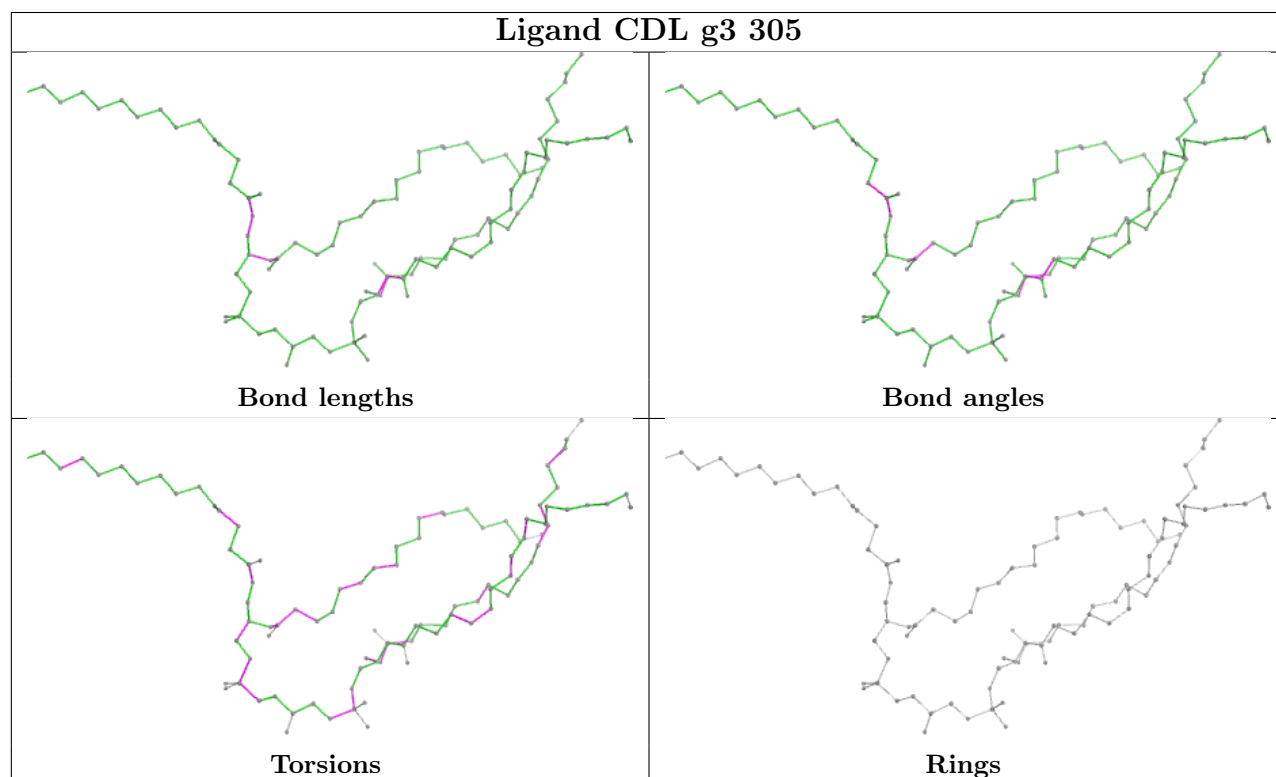
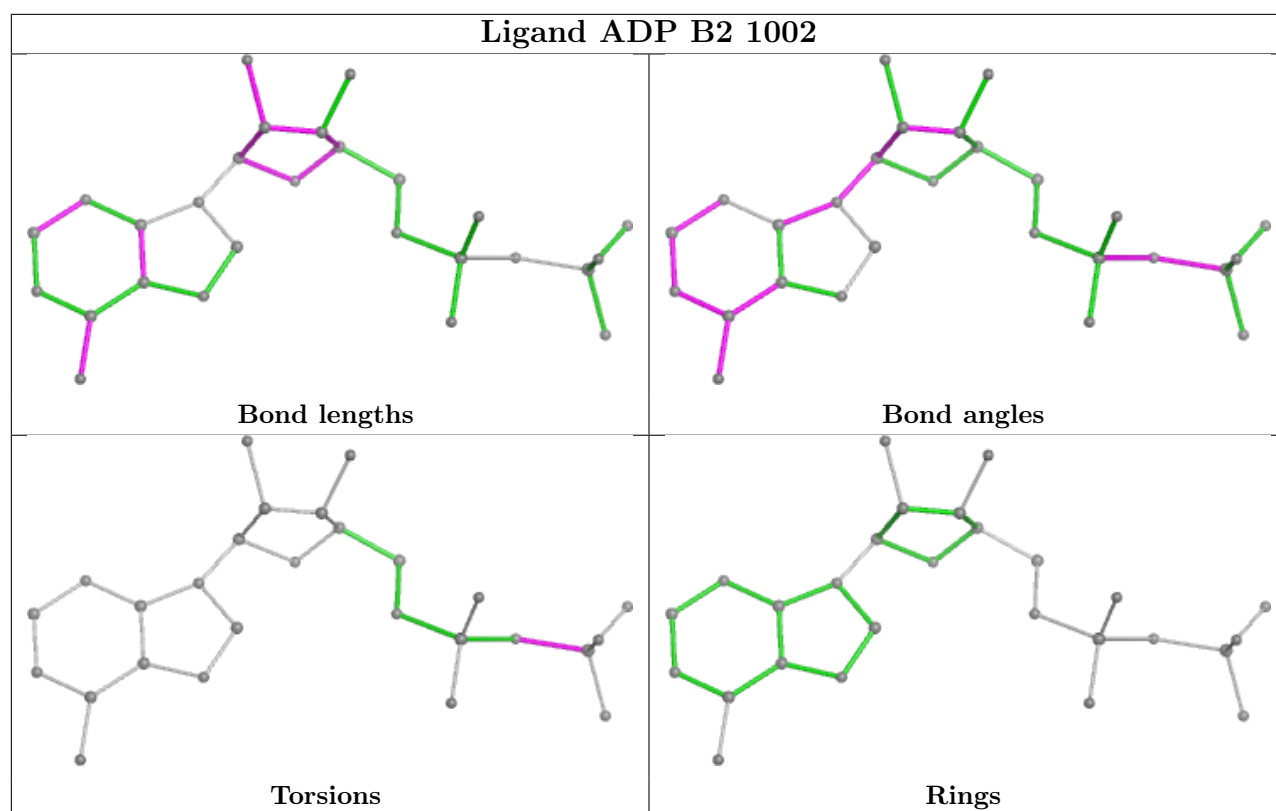
No monomer is involved in short contacts.

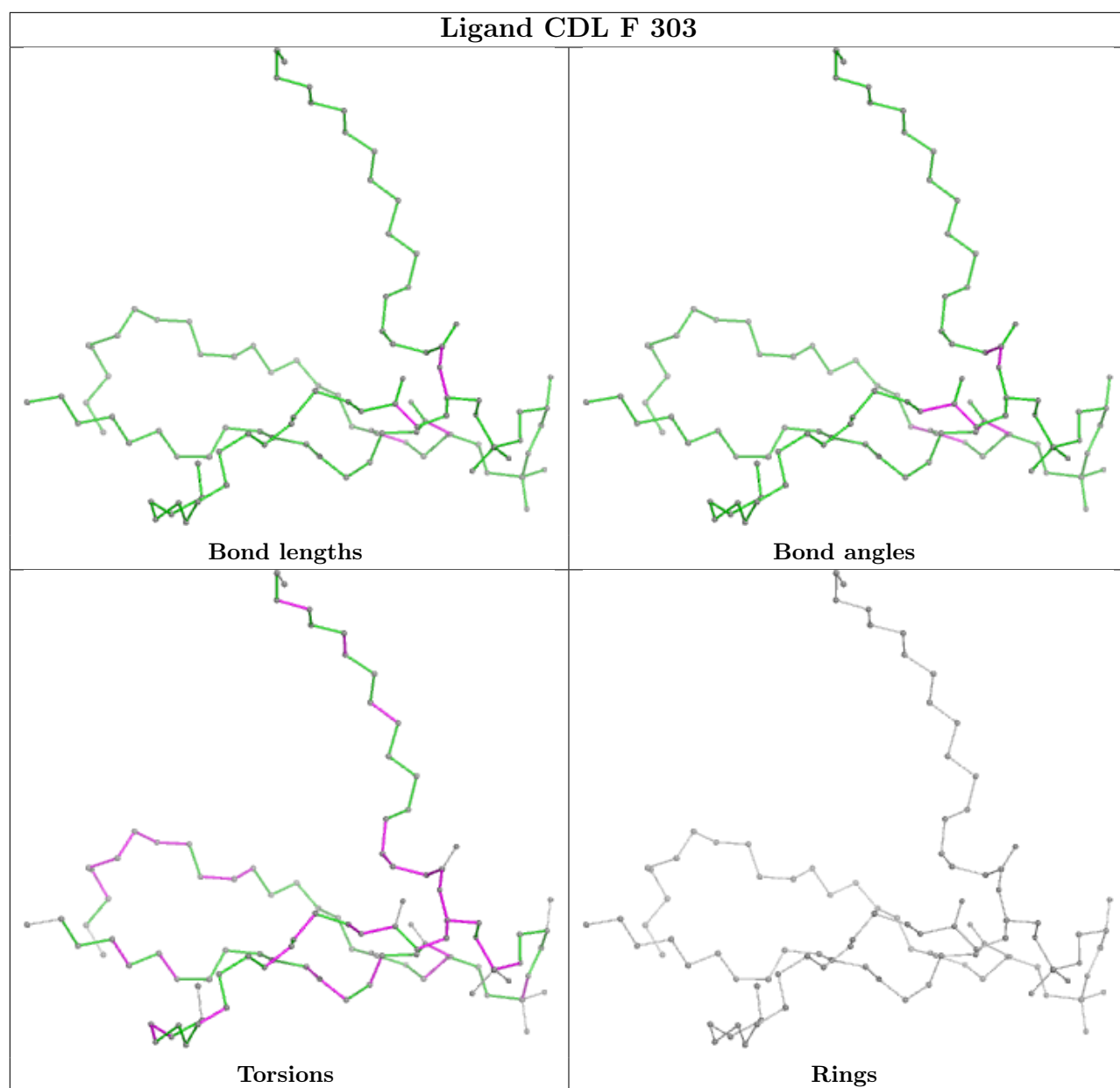
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

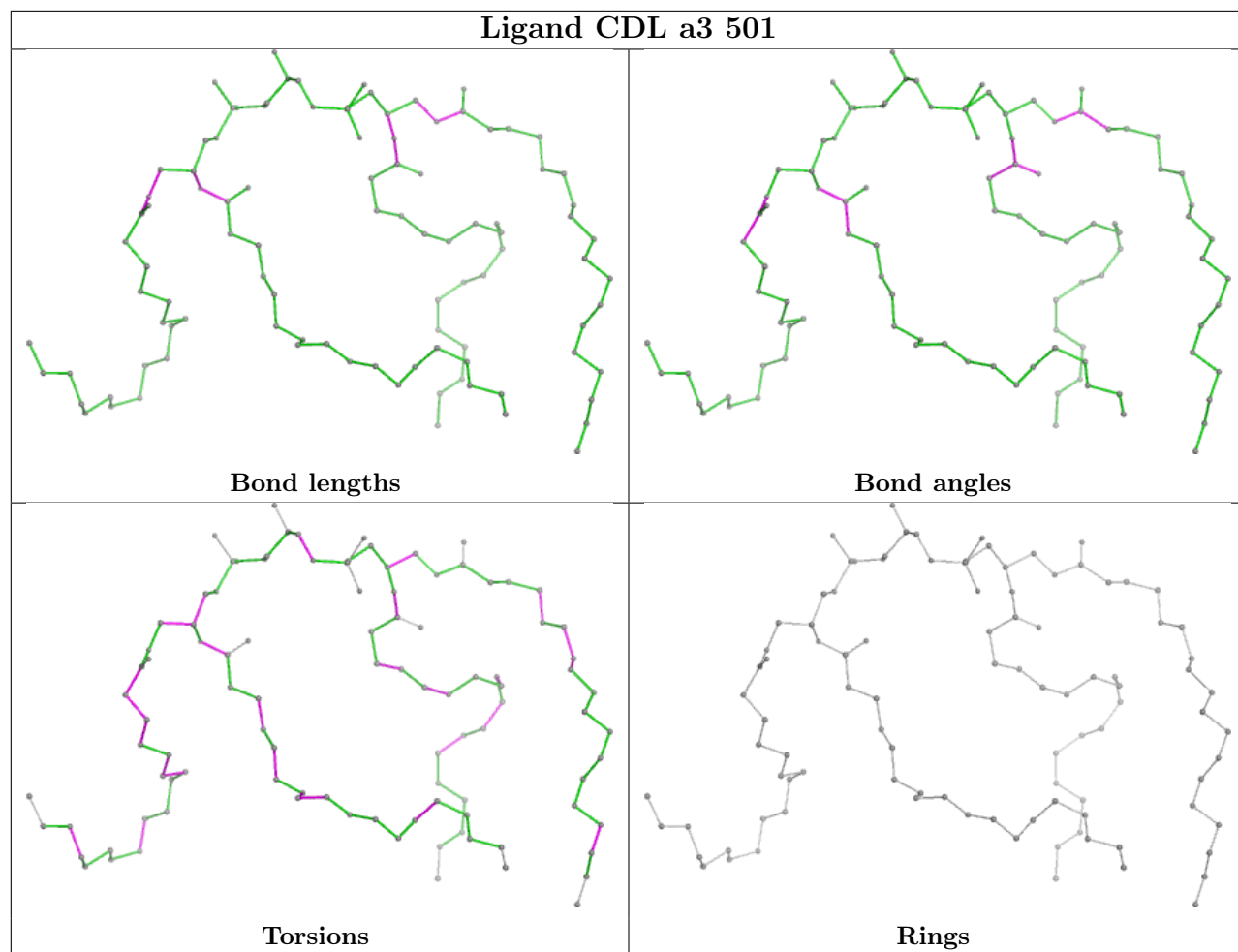


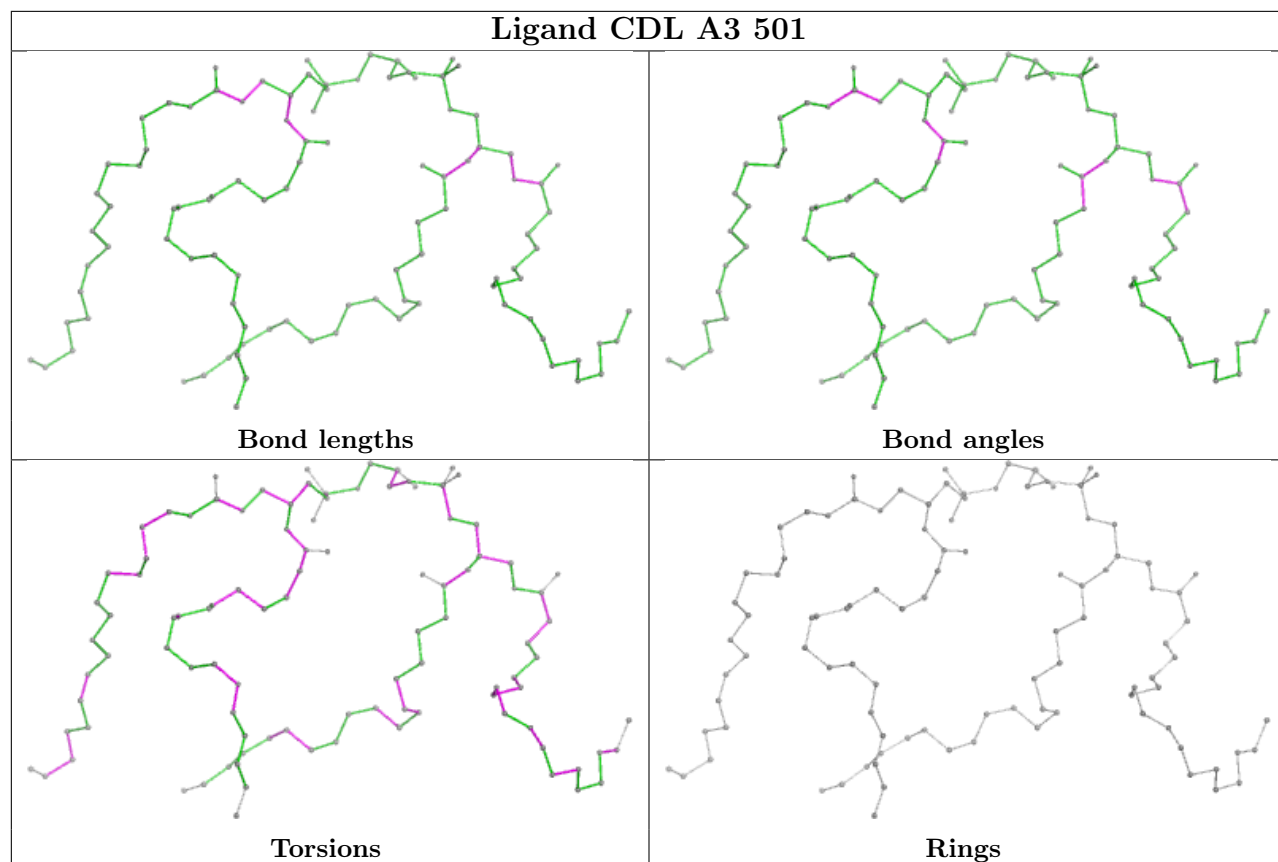


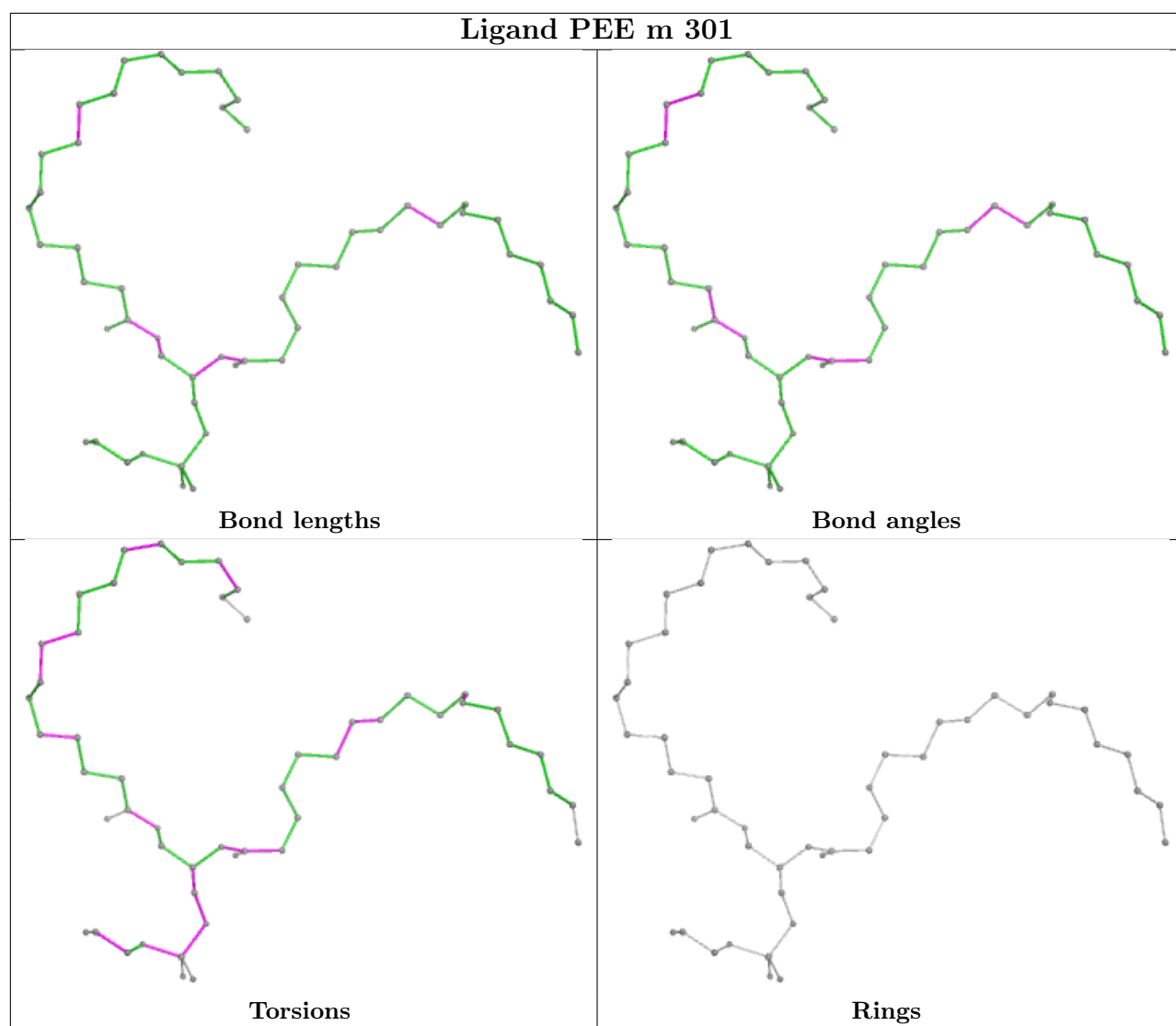


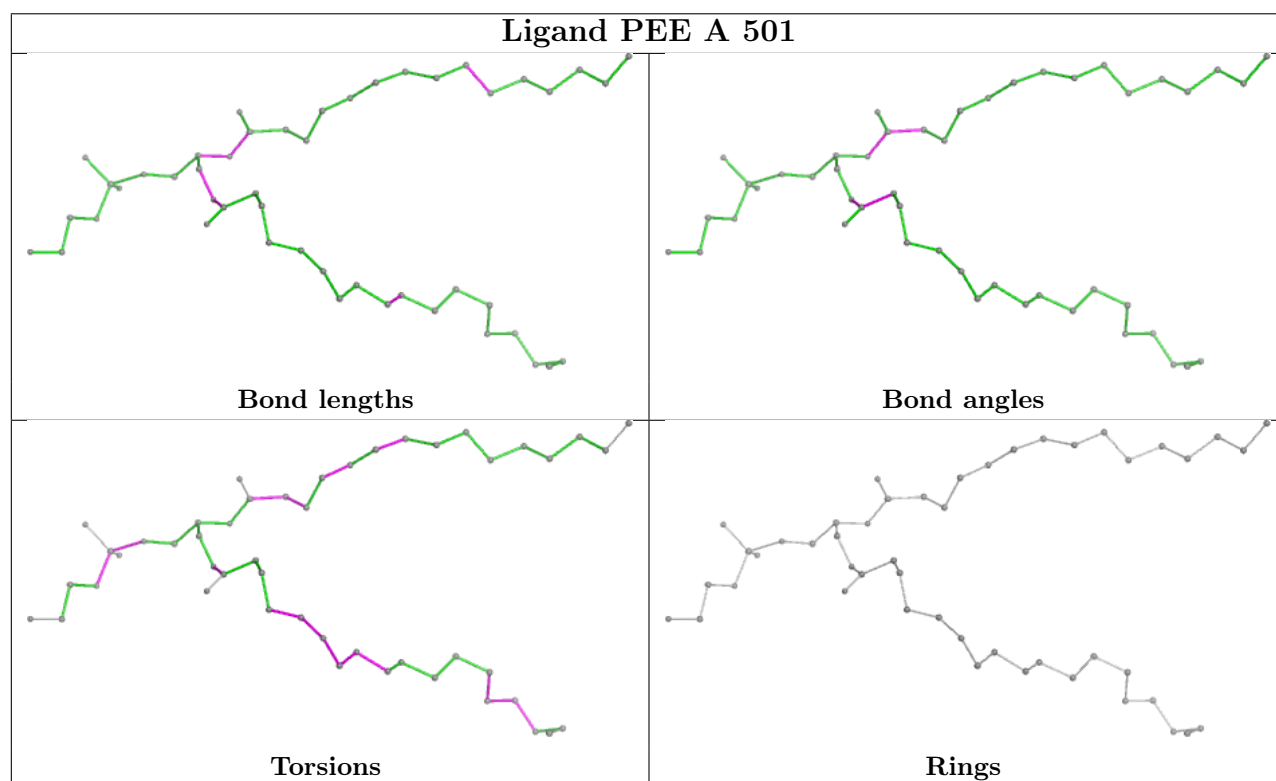
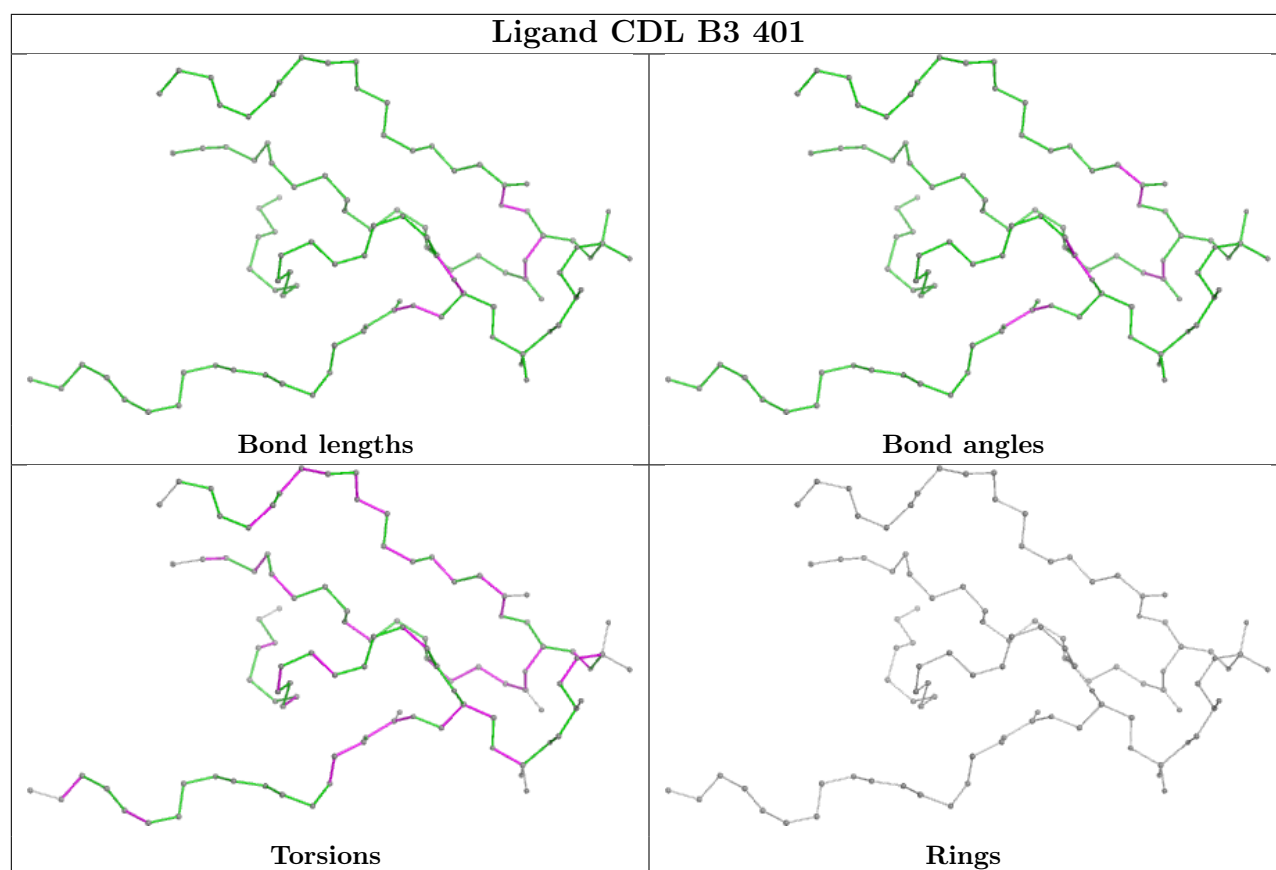


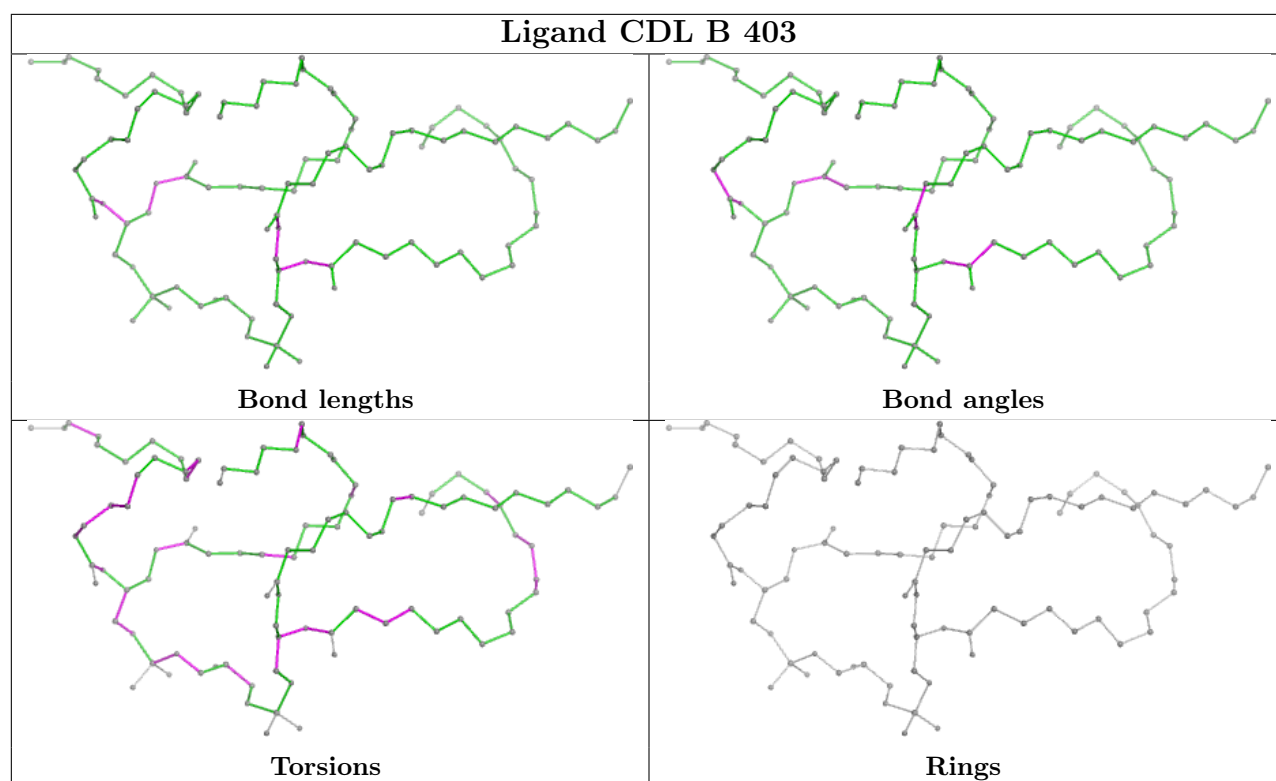


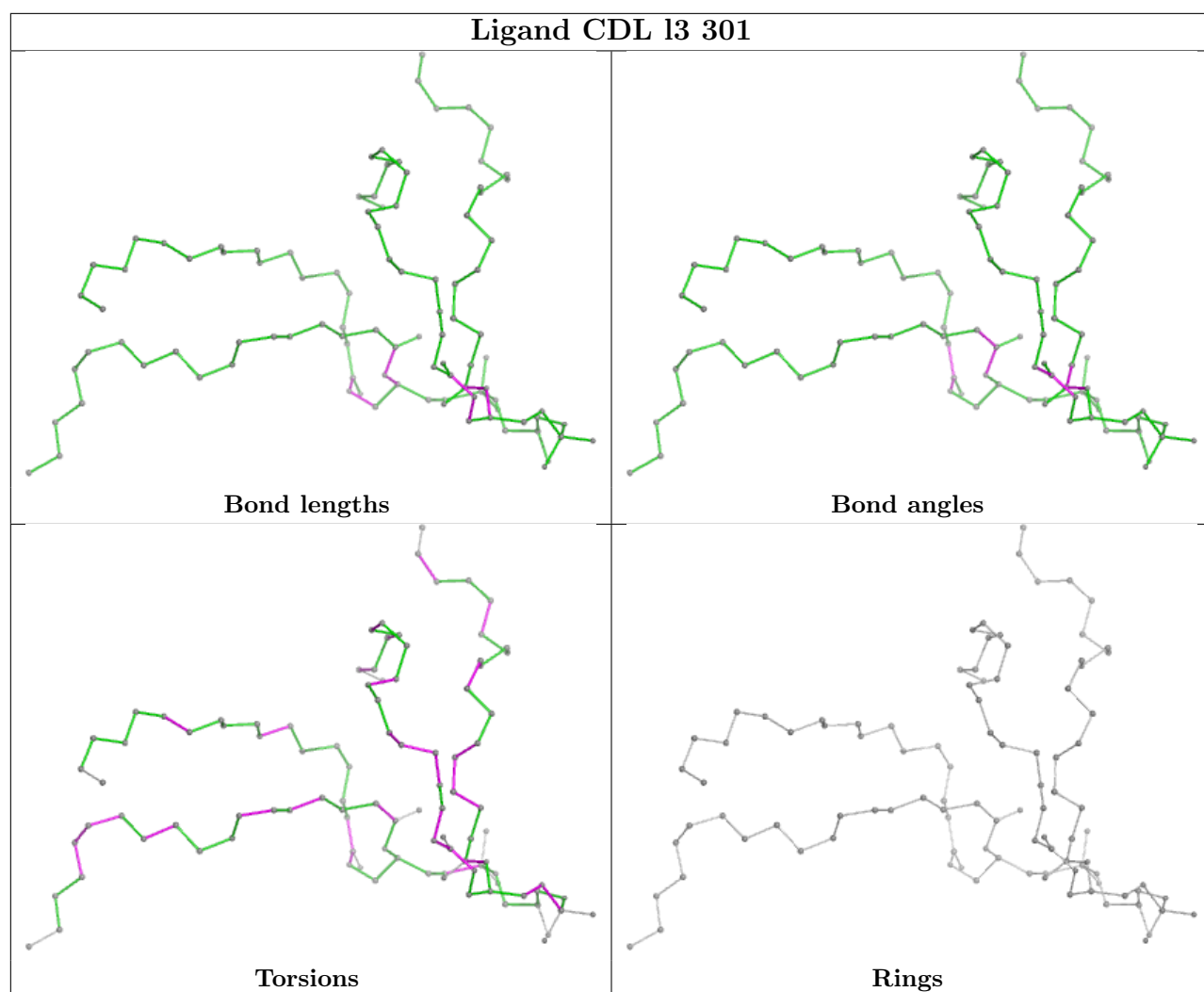


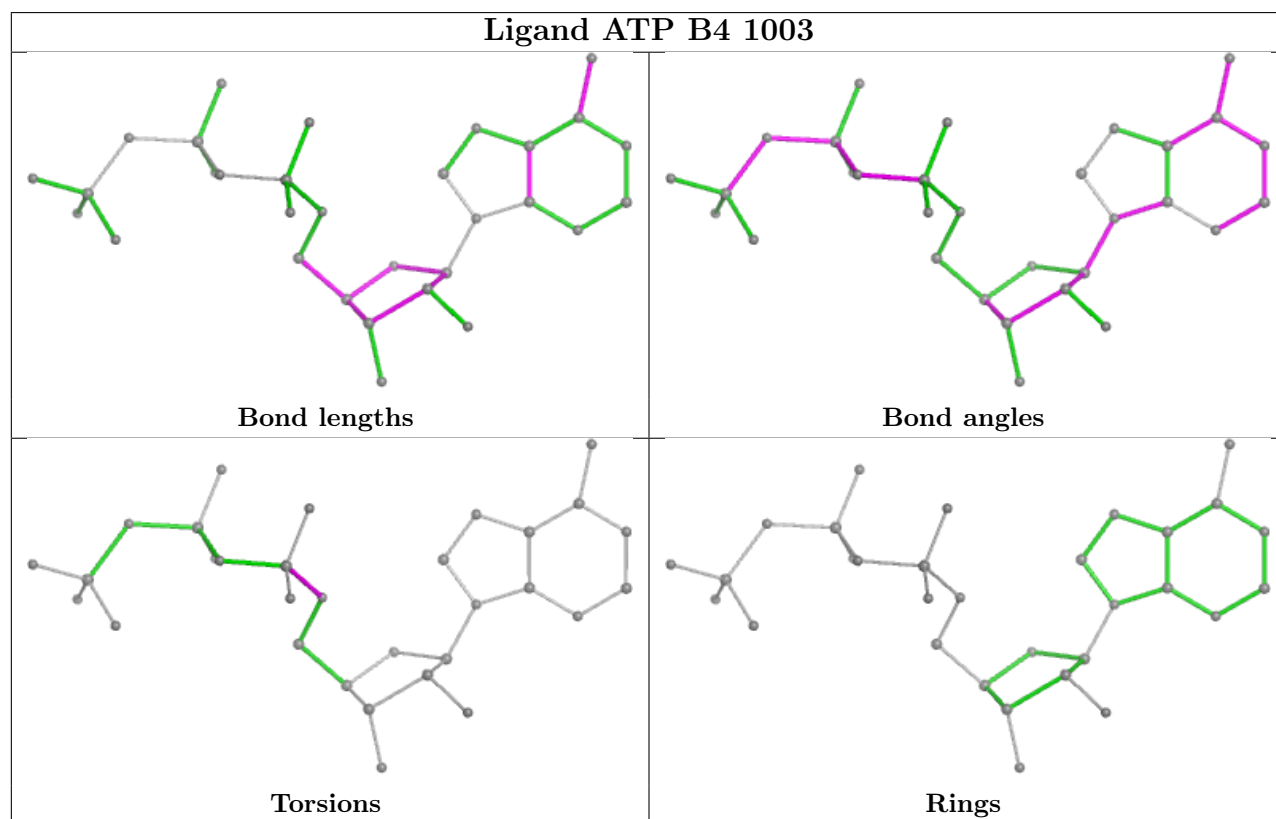
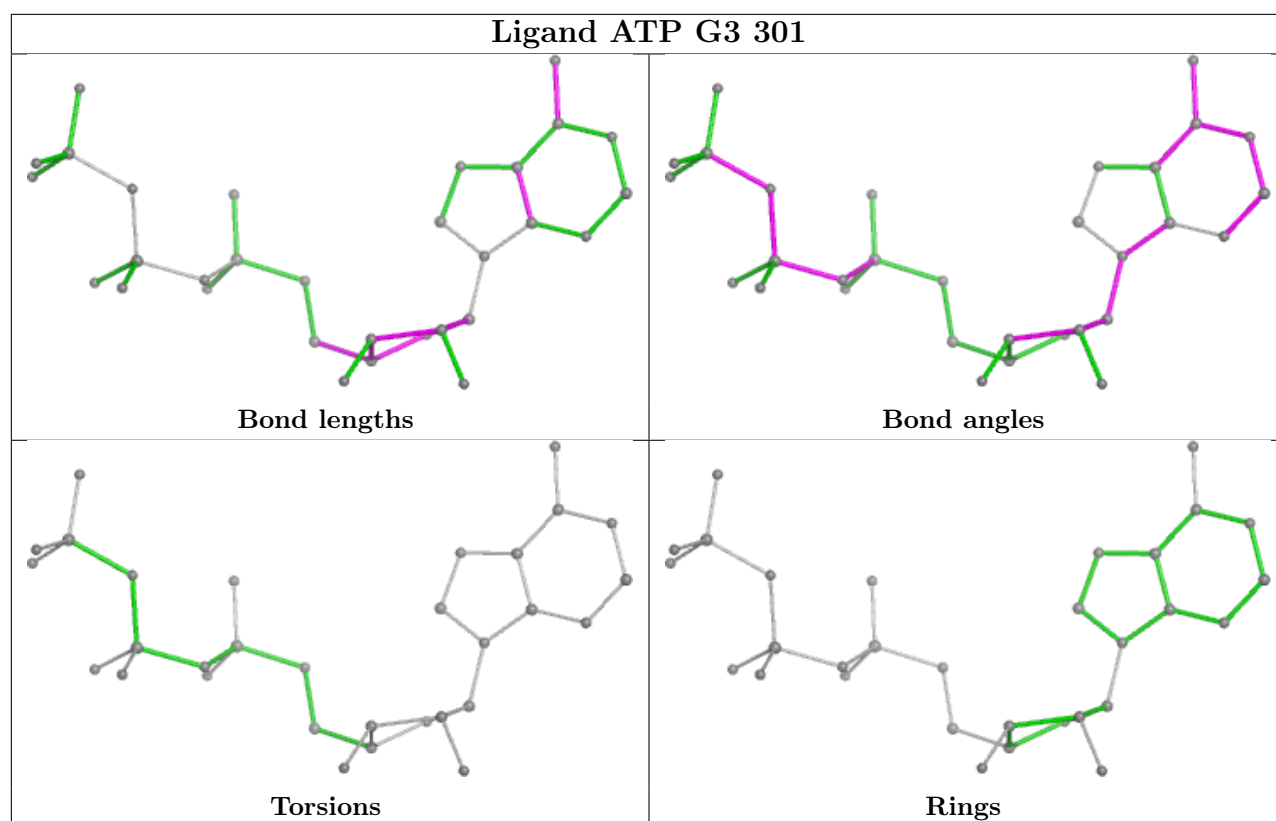


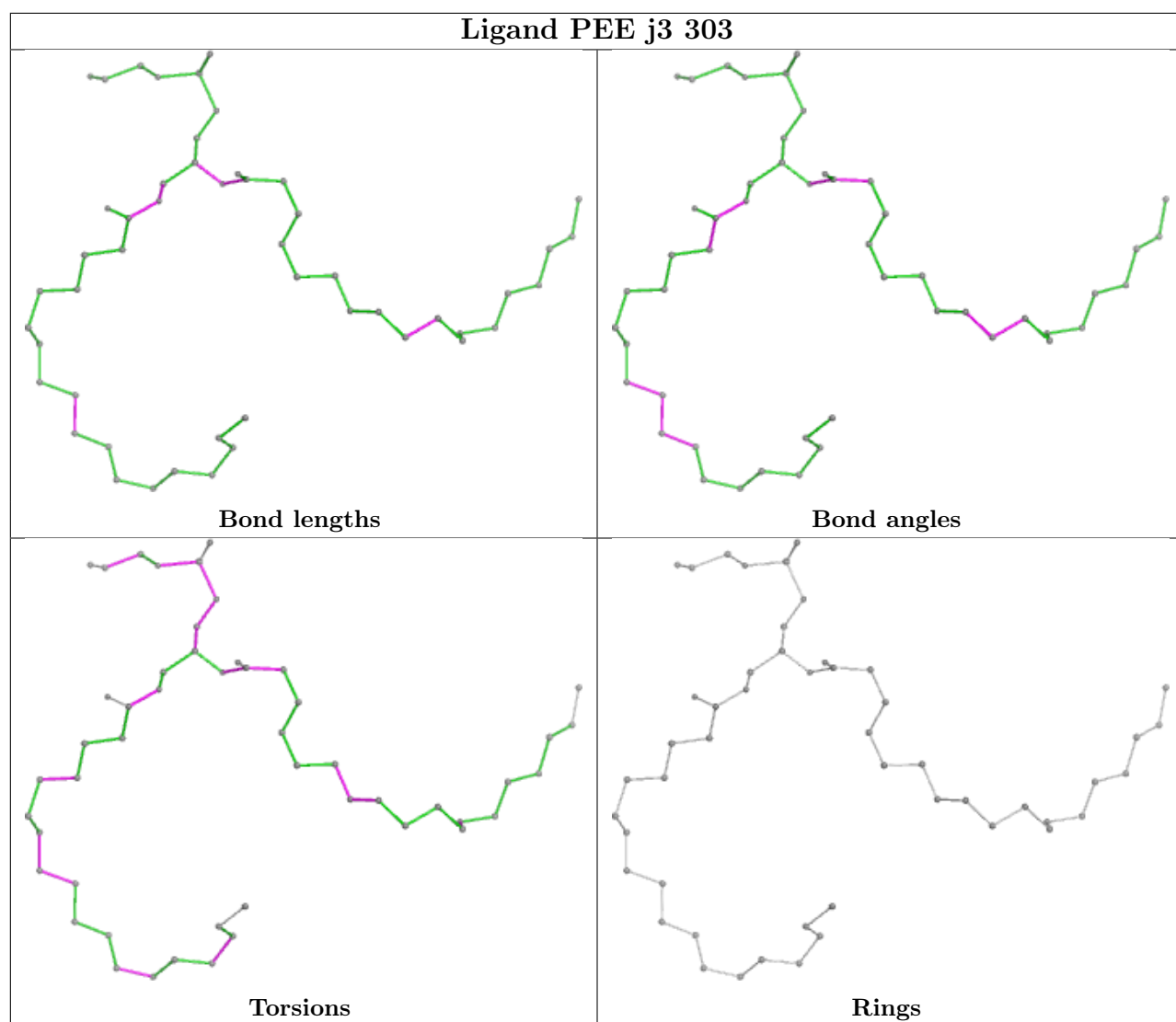


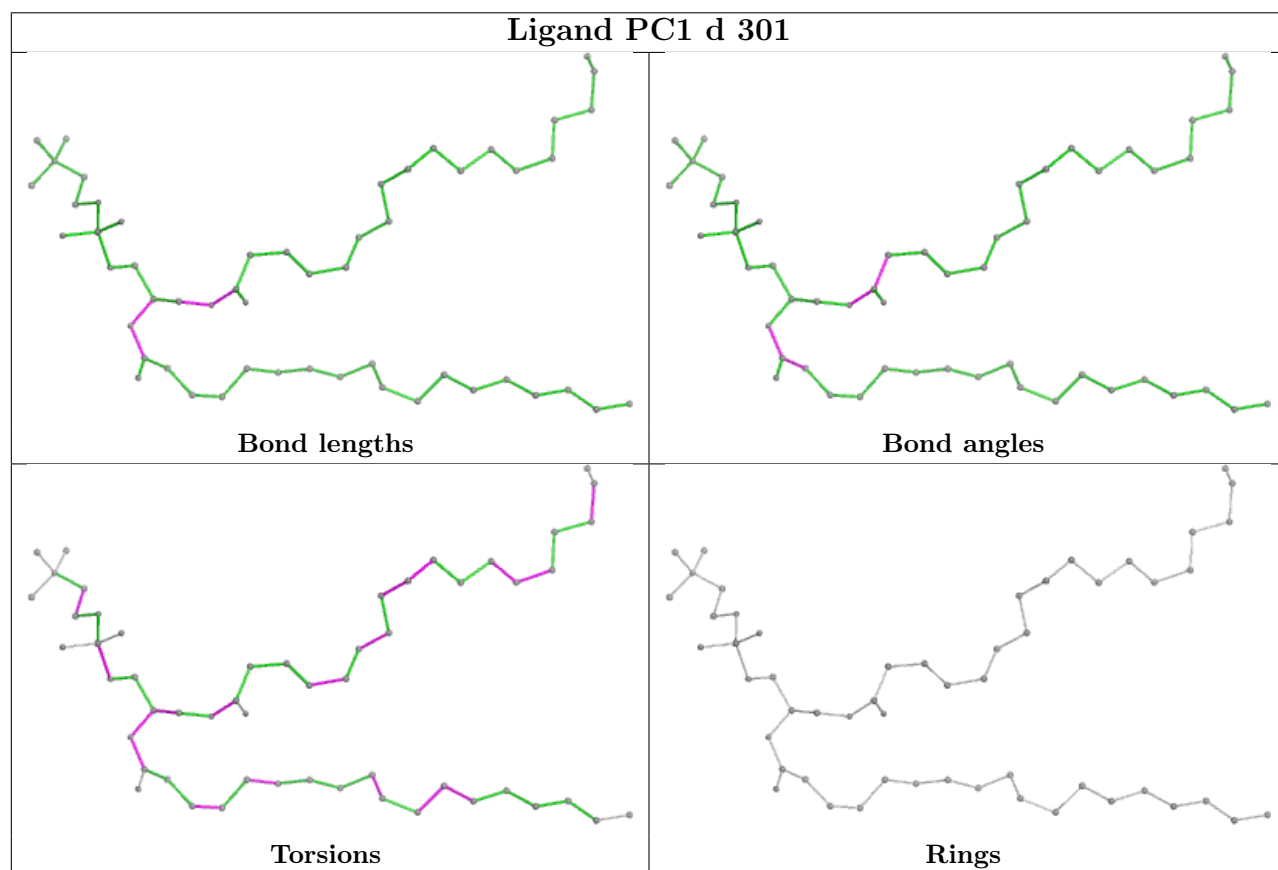
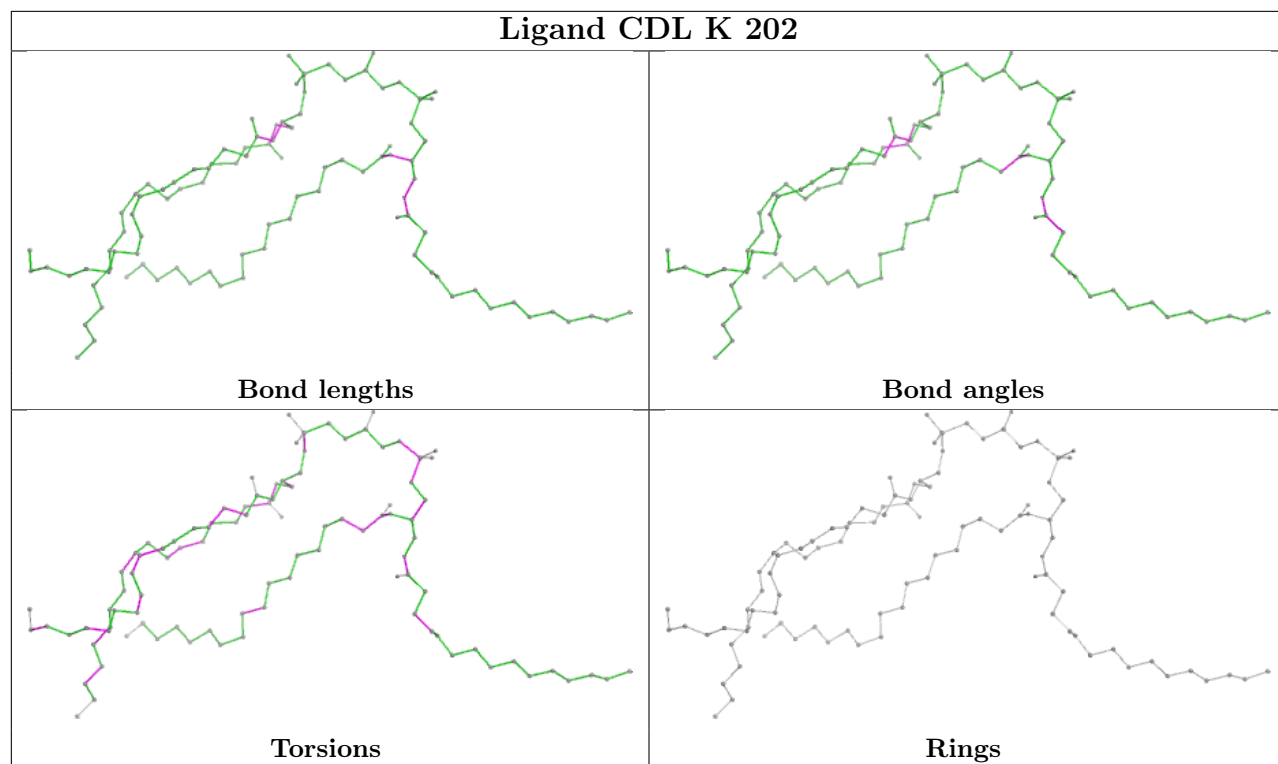


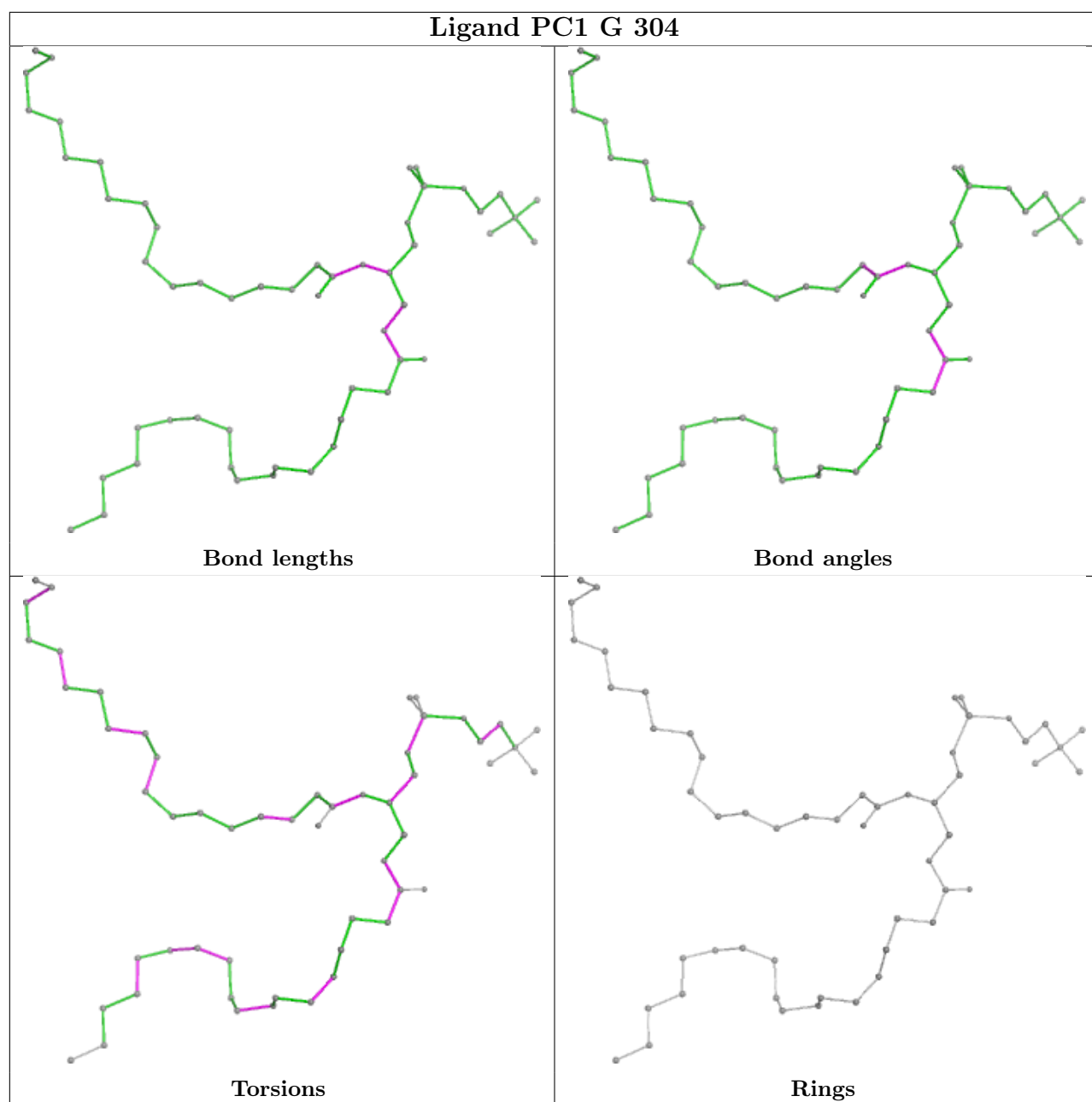


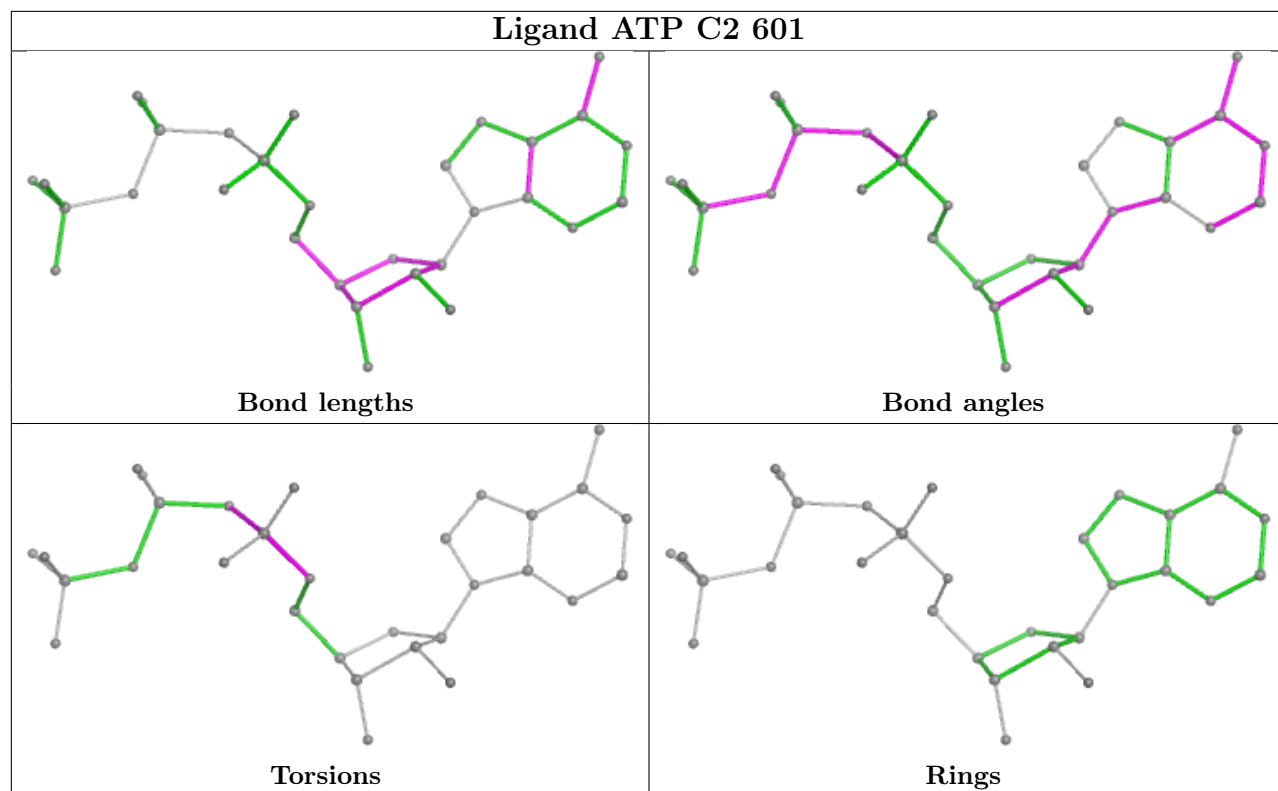


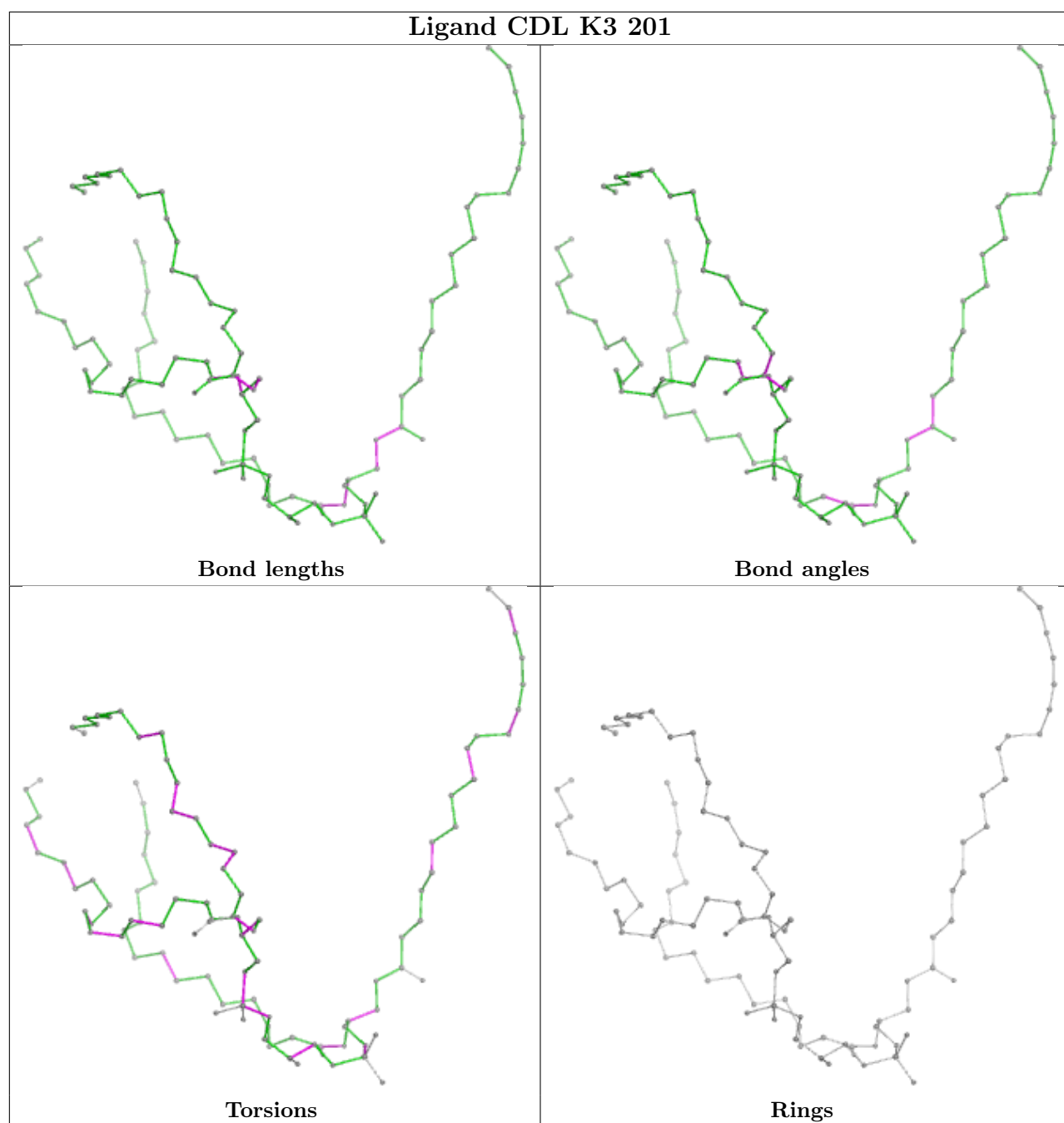




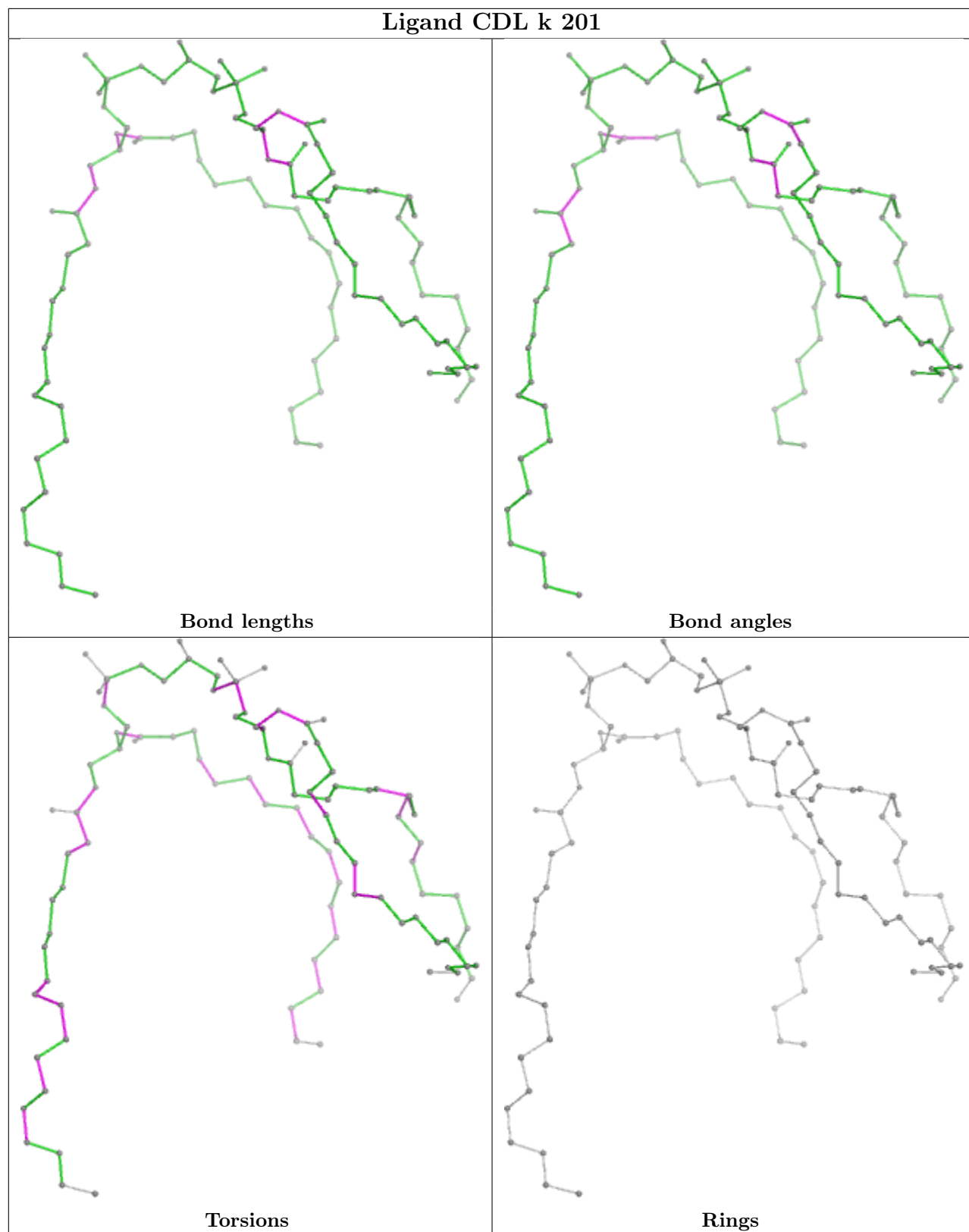


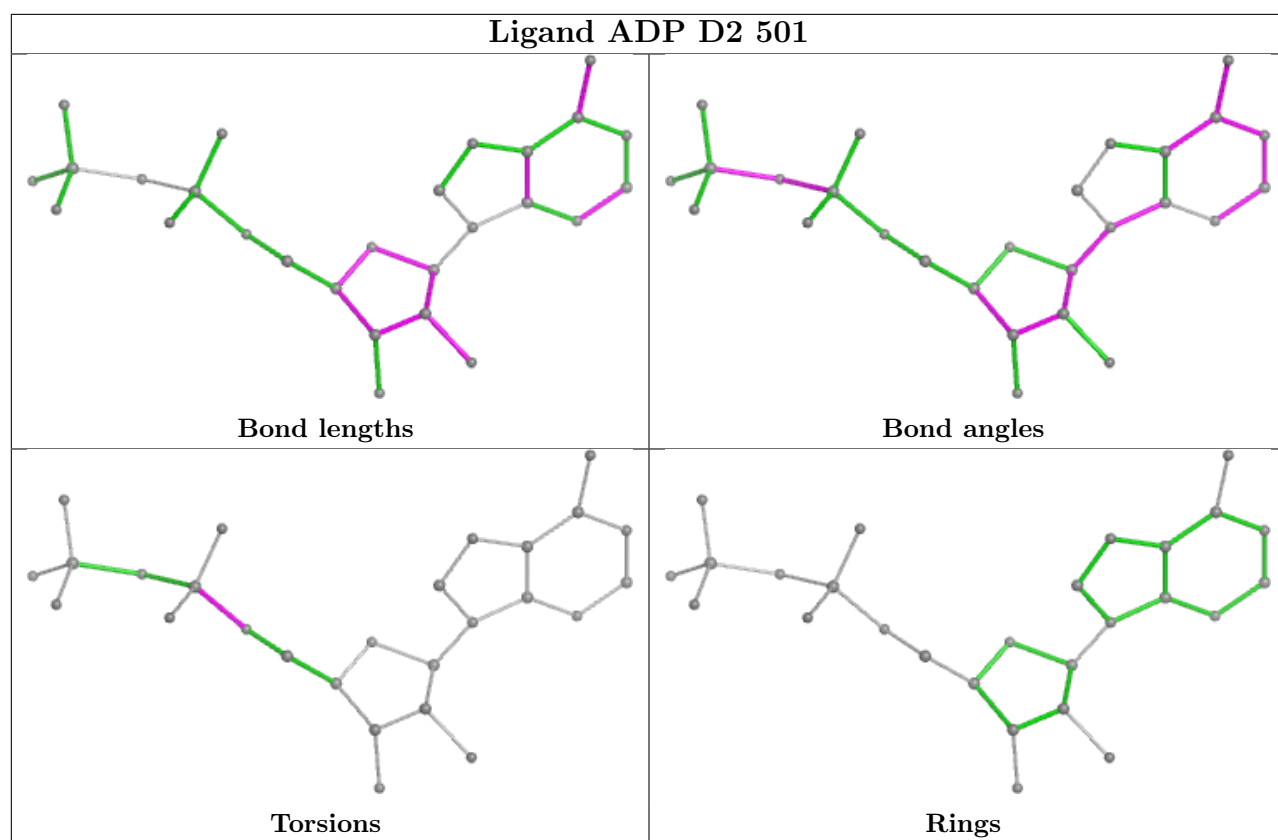


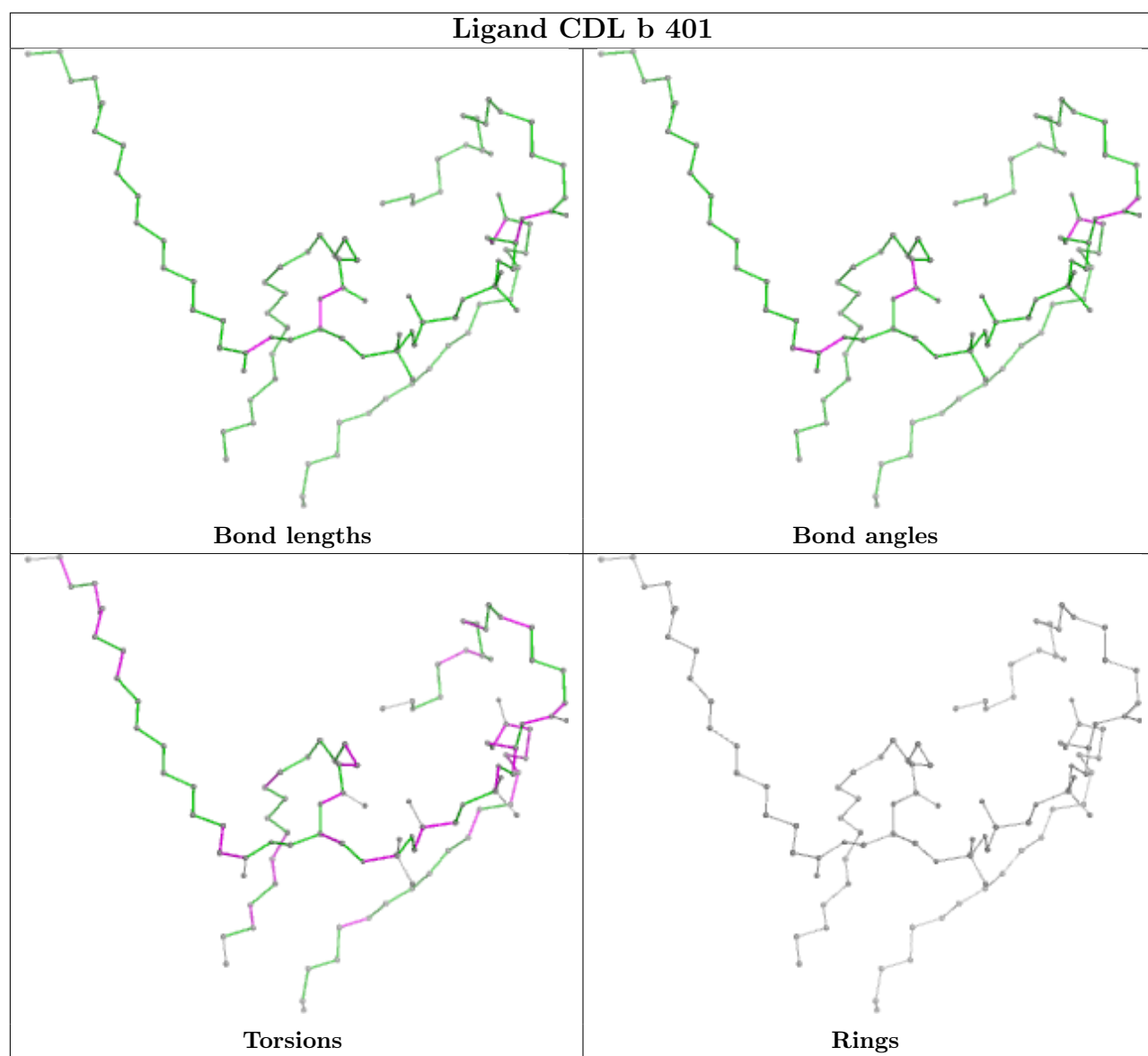


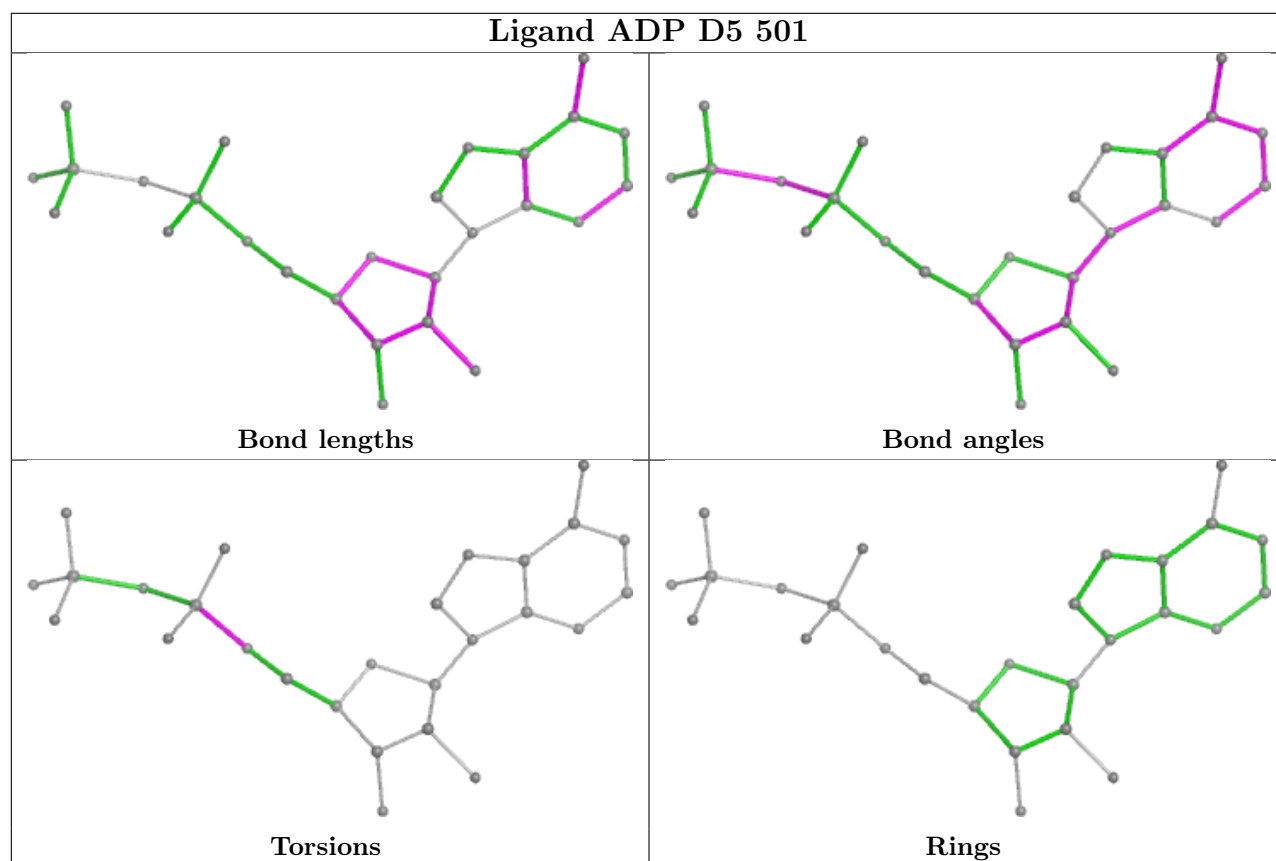
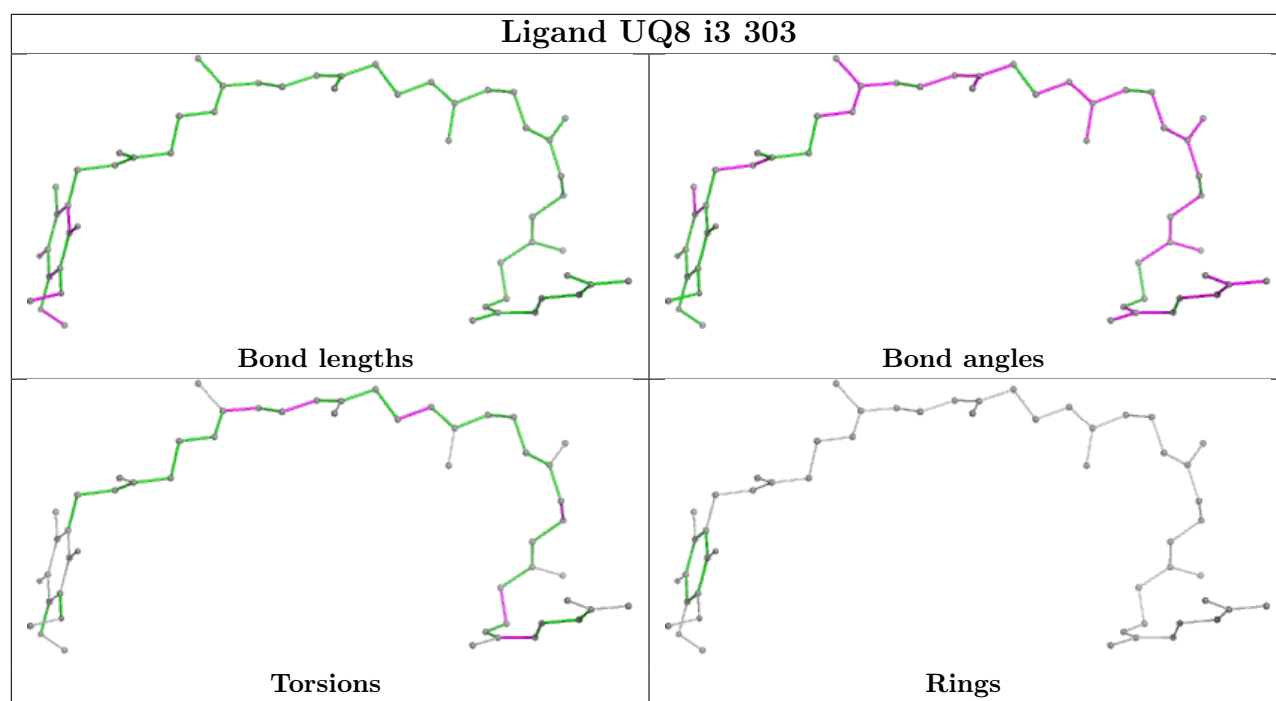


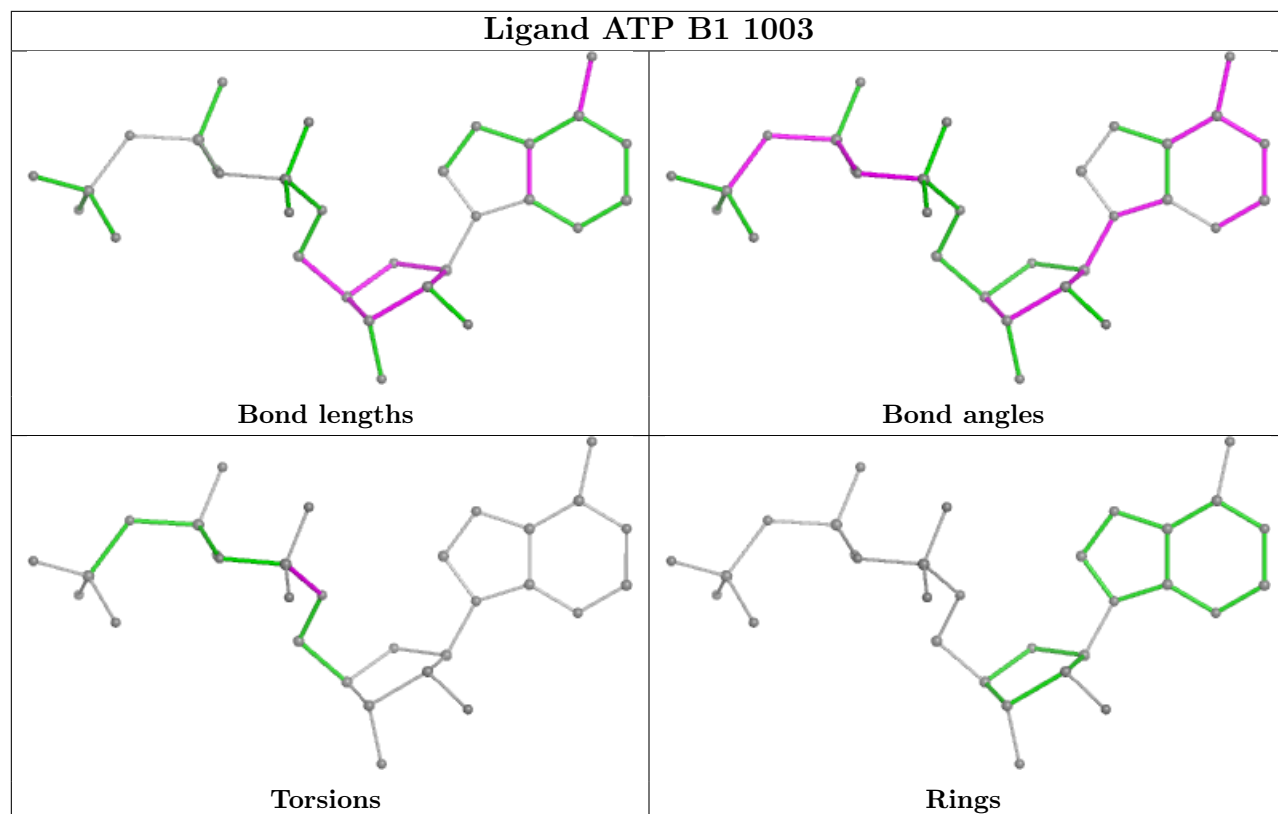
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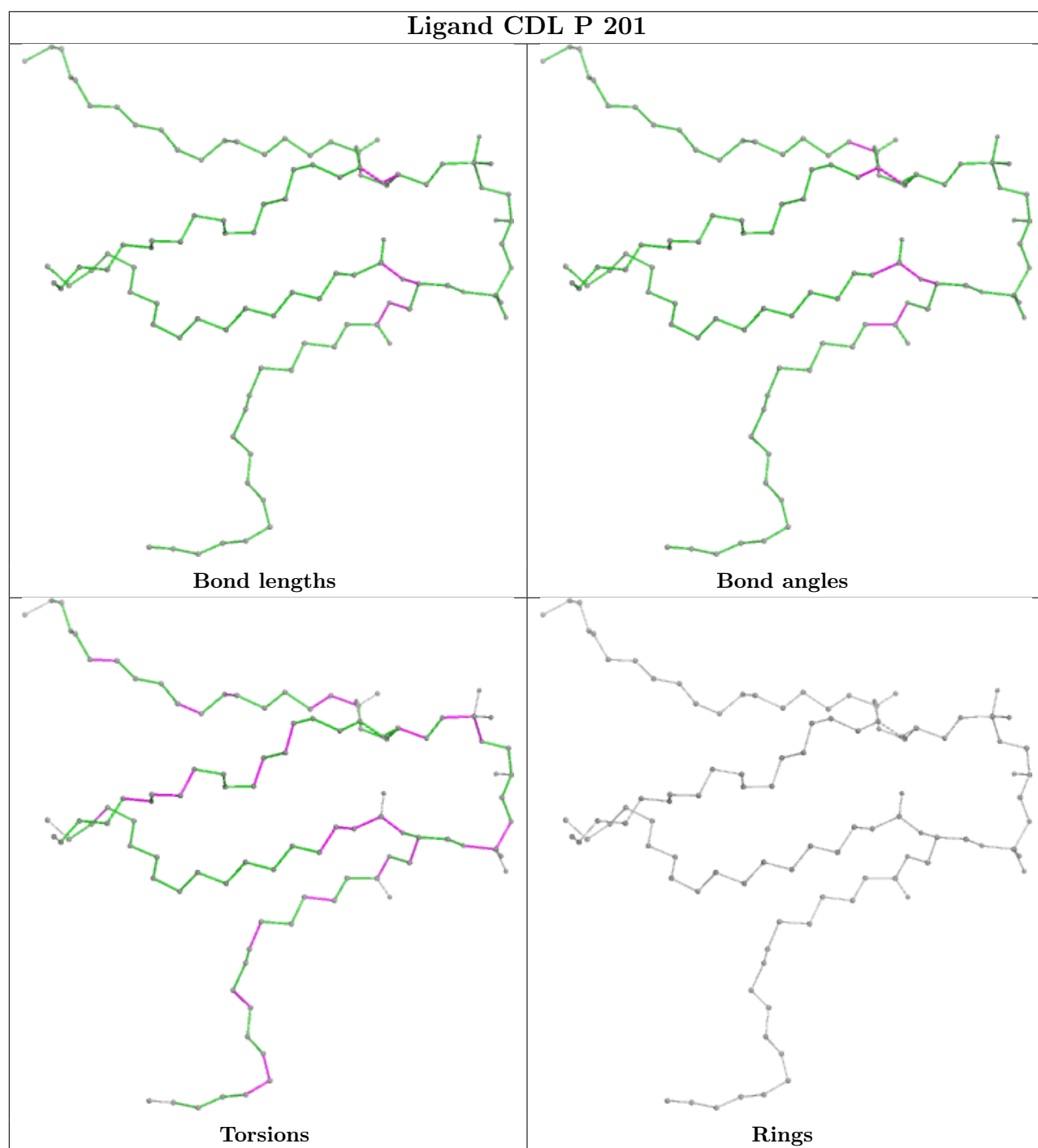


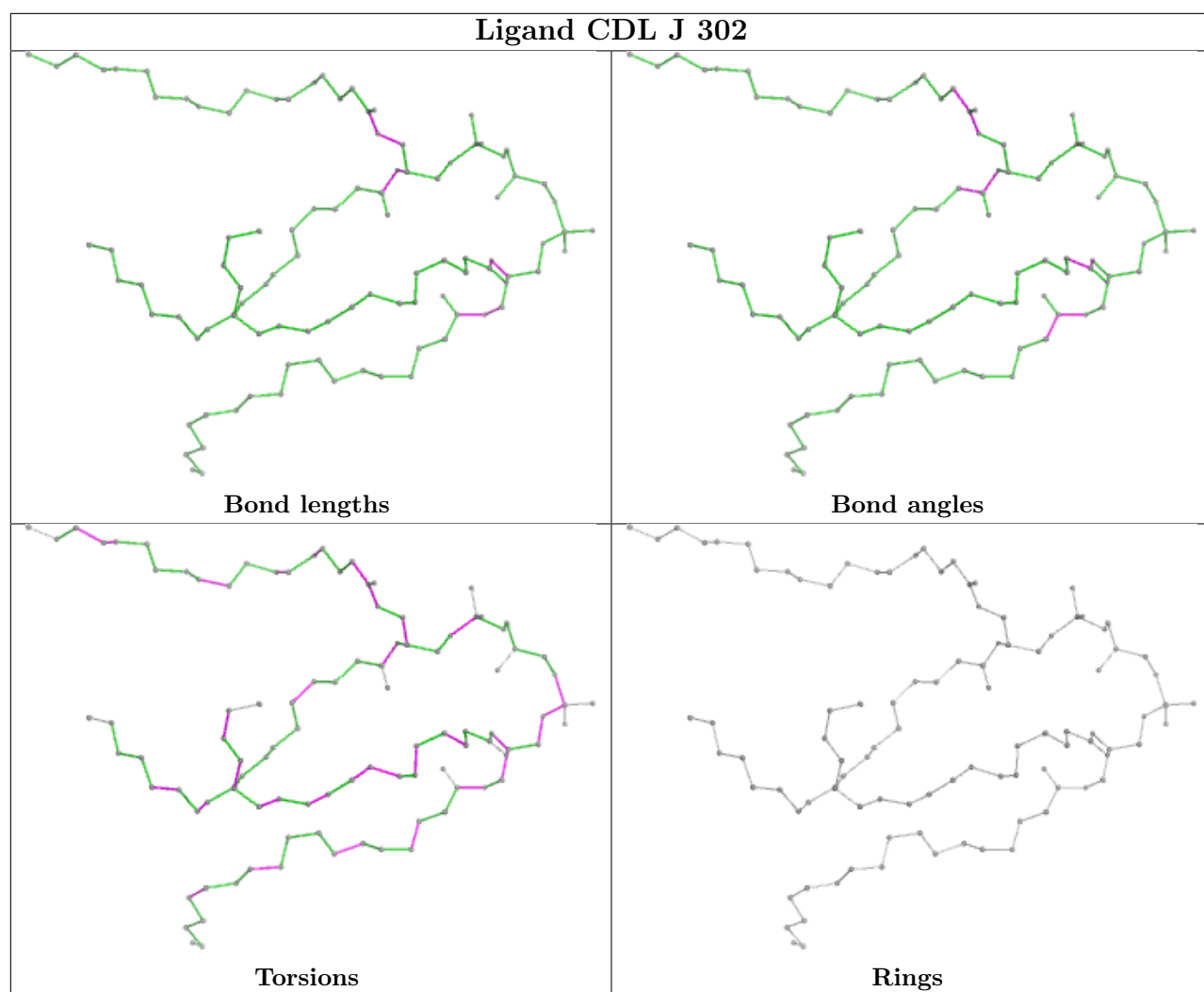


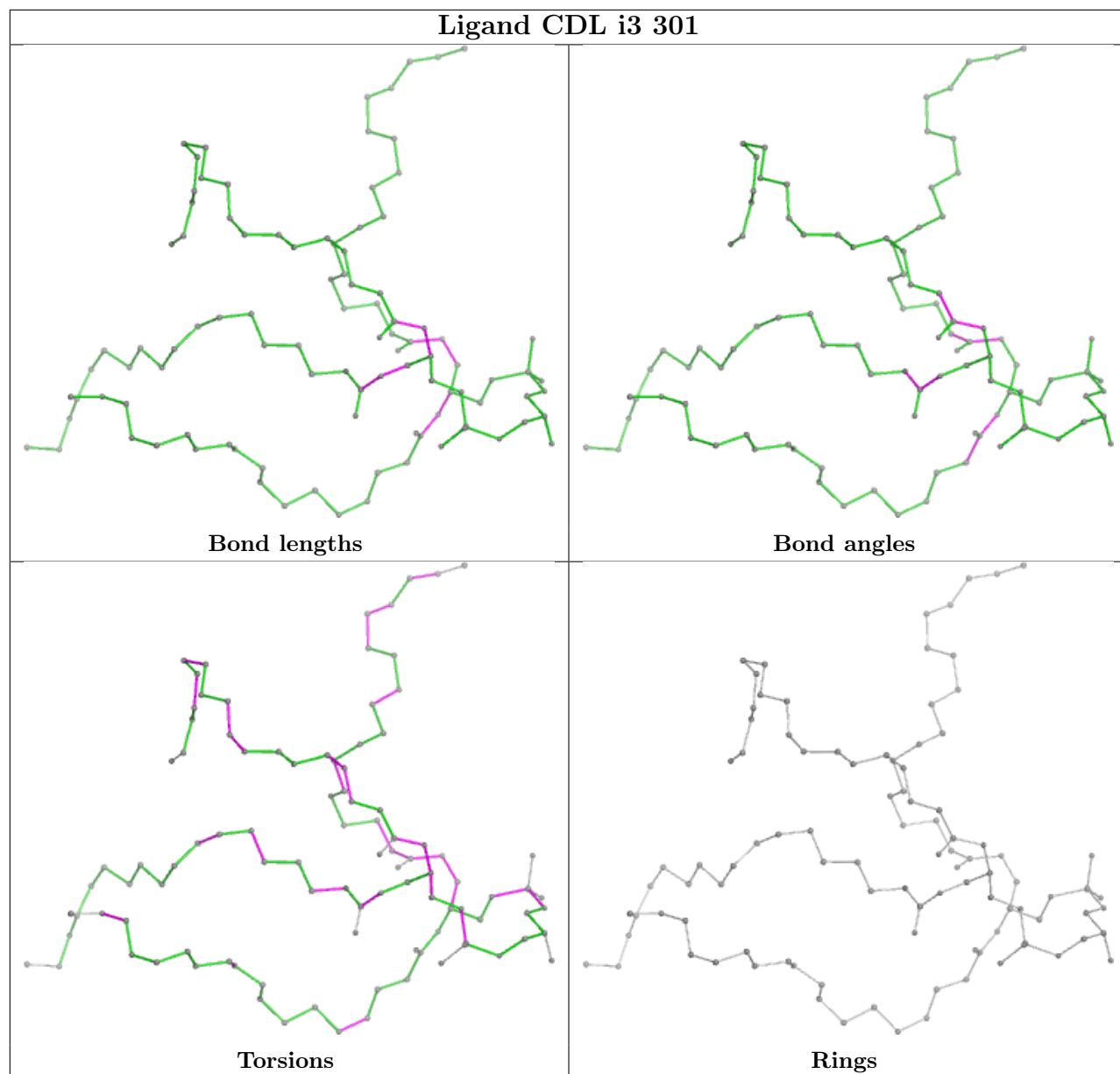


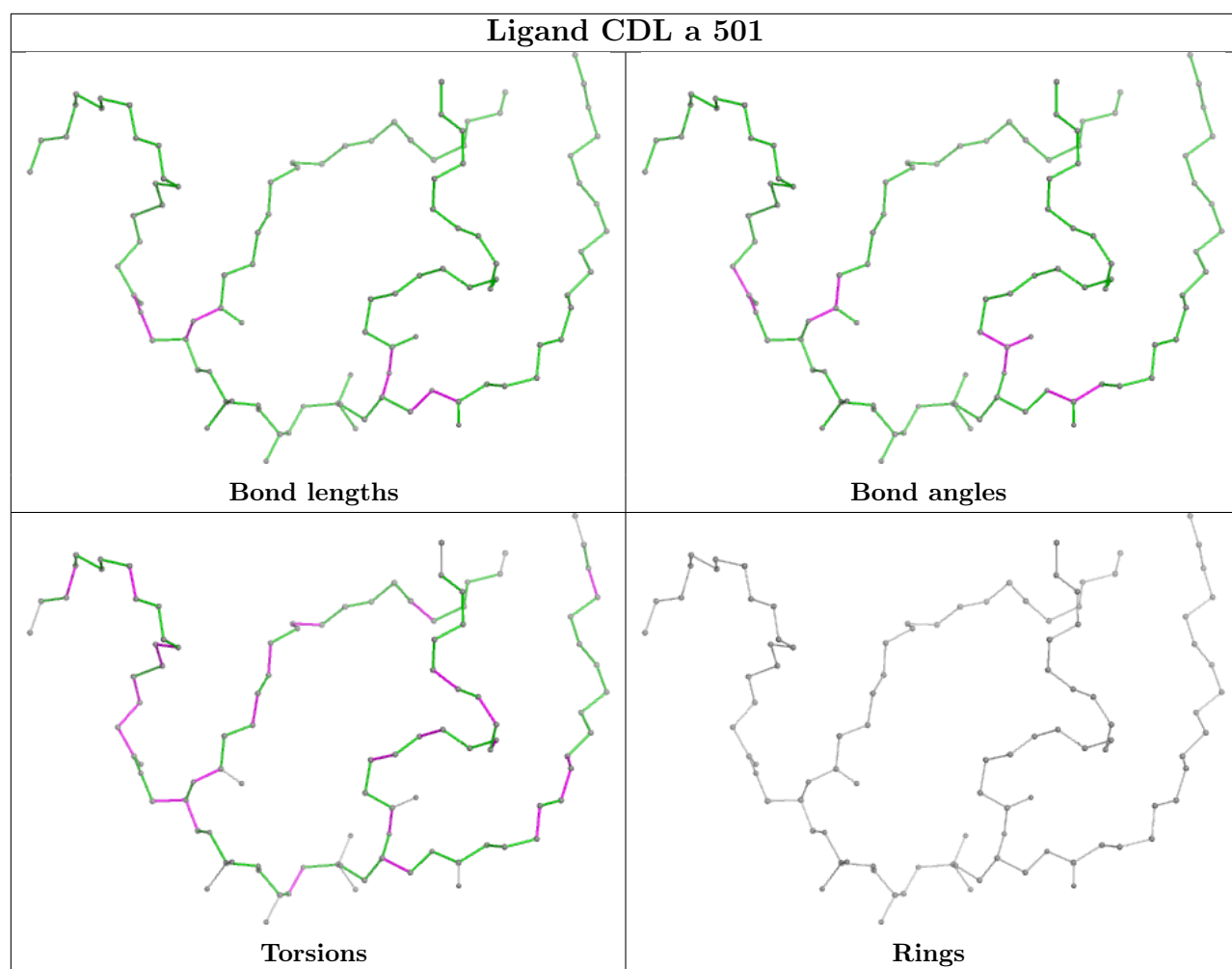


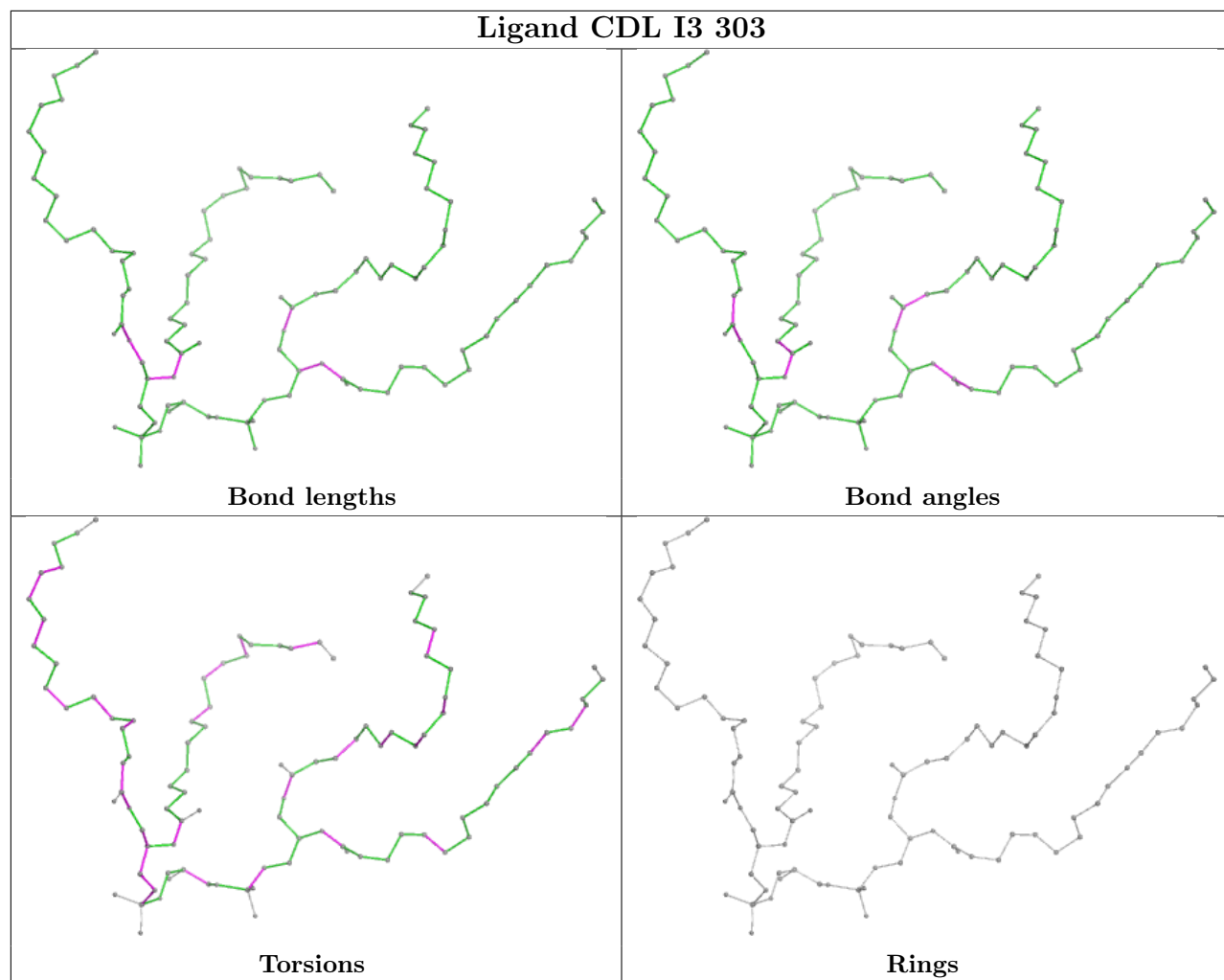


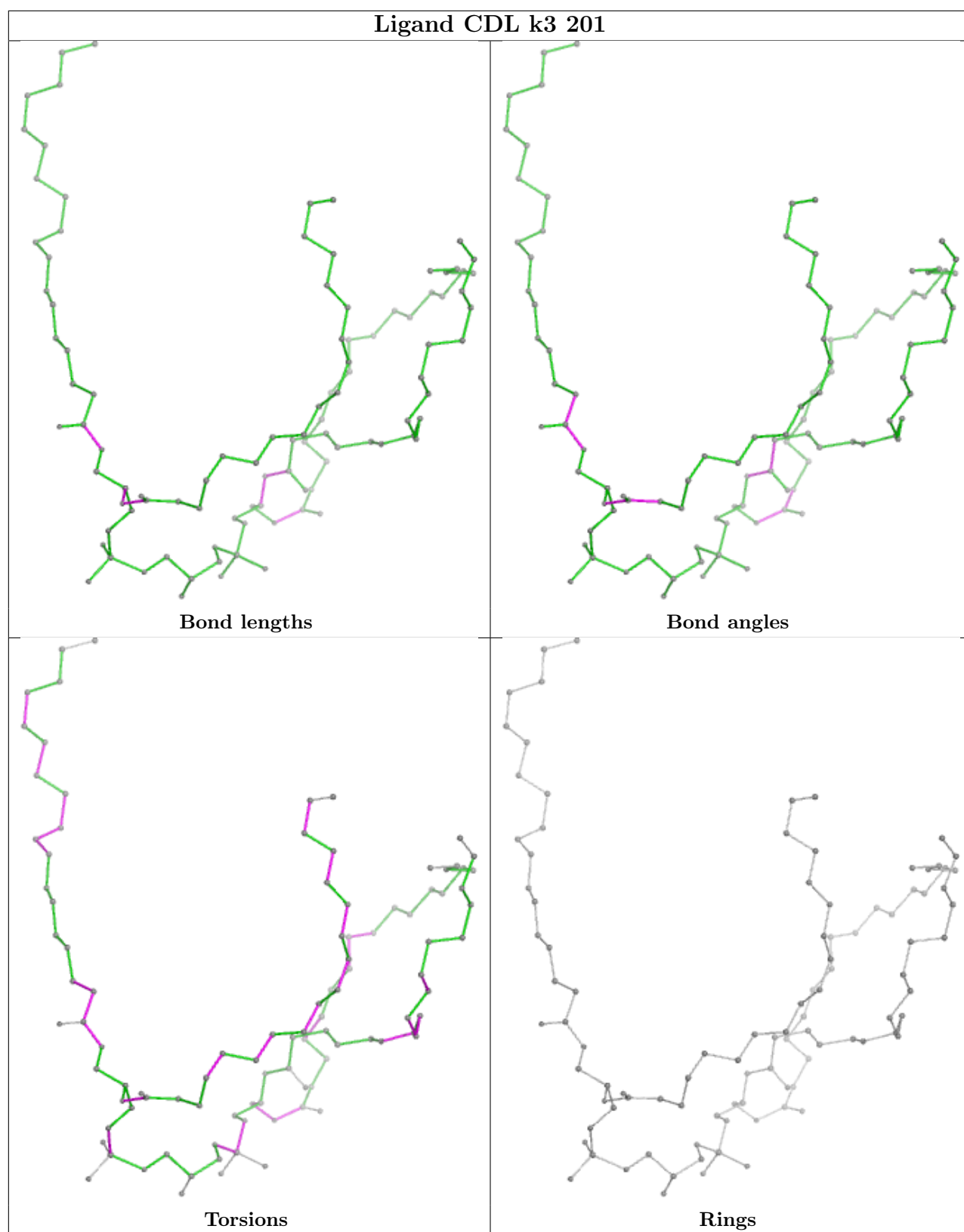


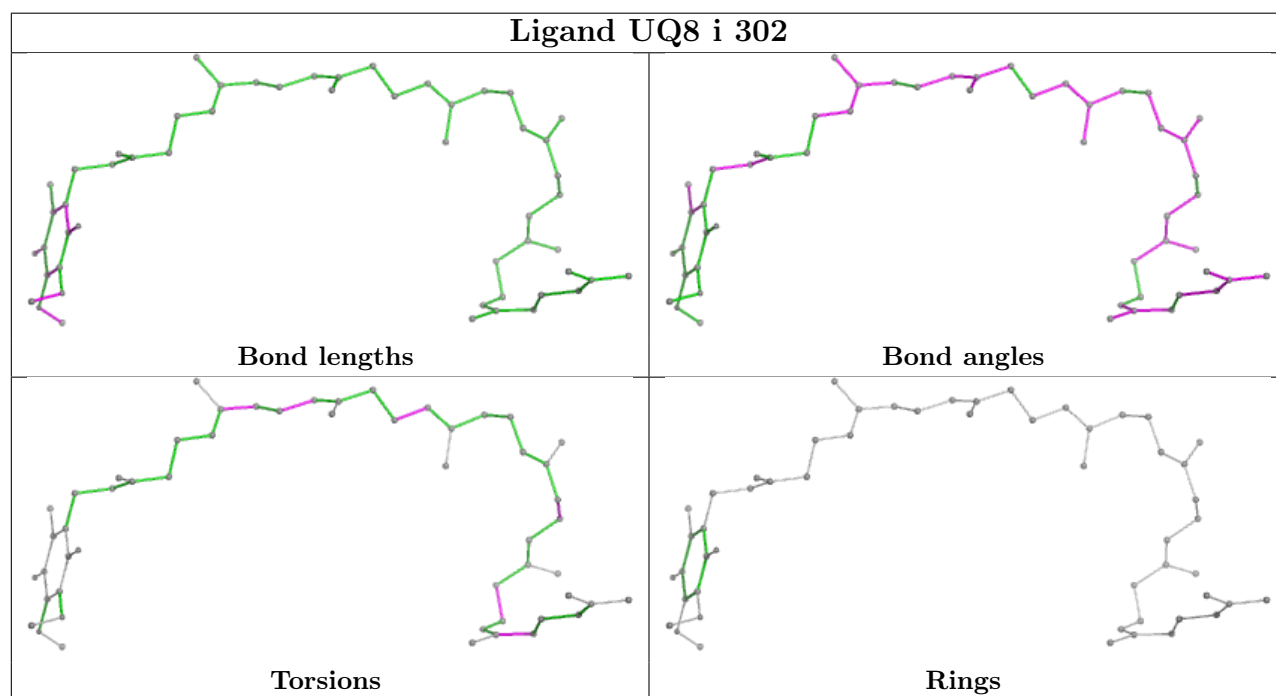
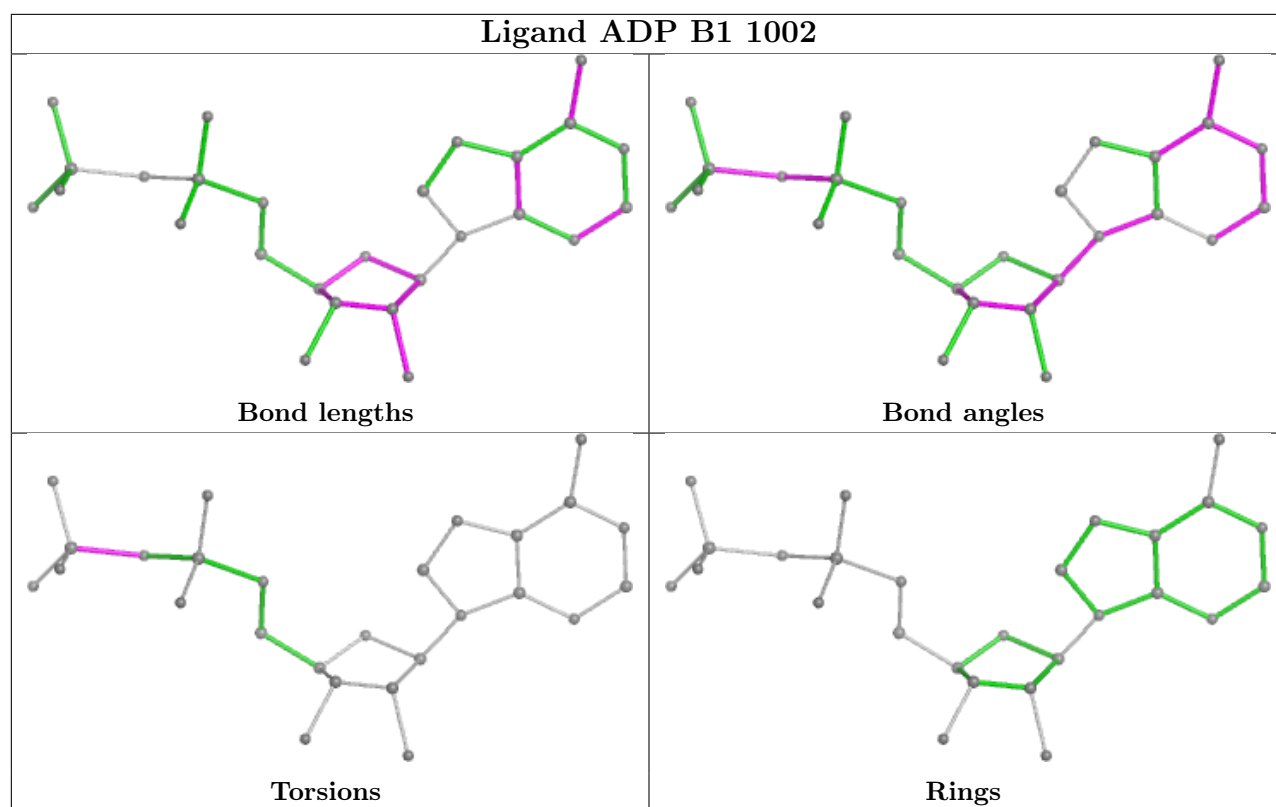


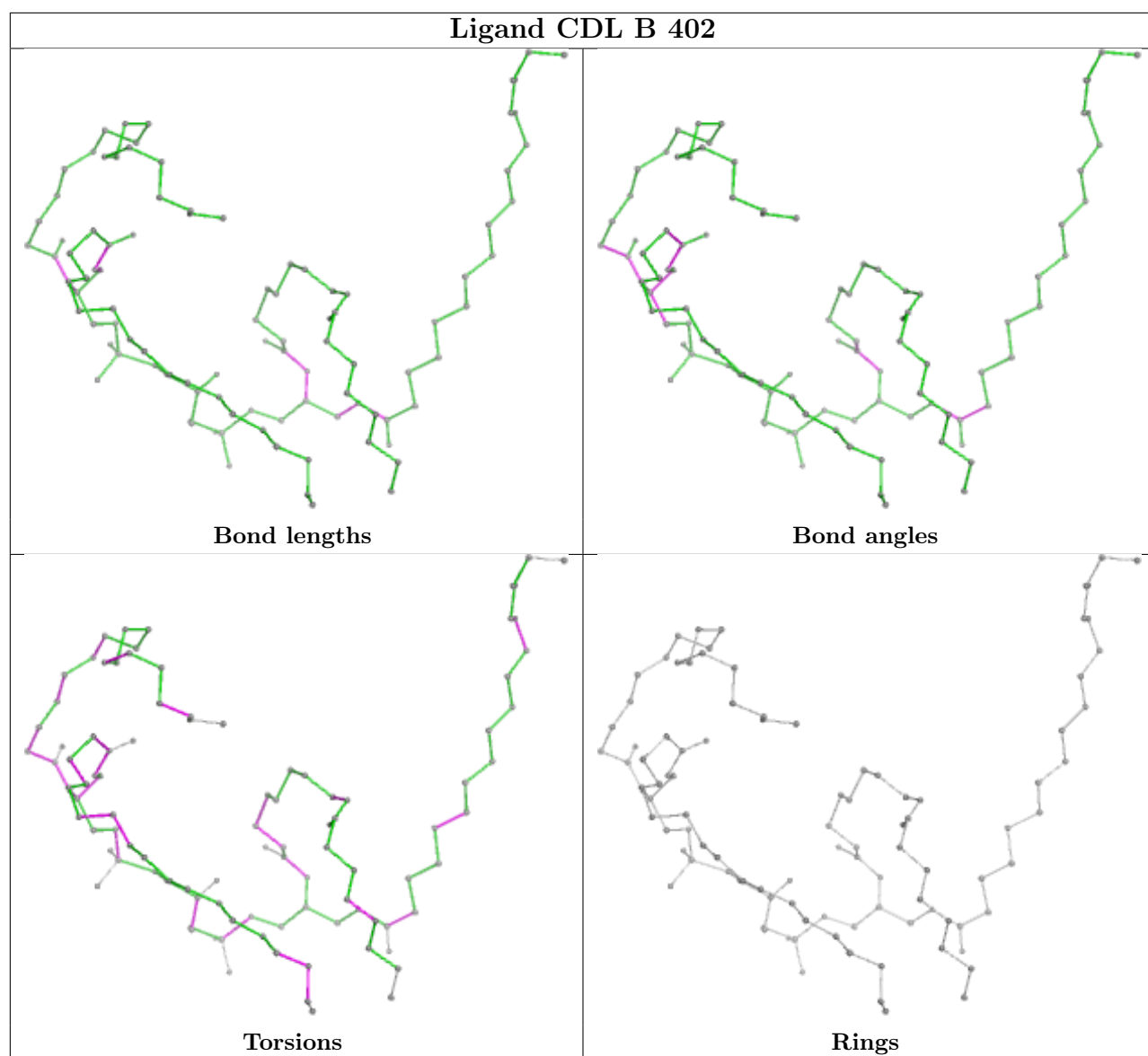


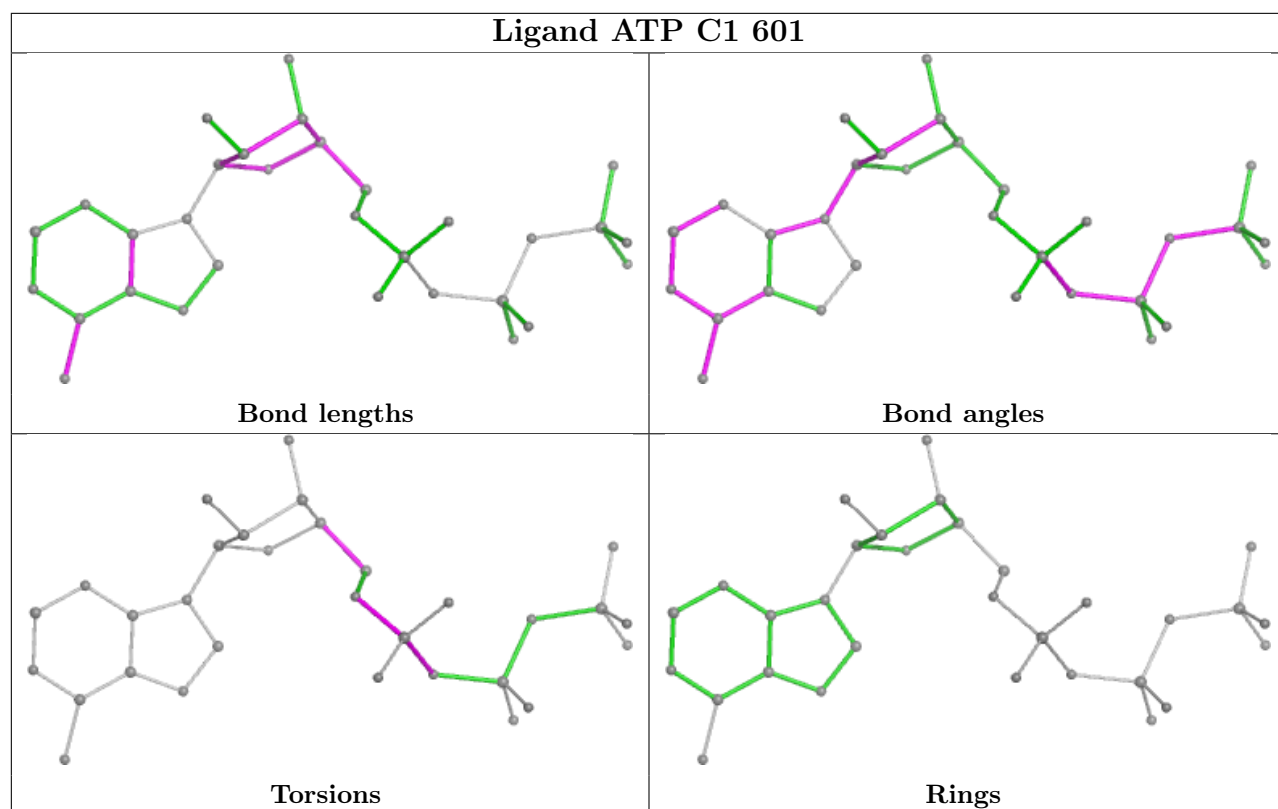
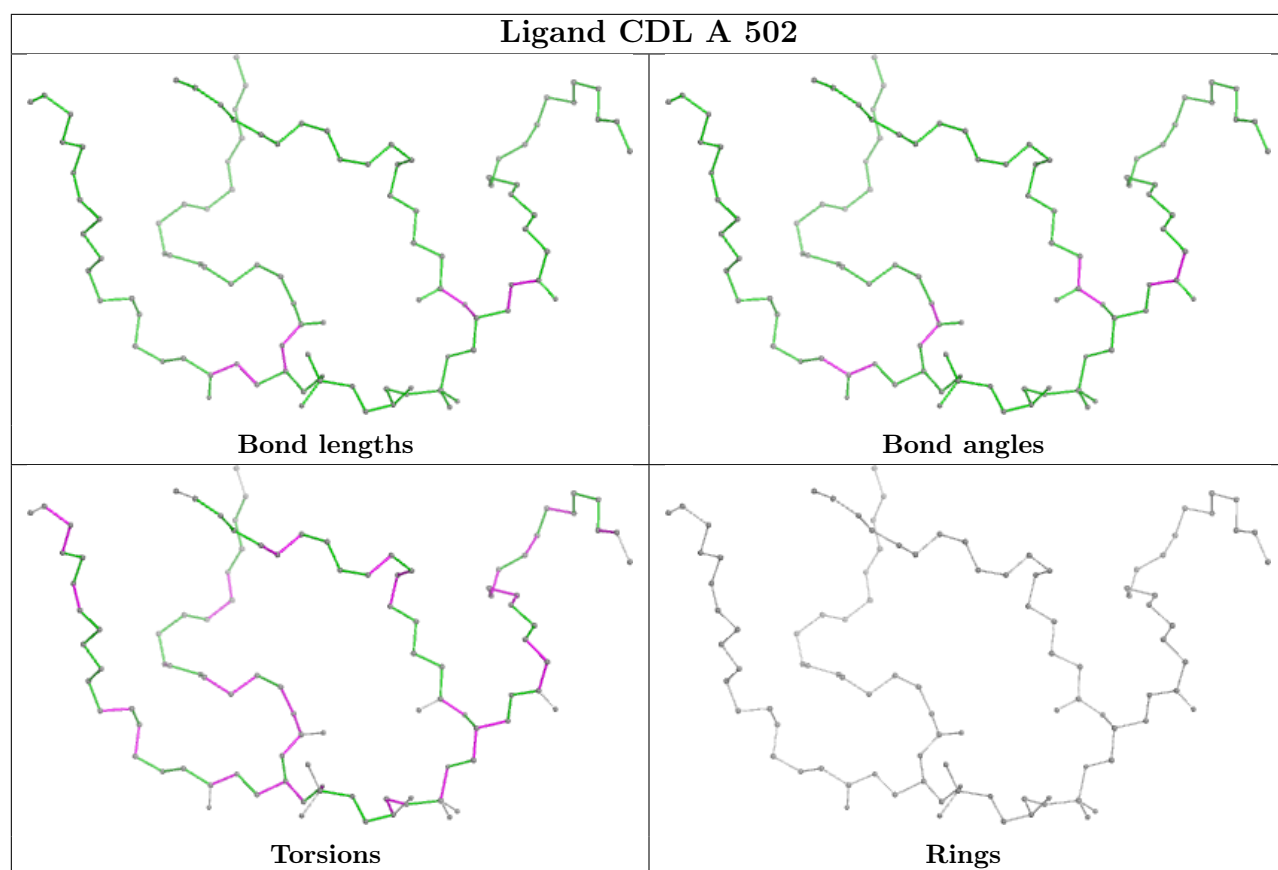


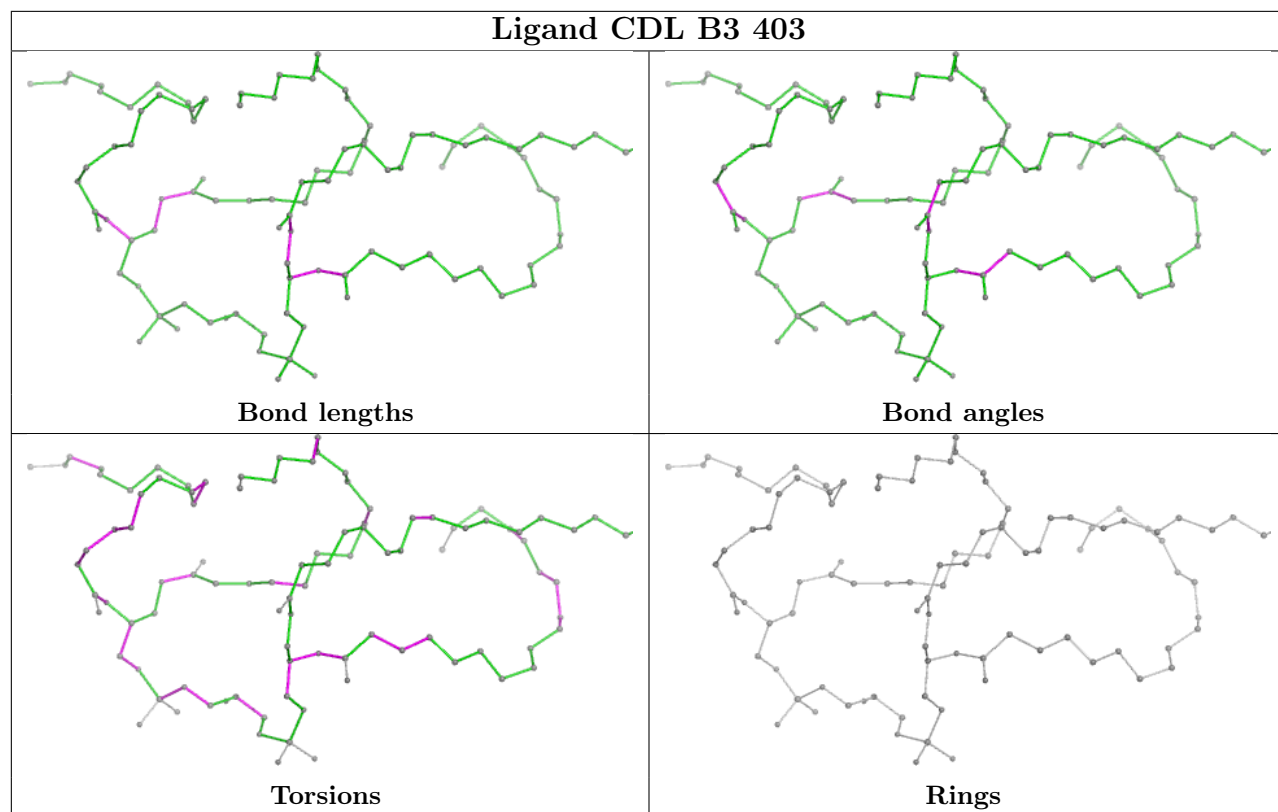


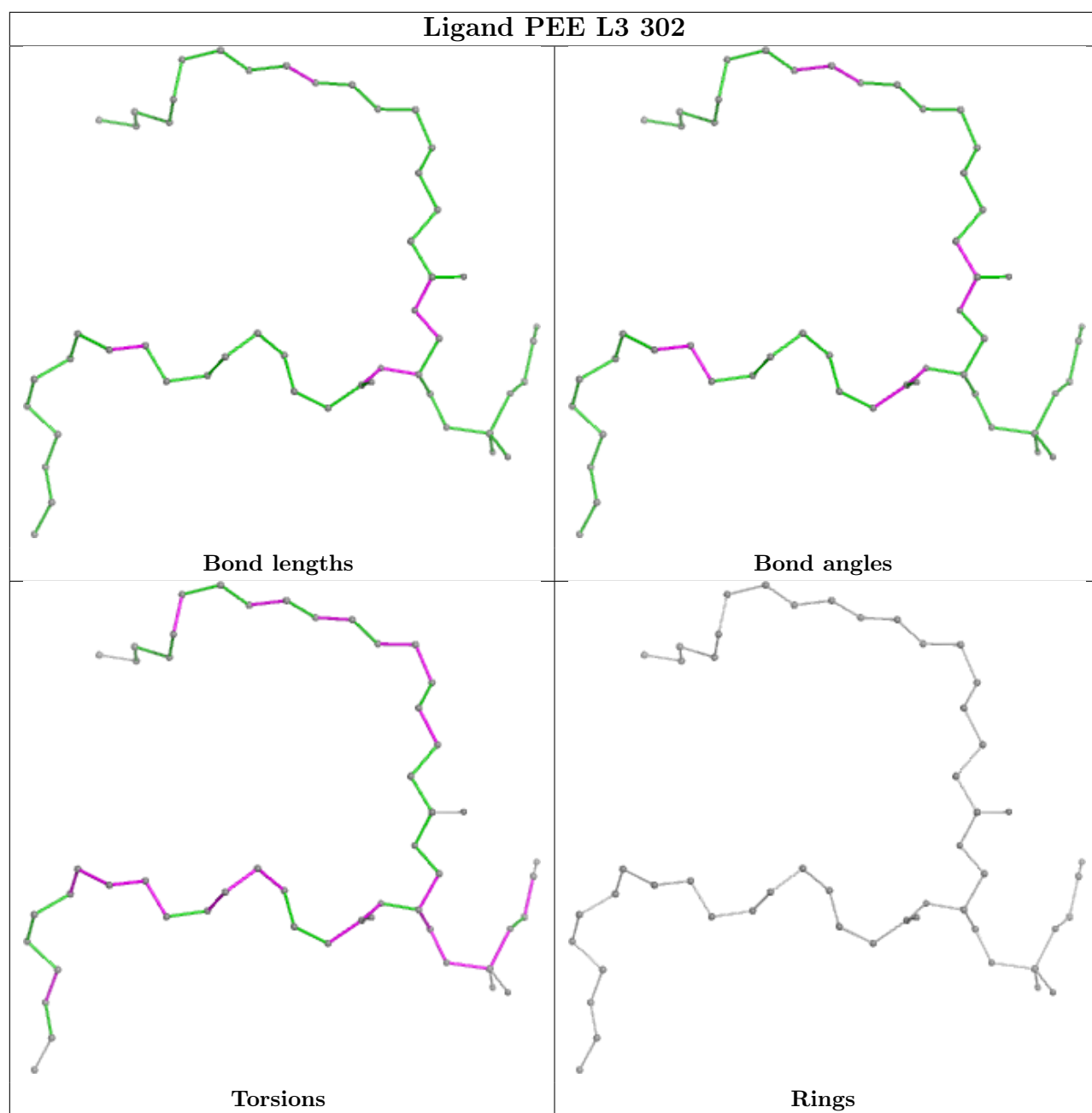


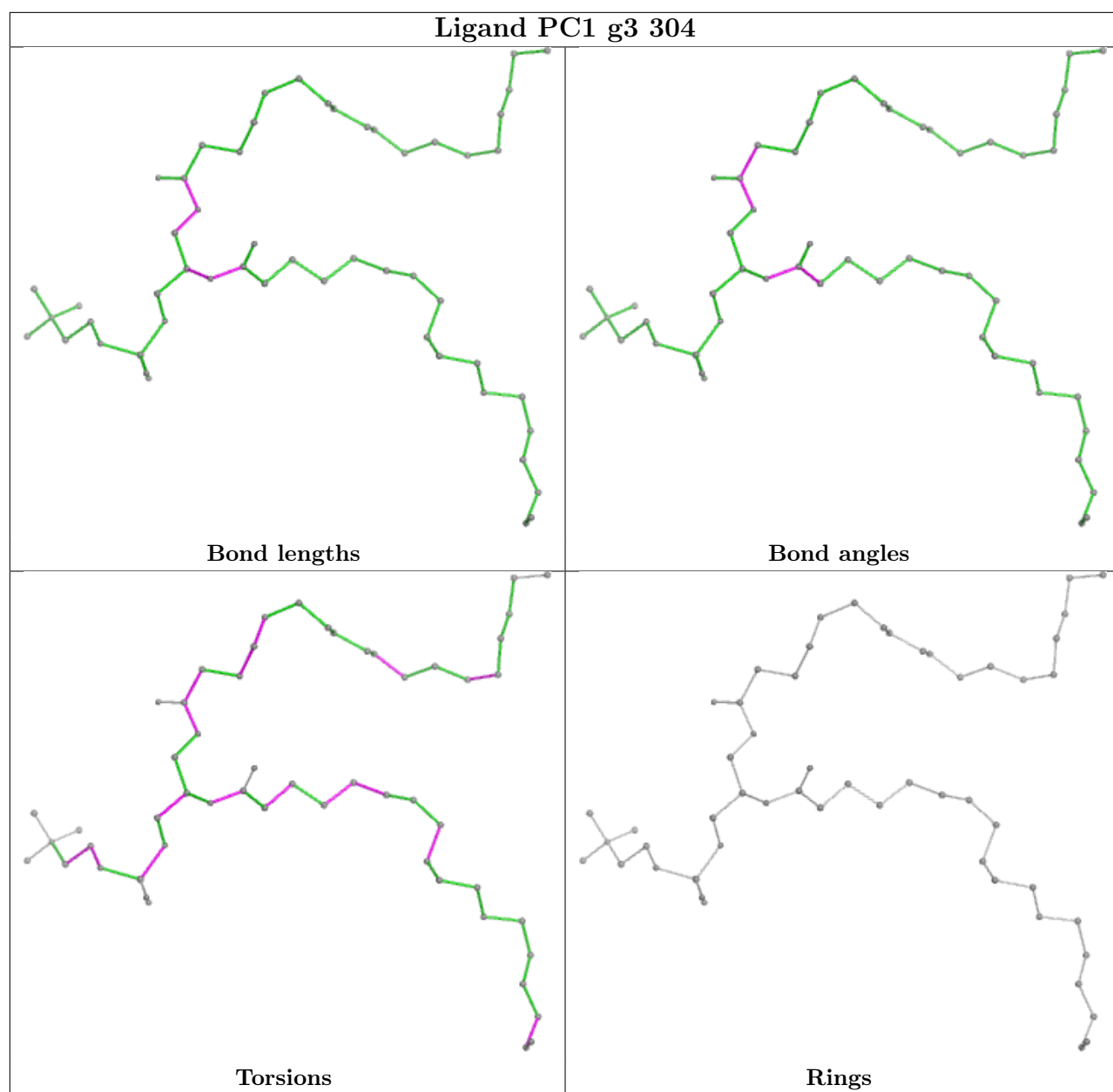


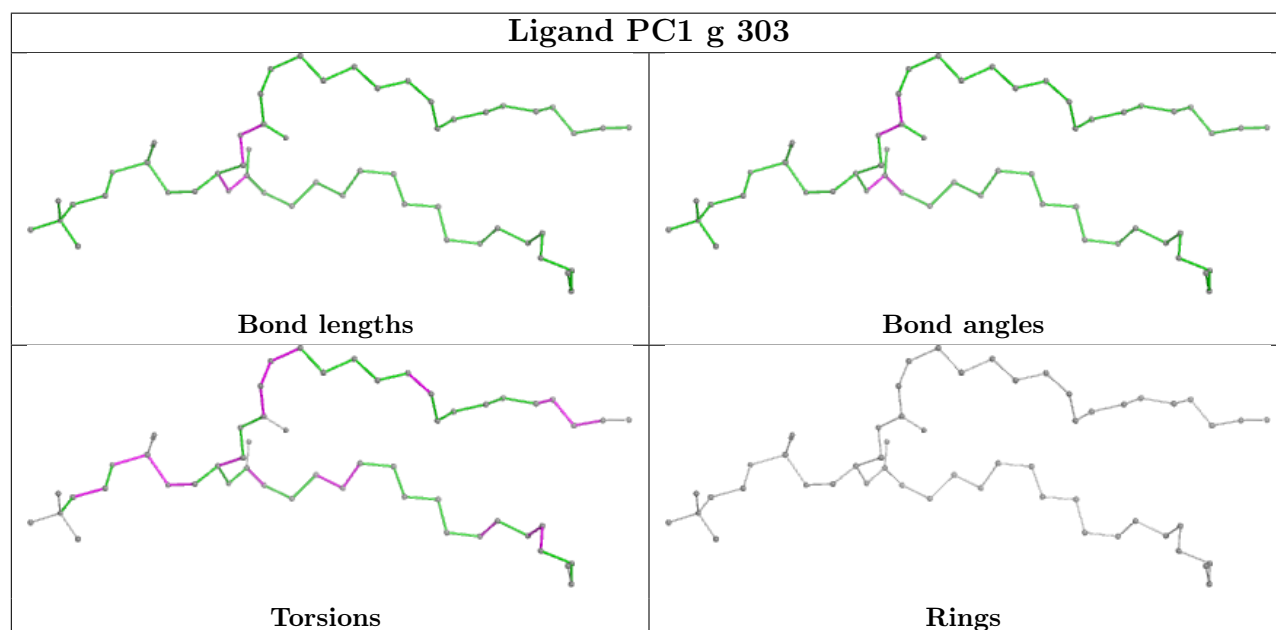
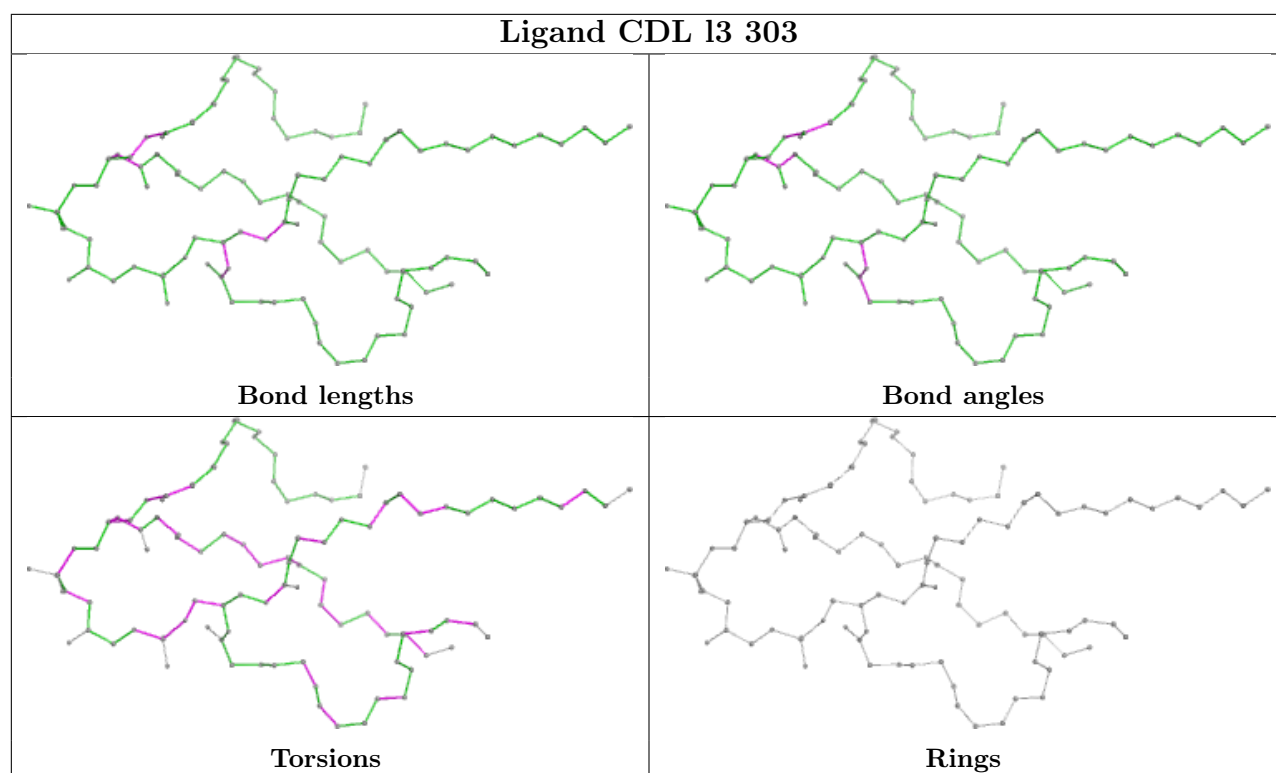


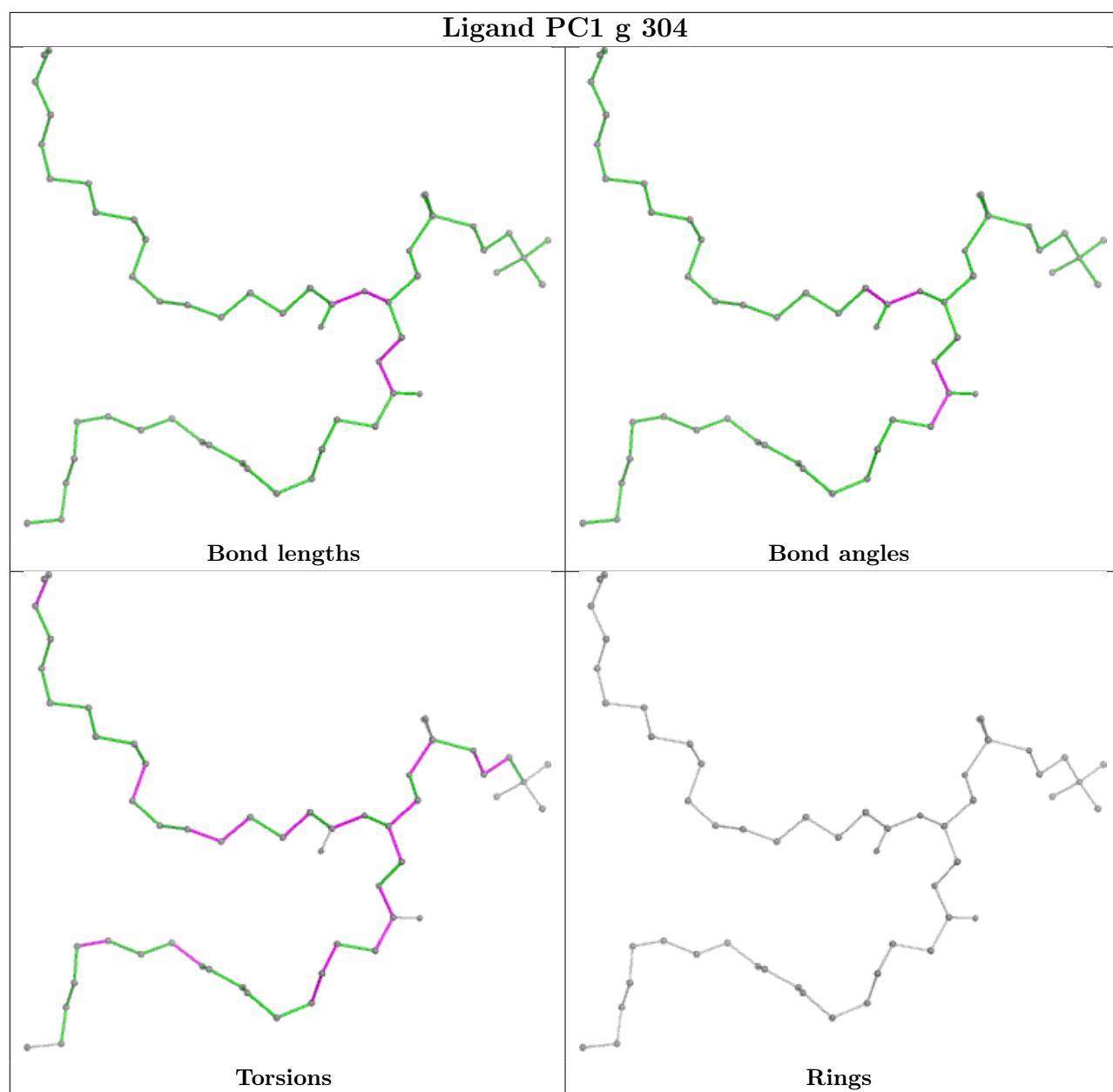


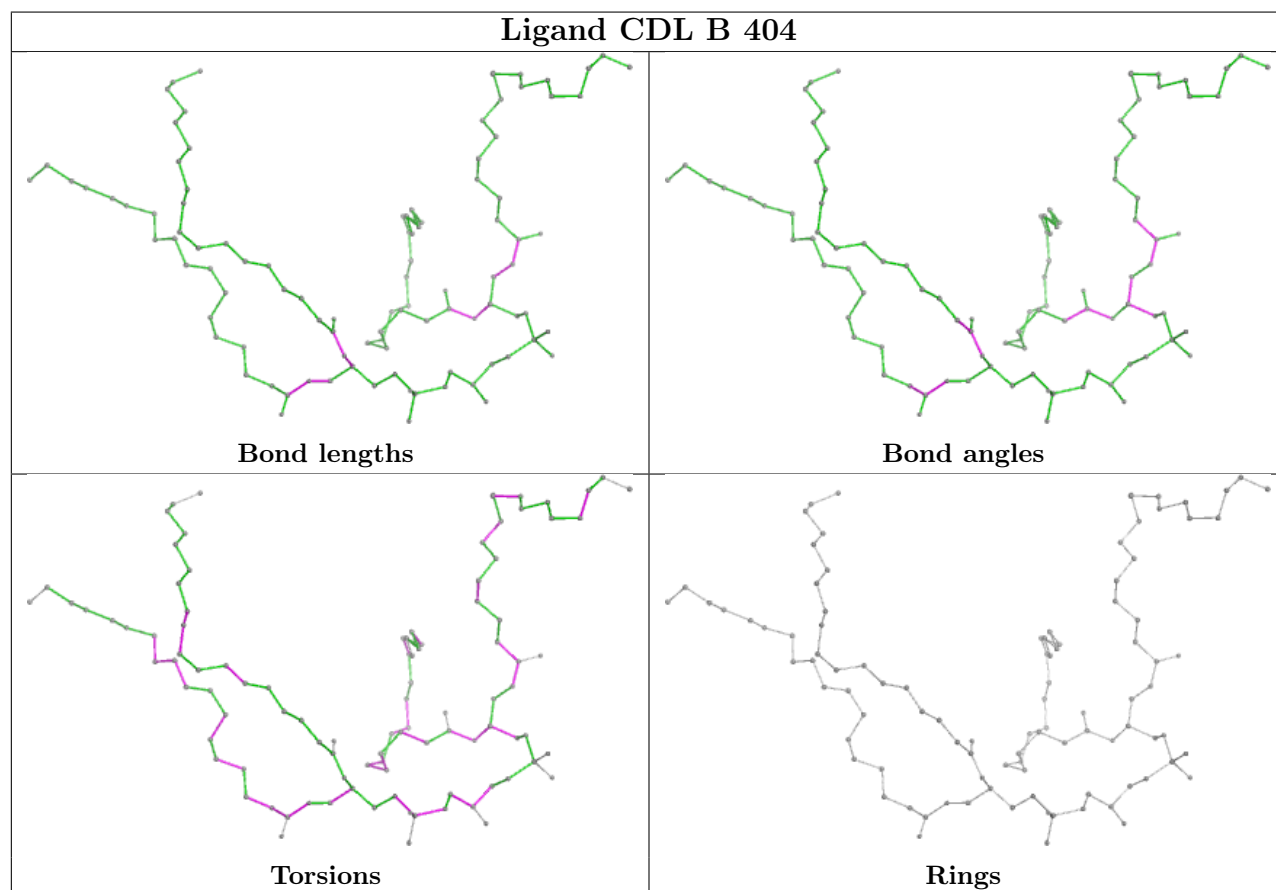
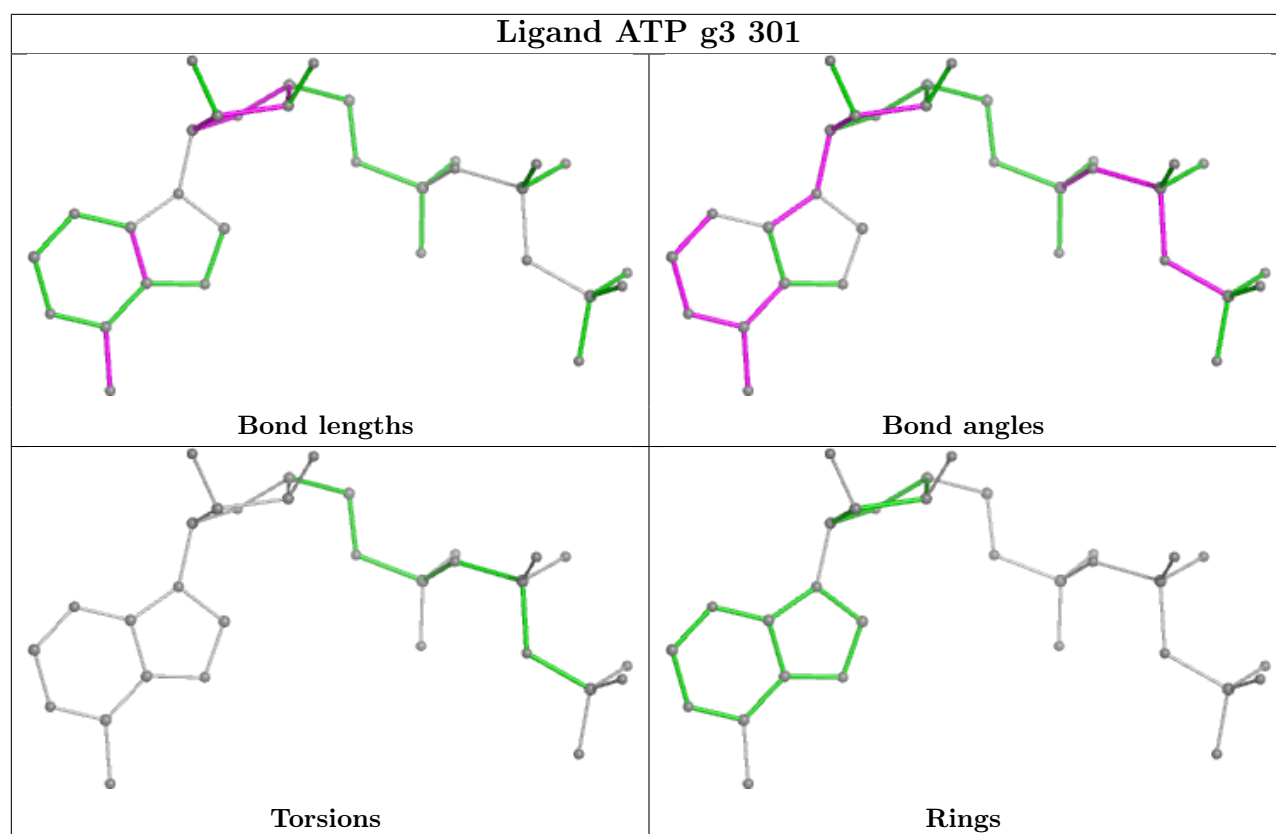


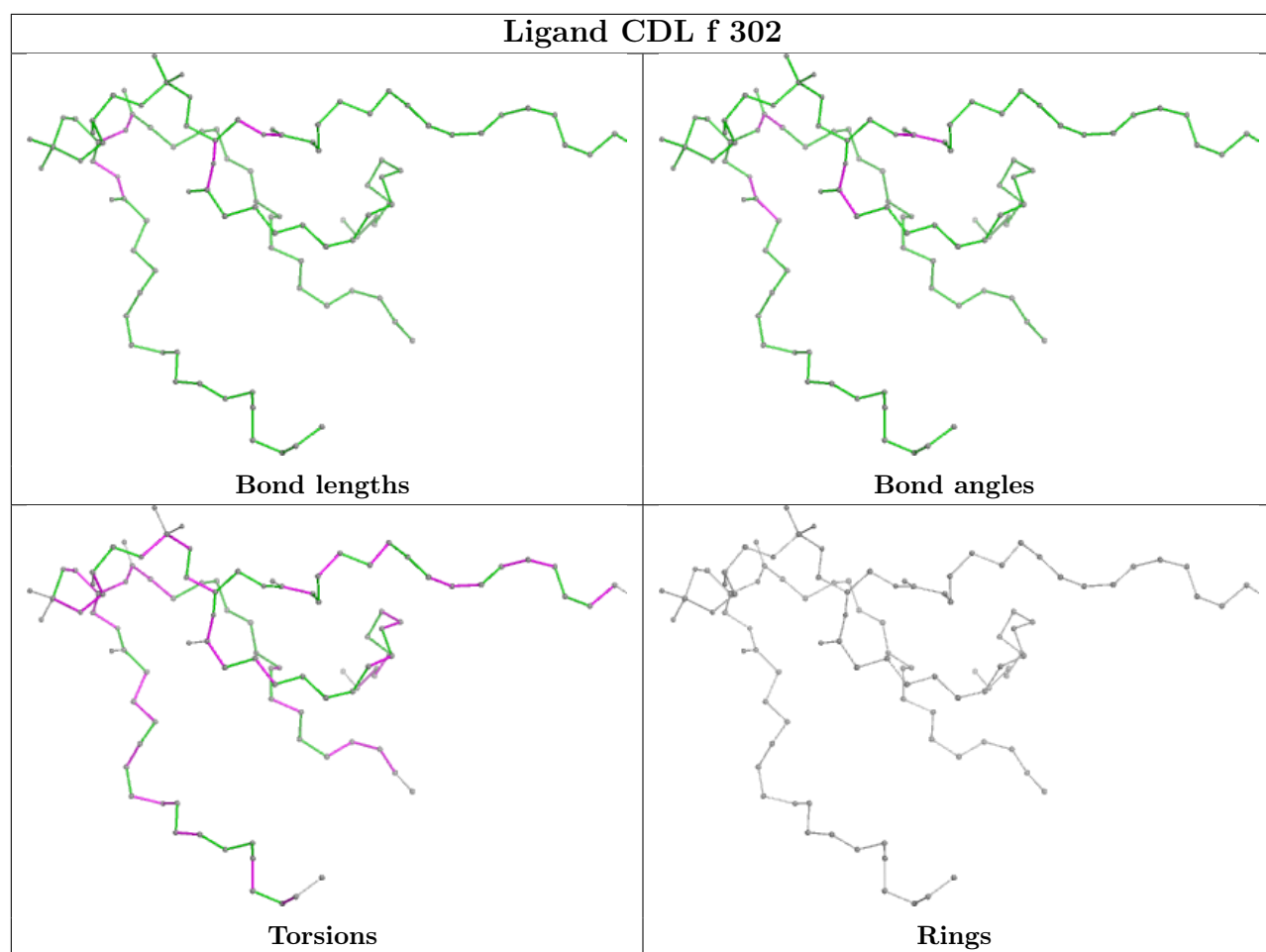


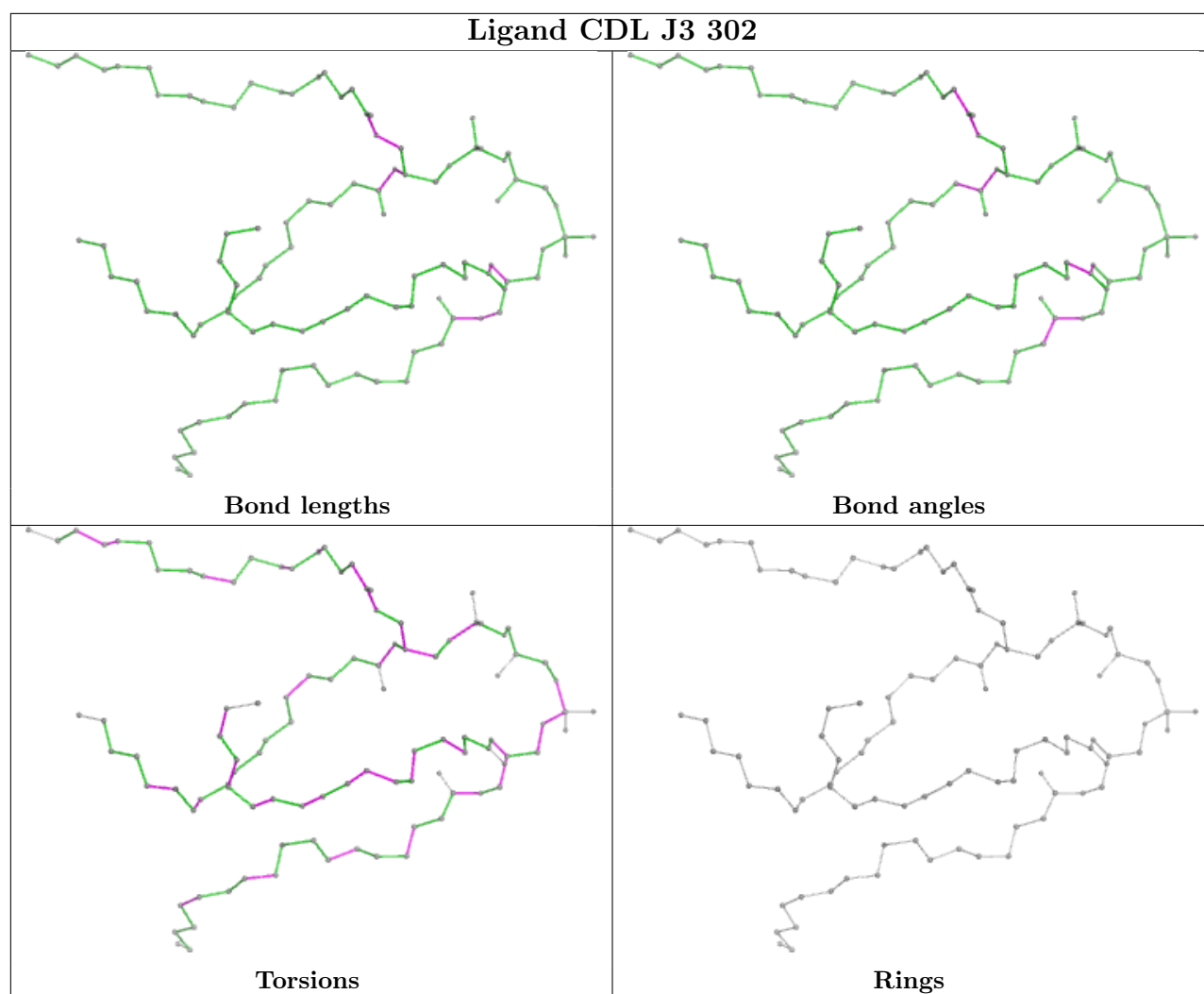


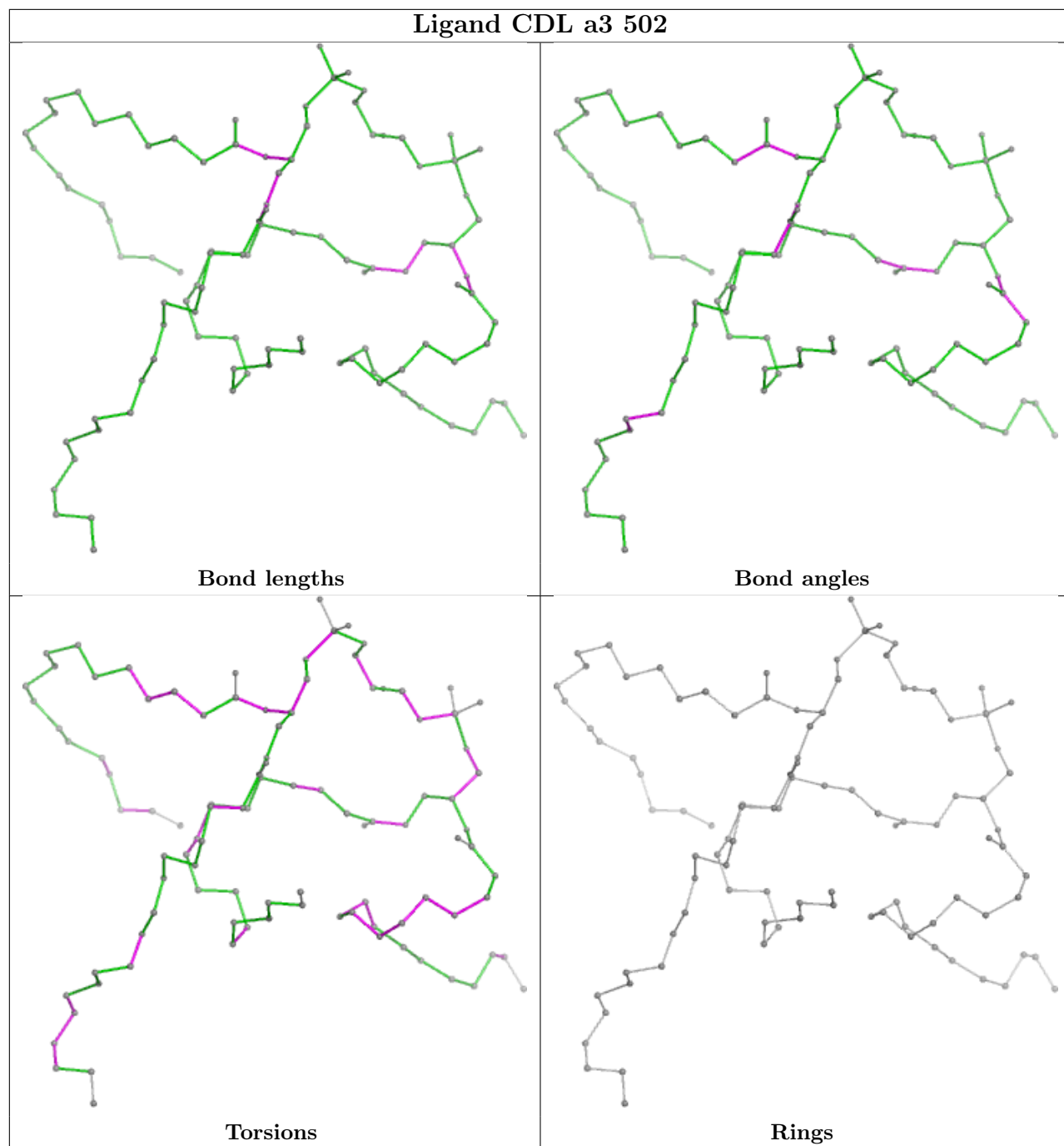


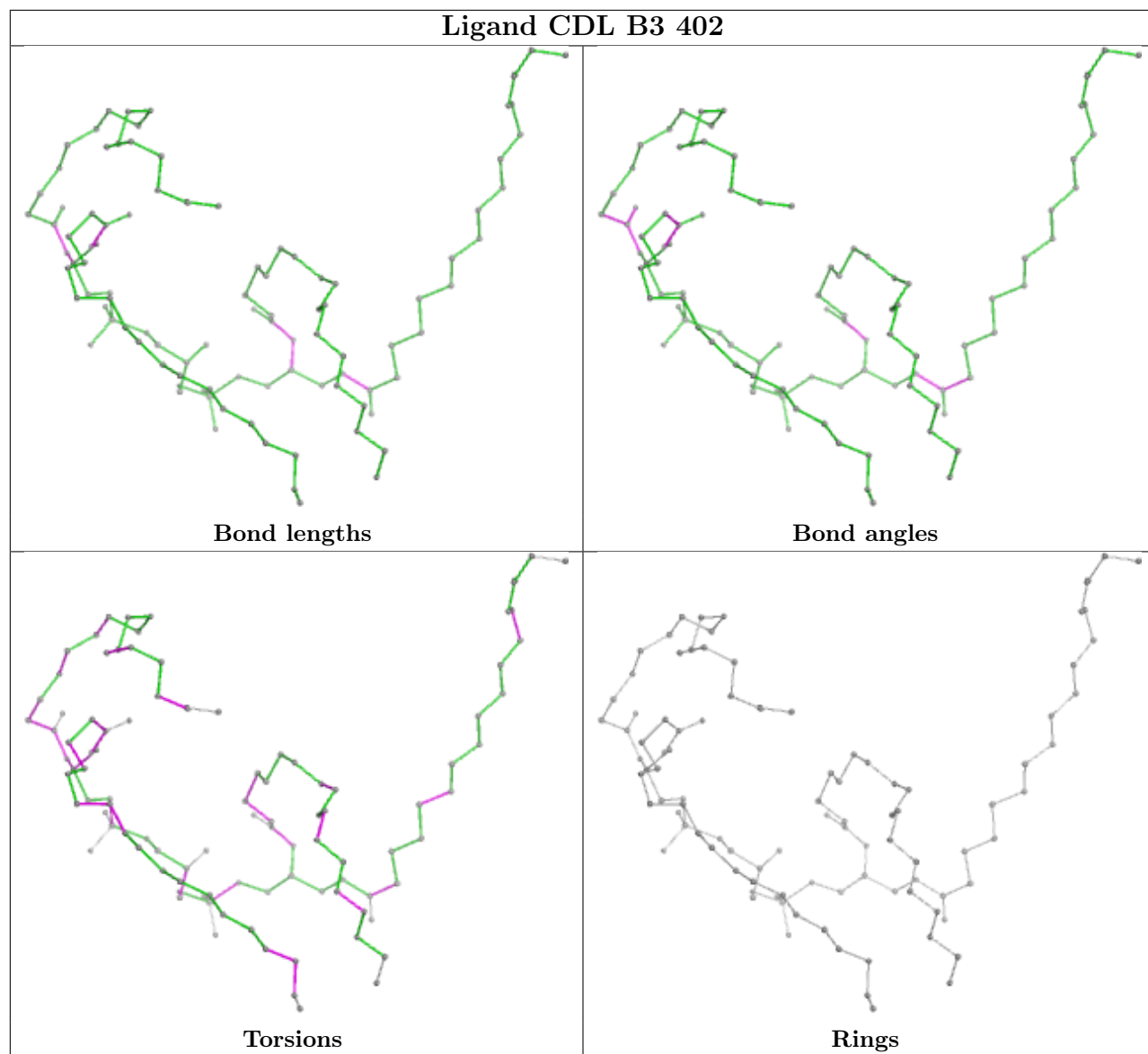


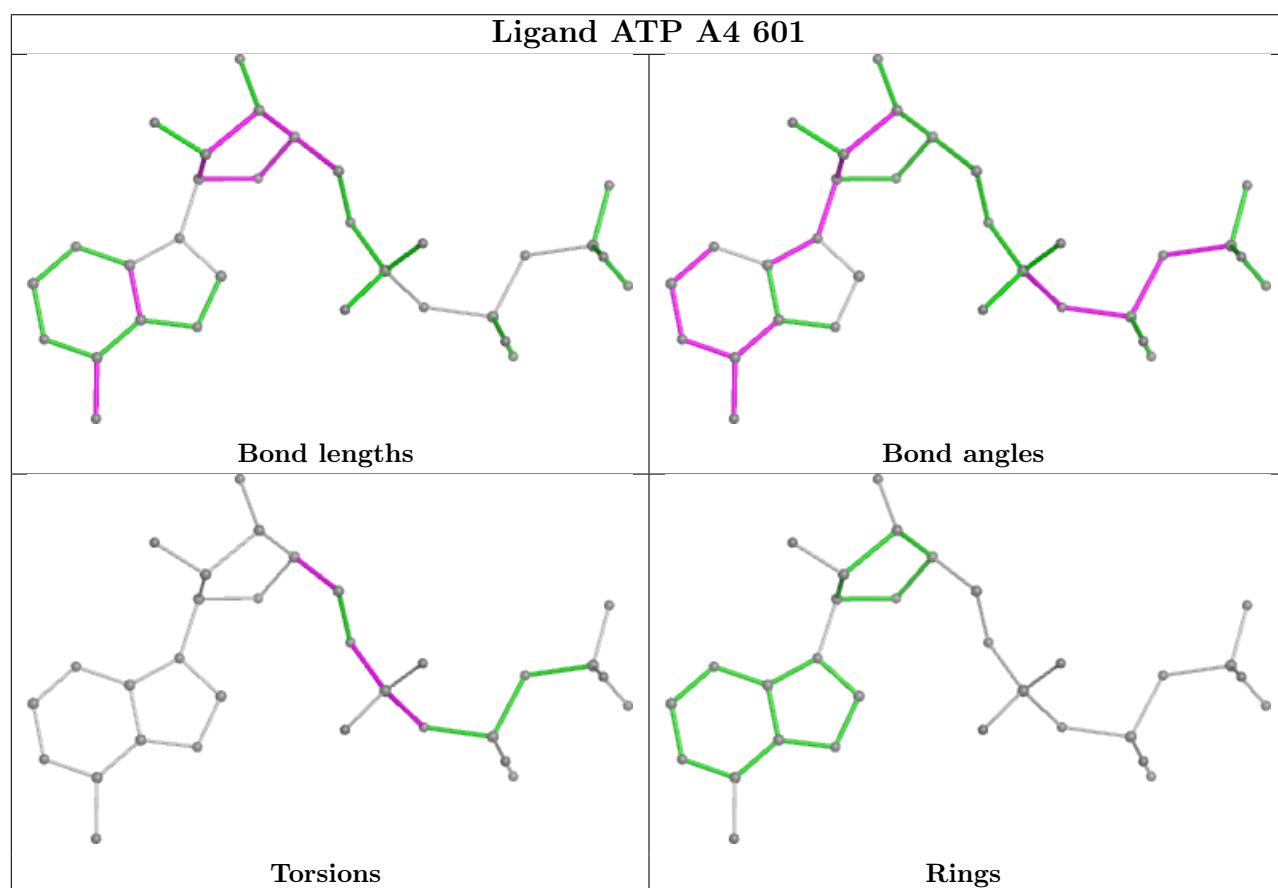
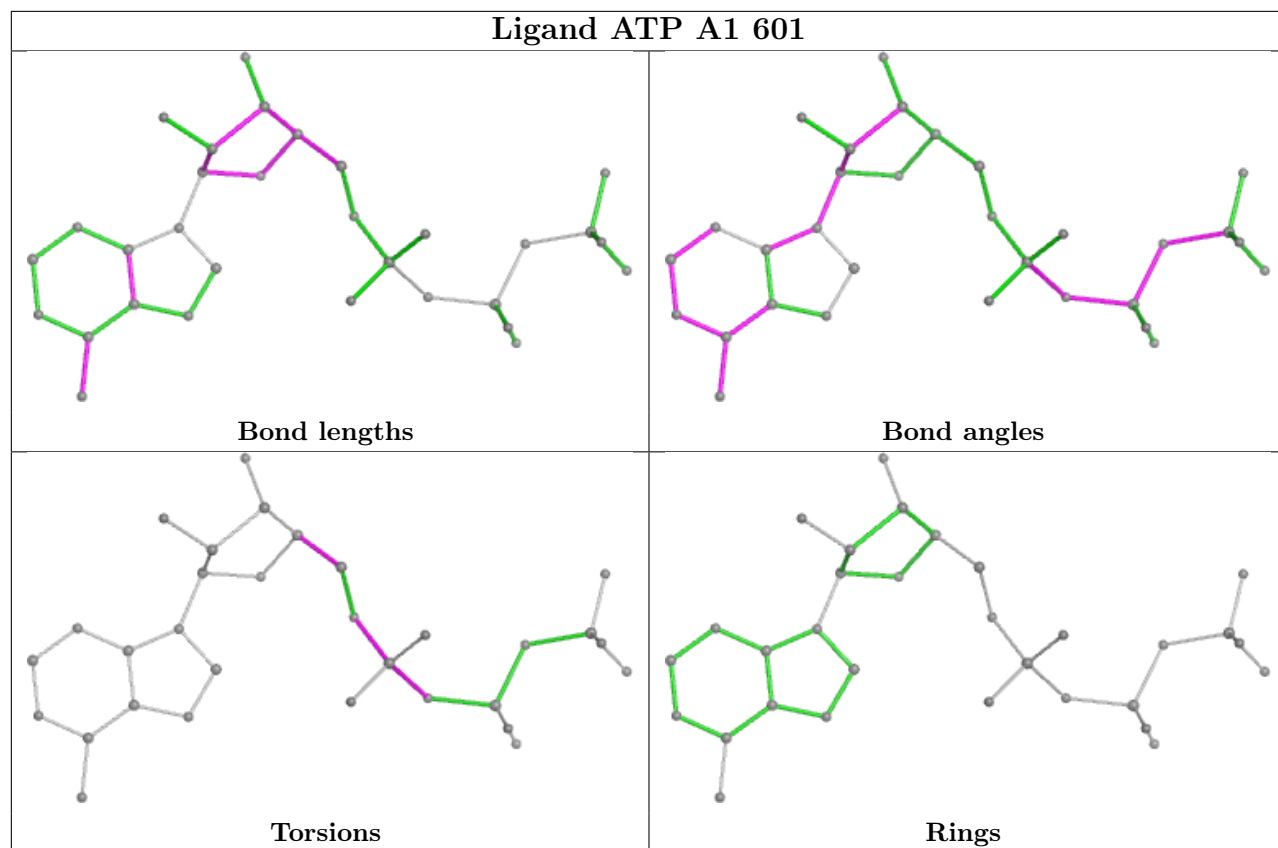


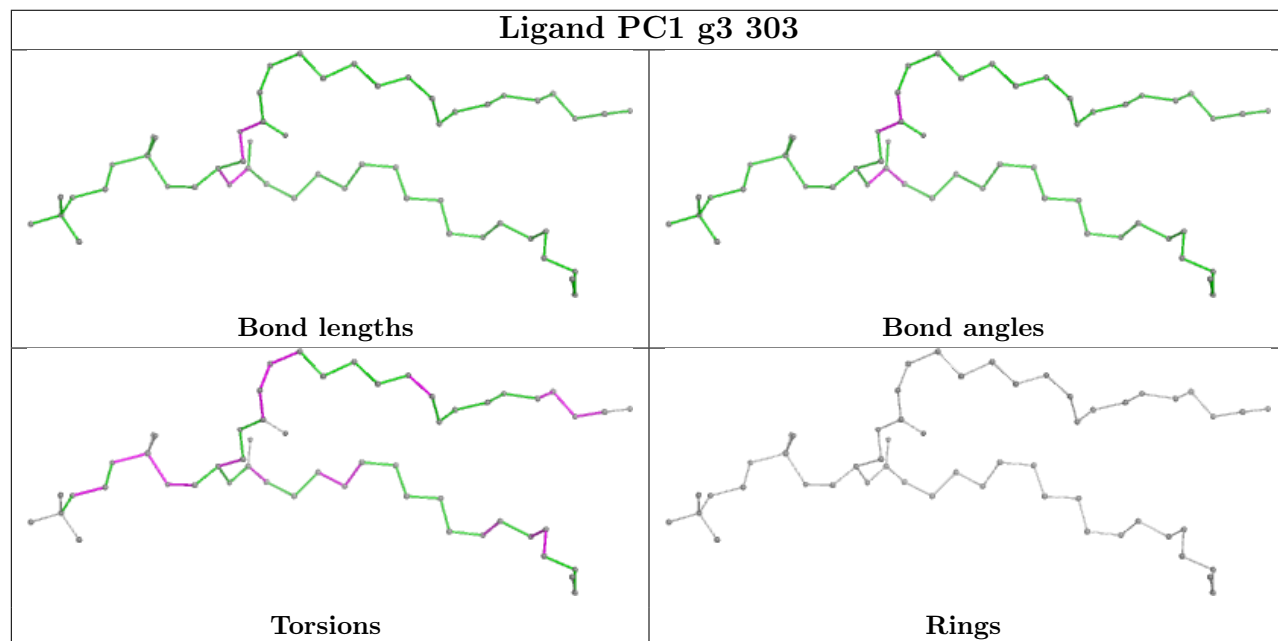
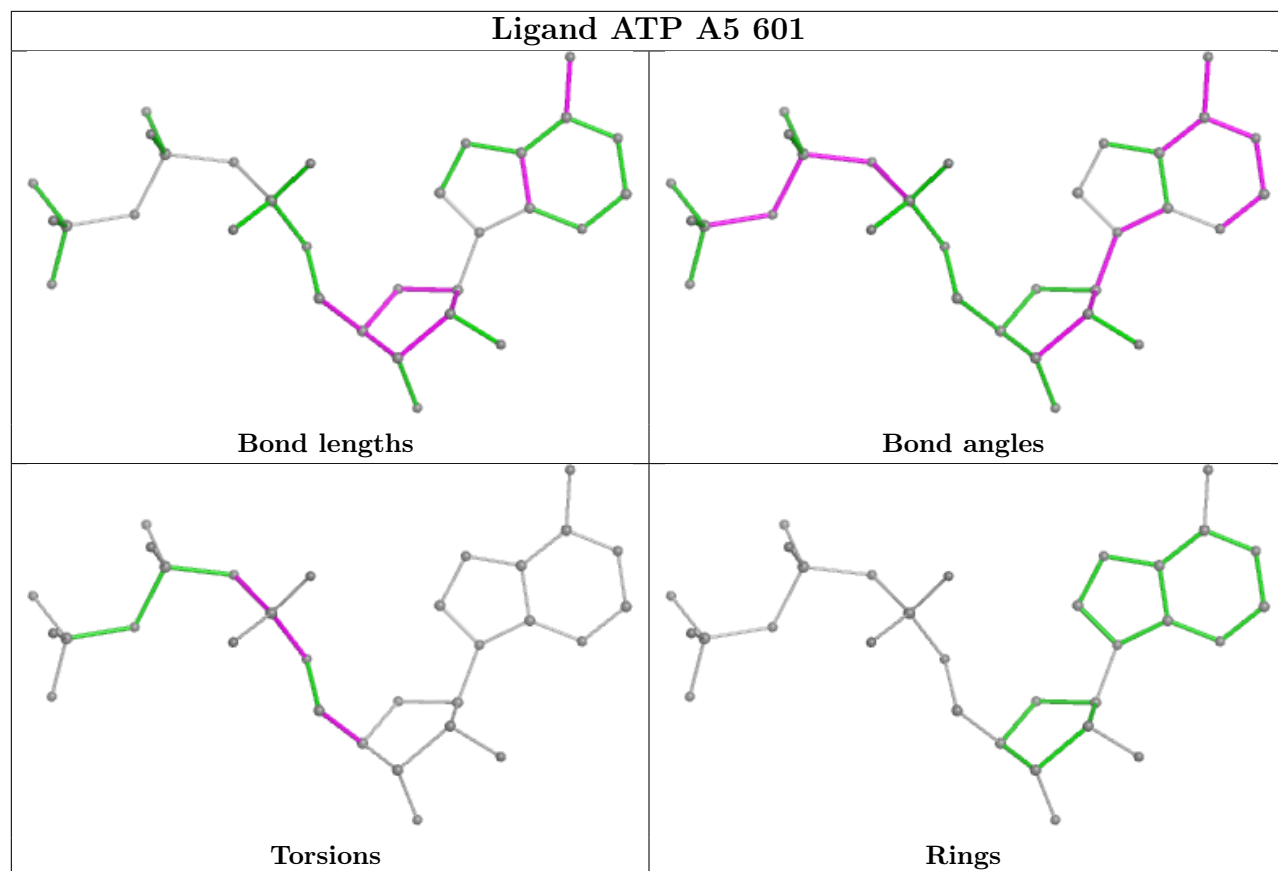


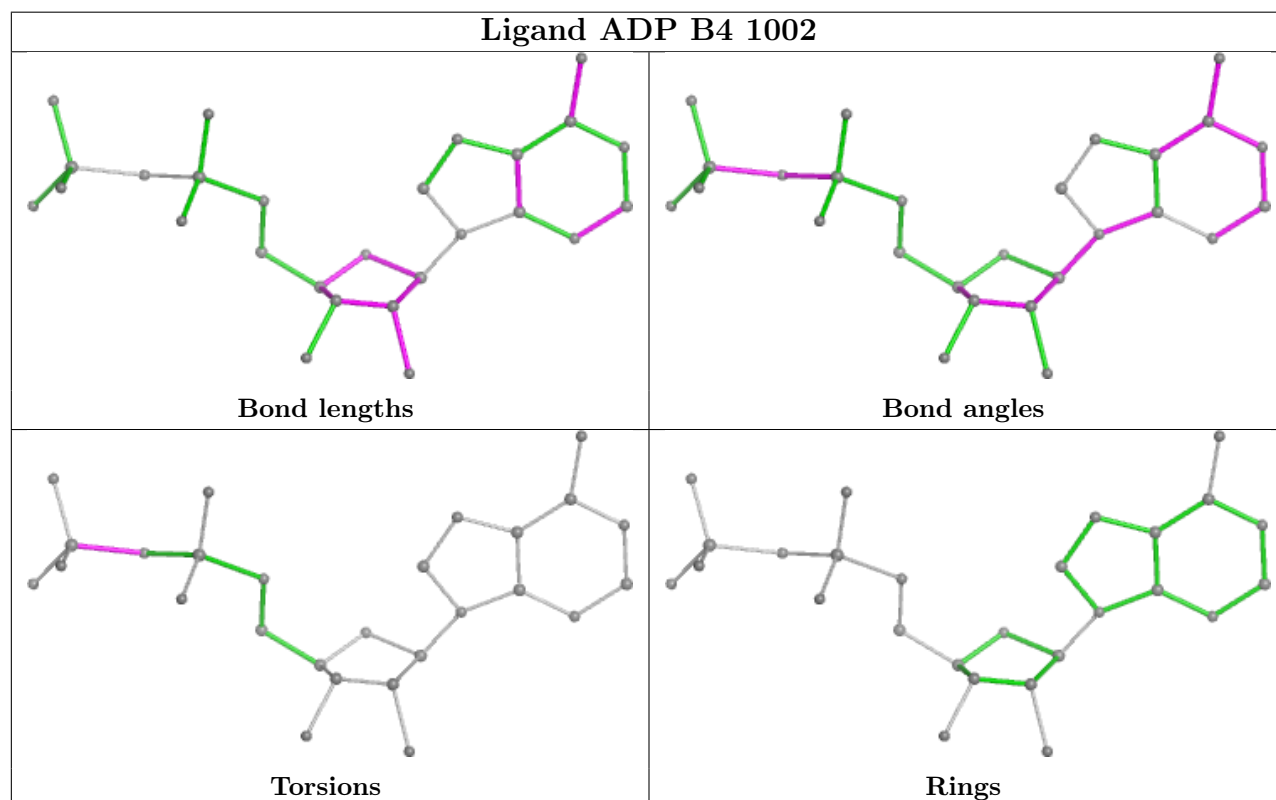
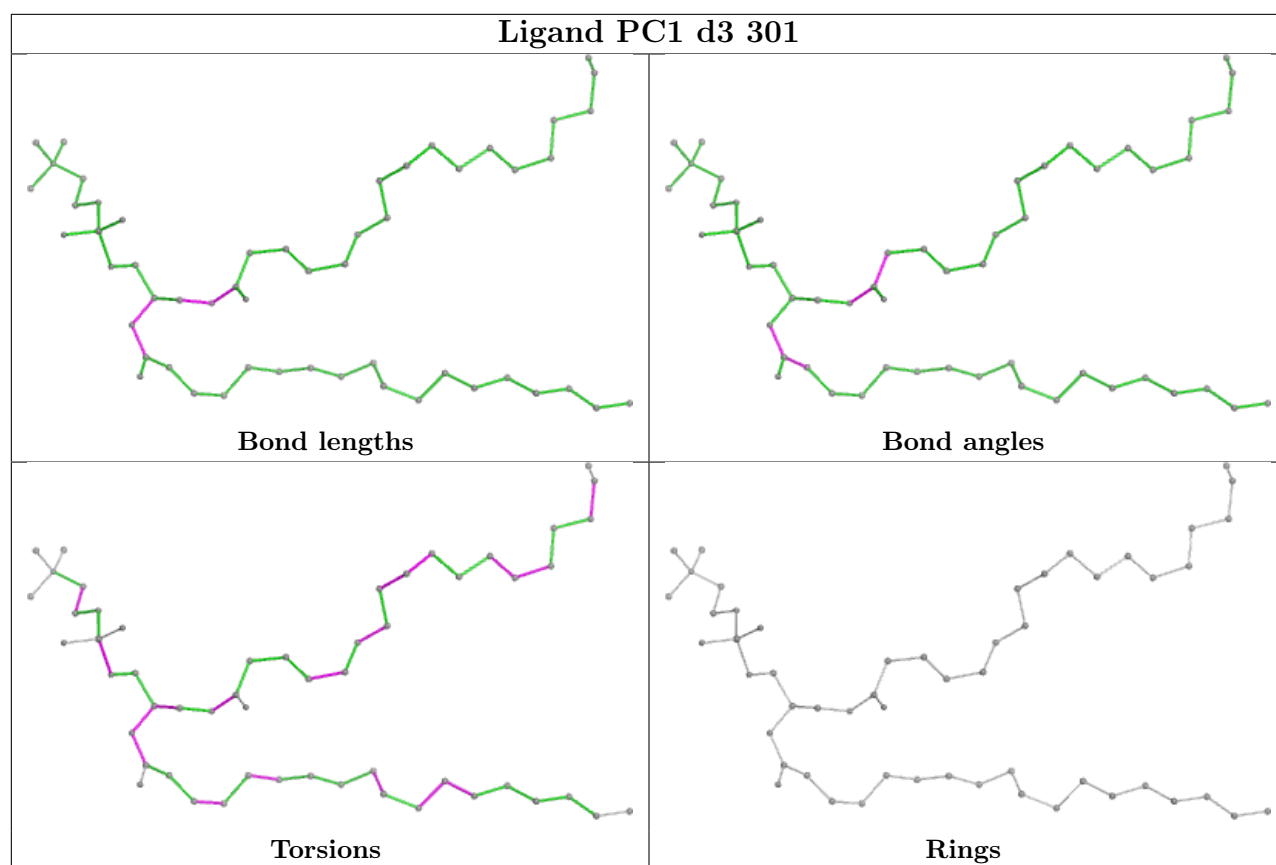


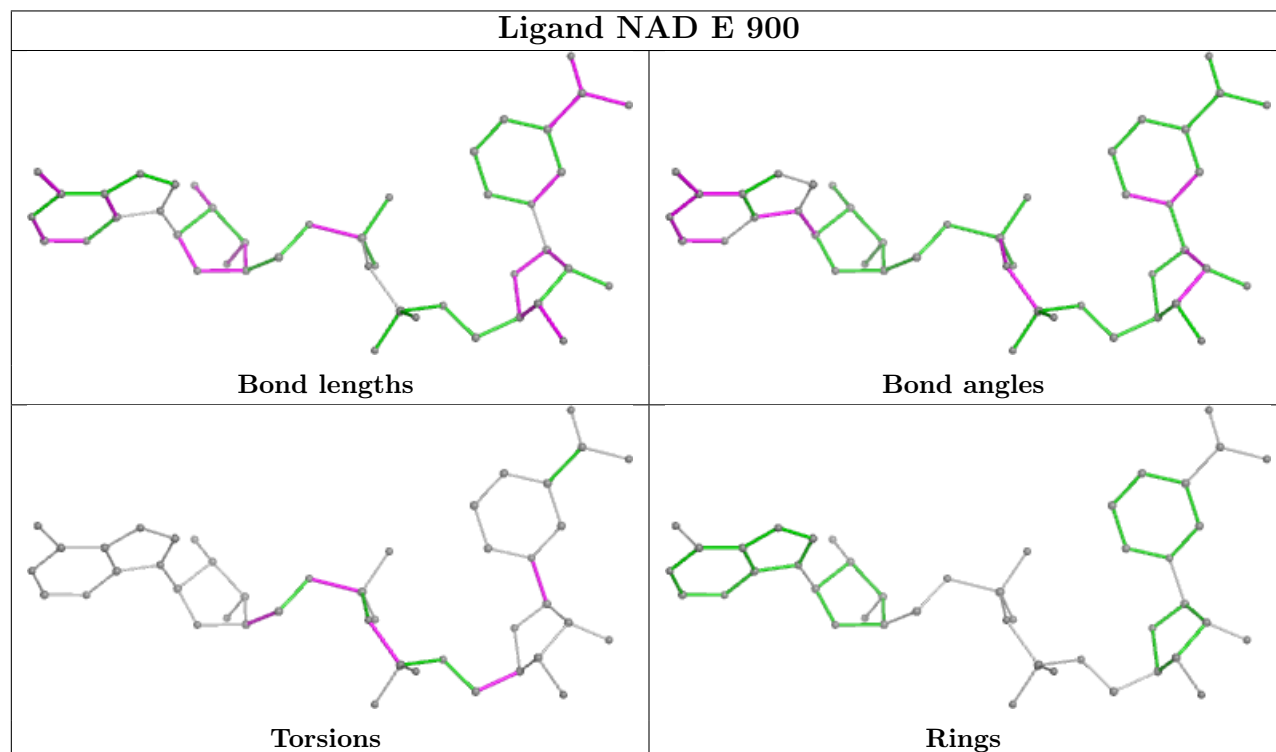
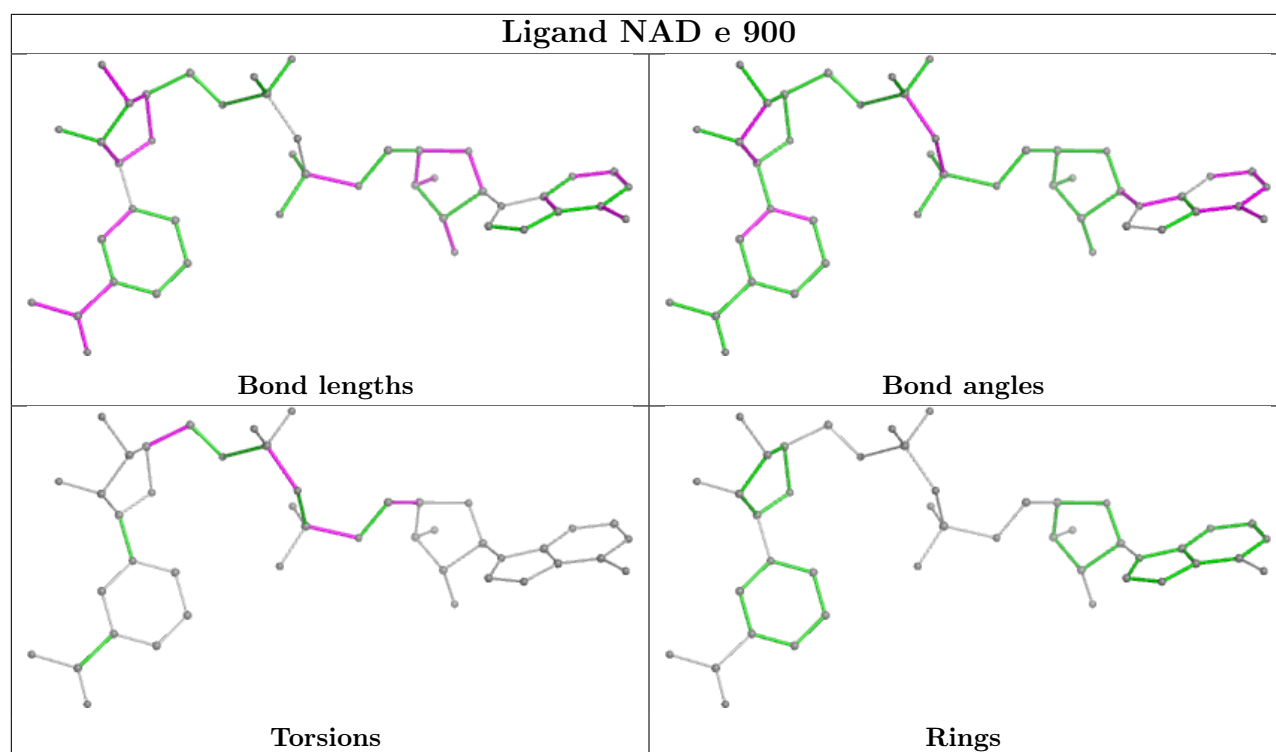


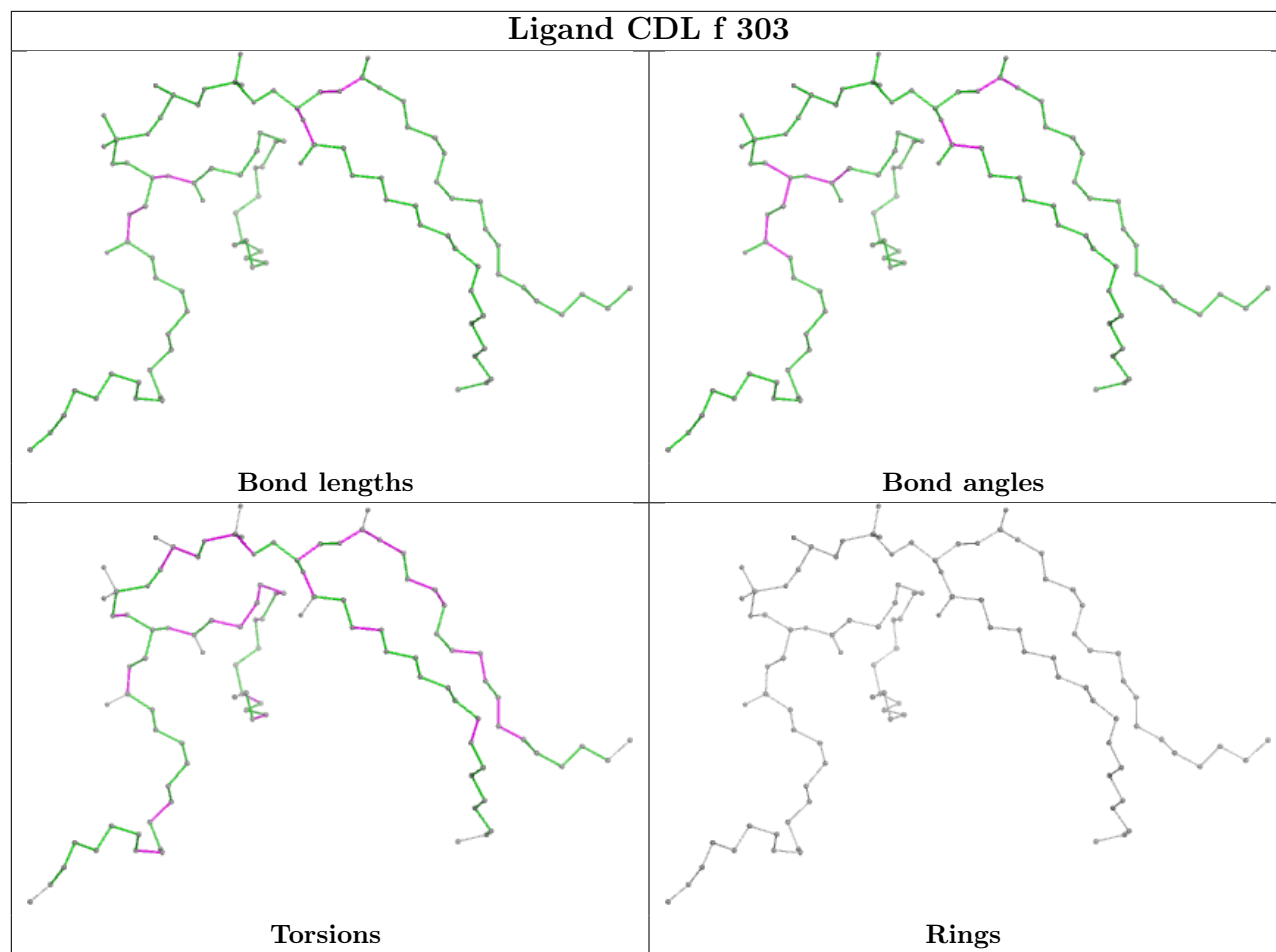


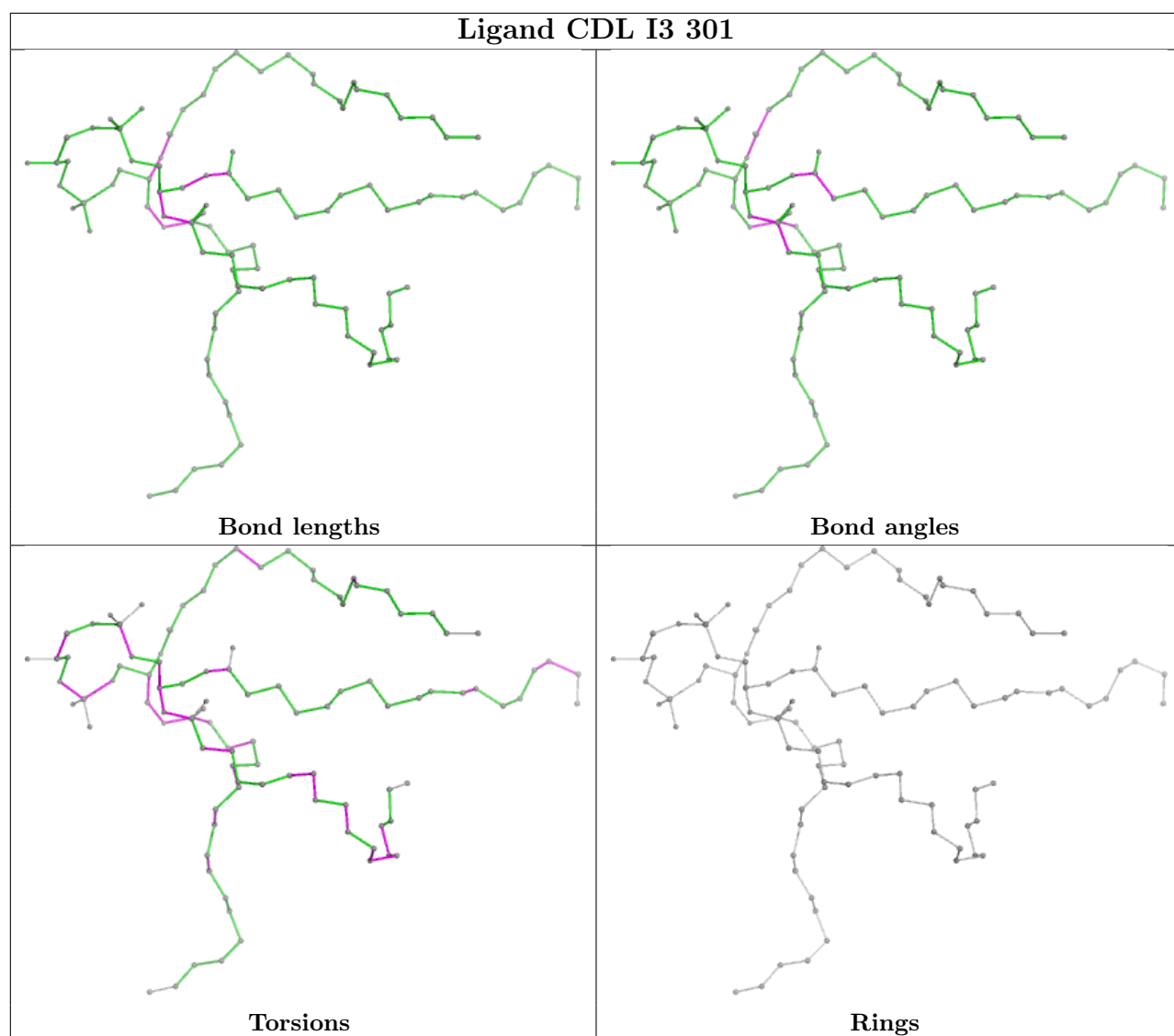


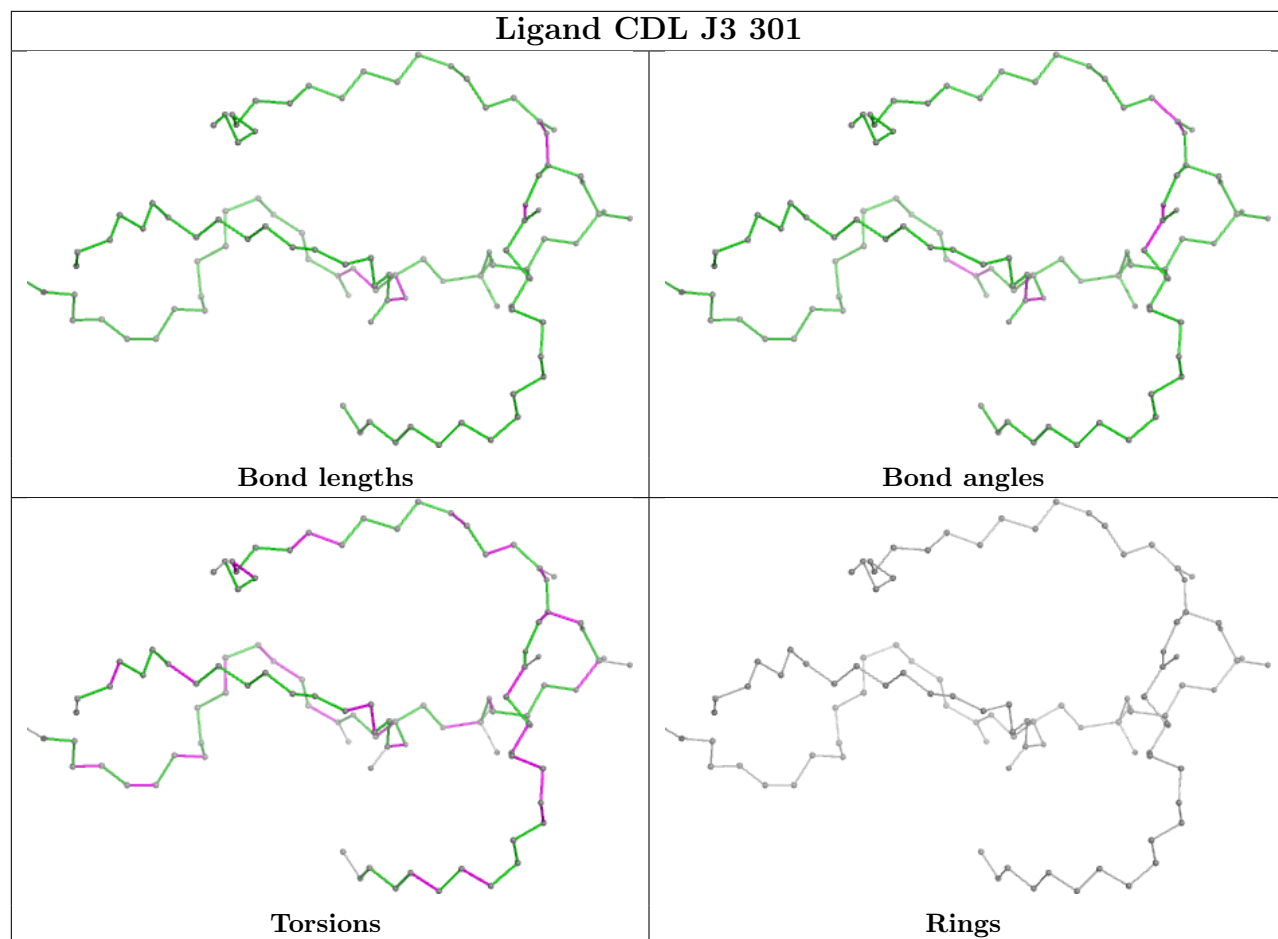


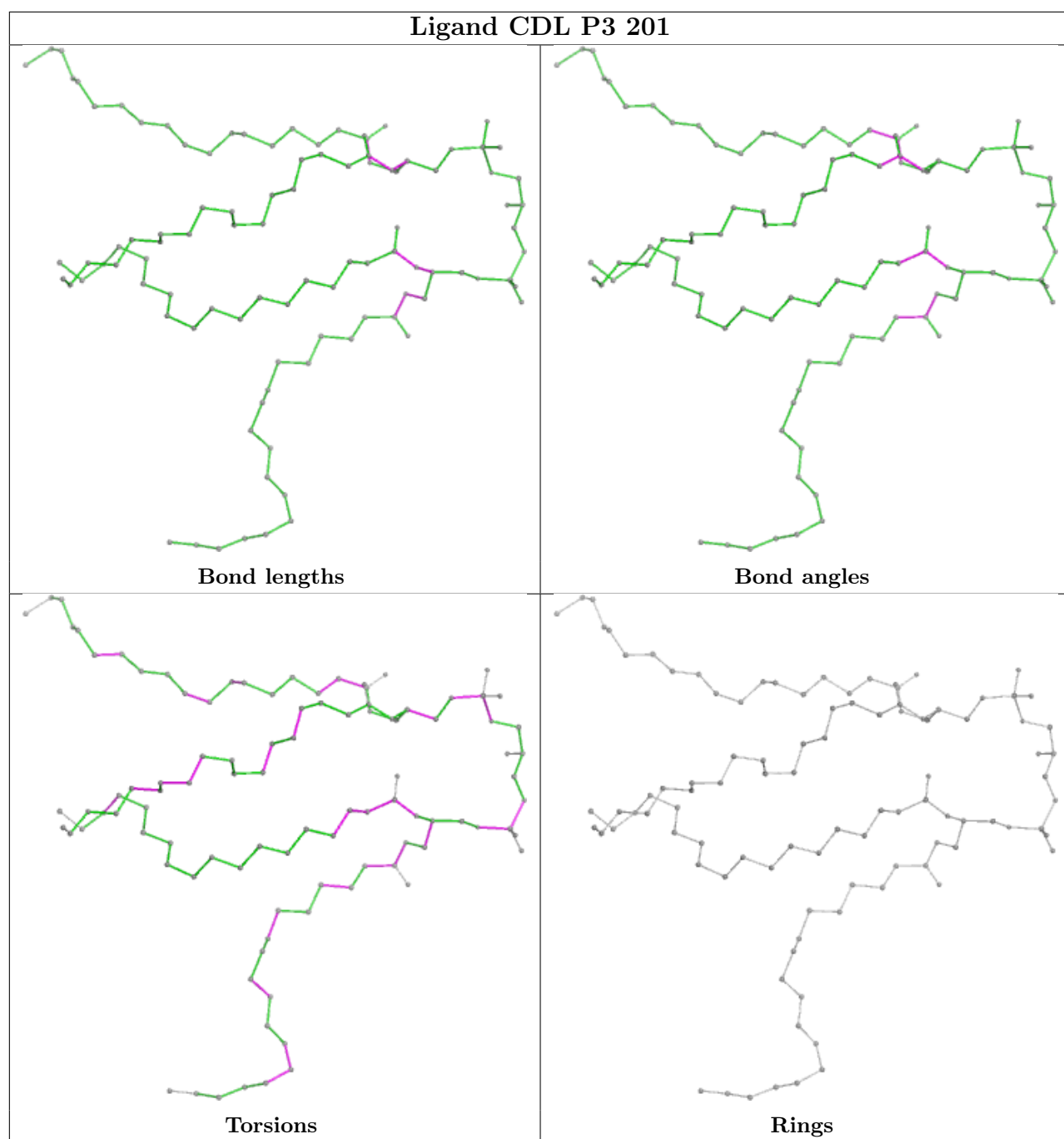


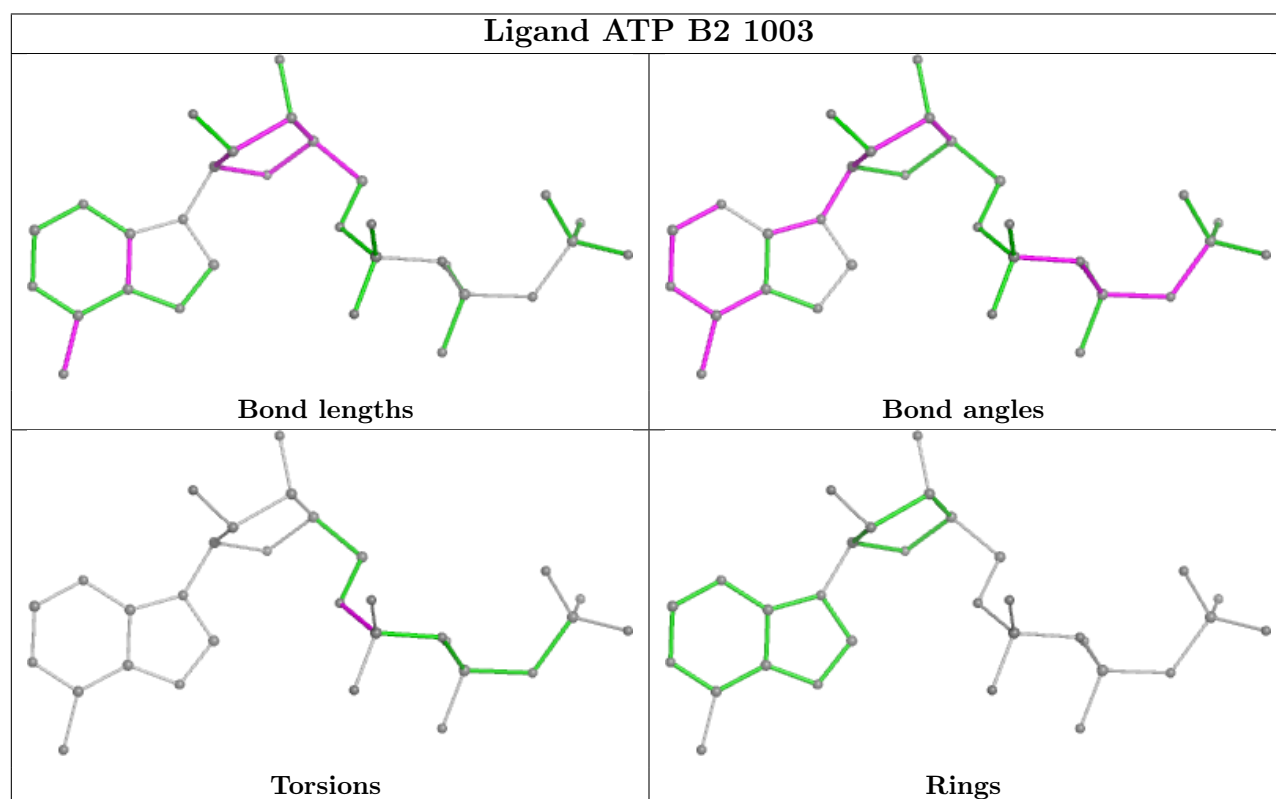
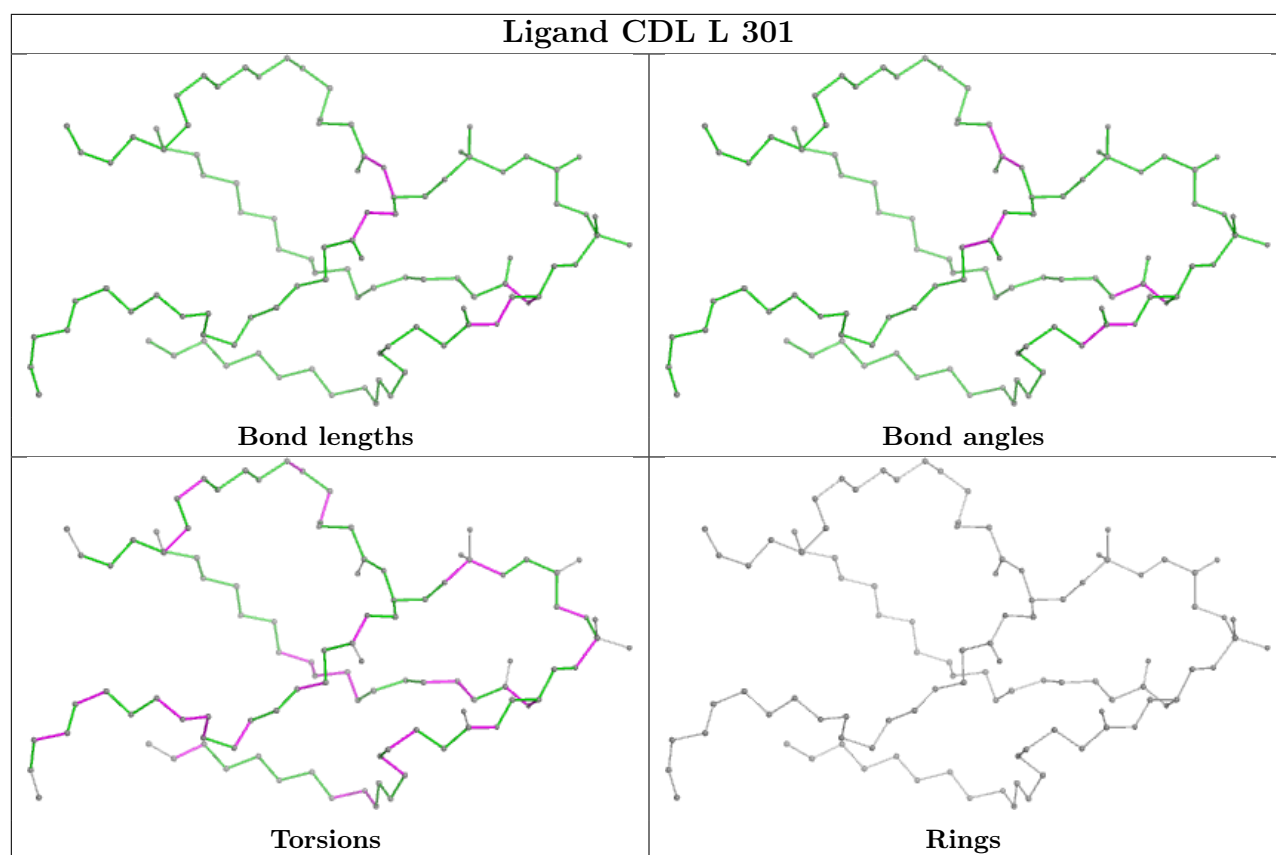


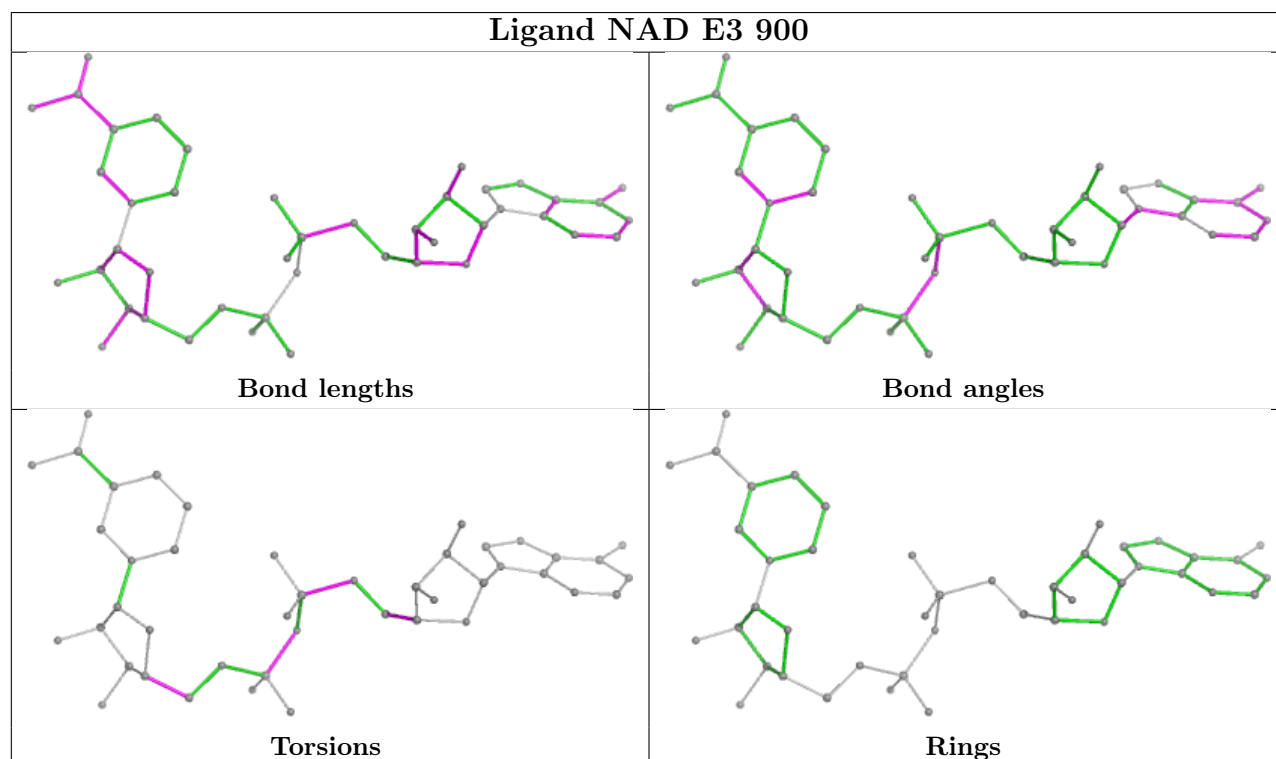
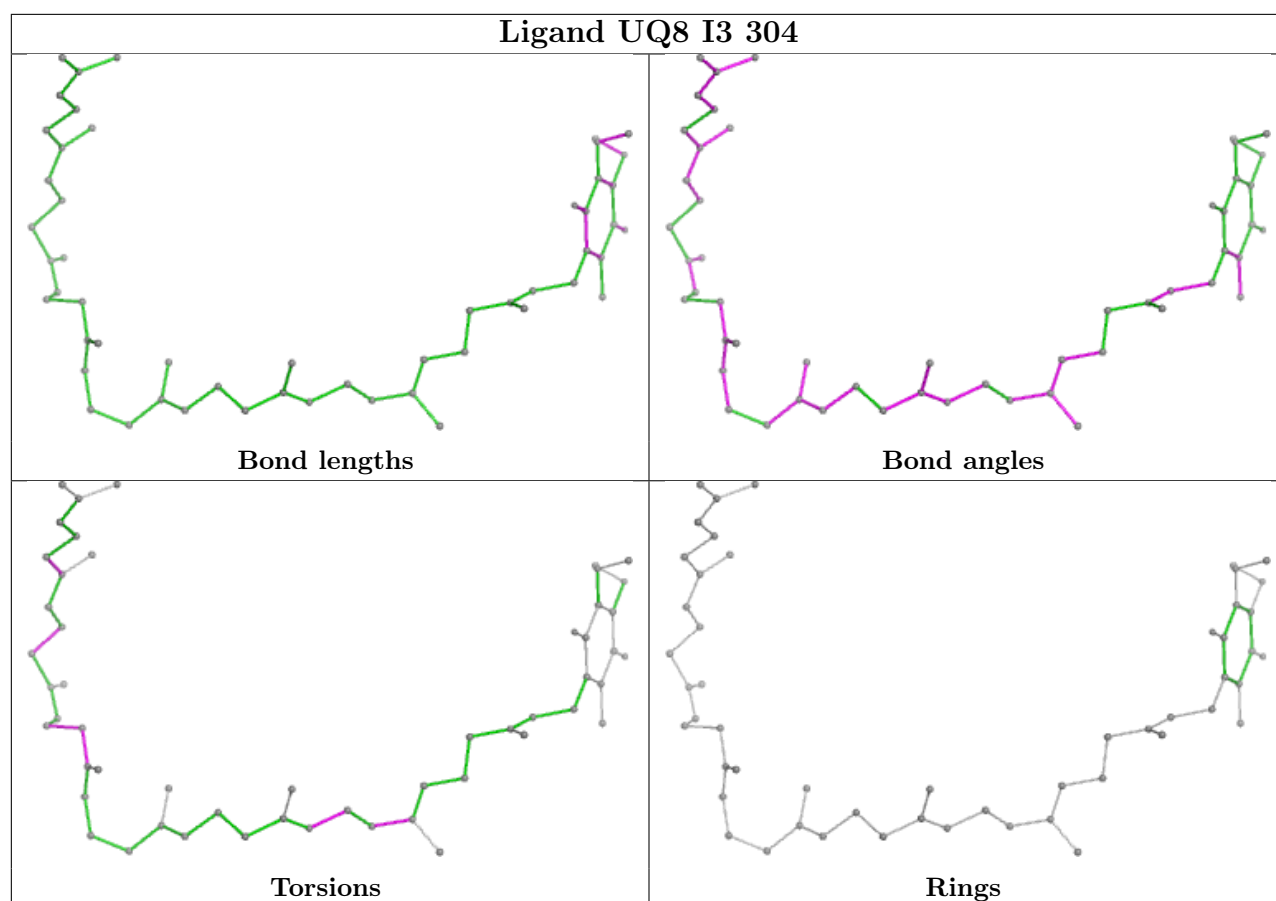


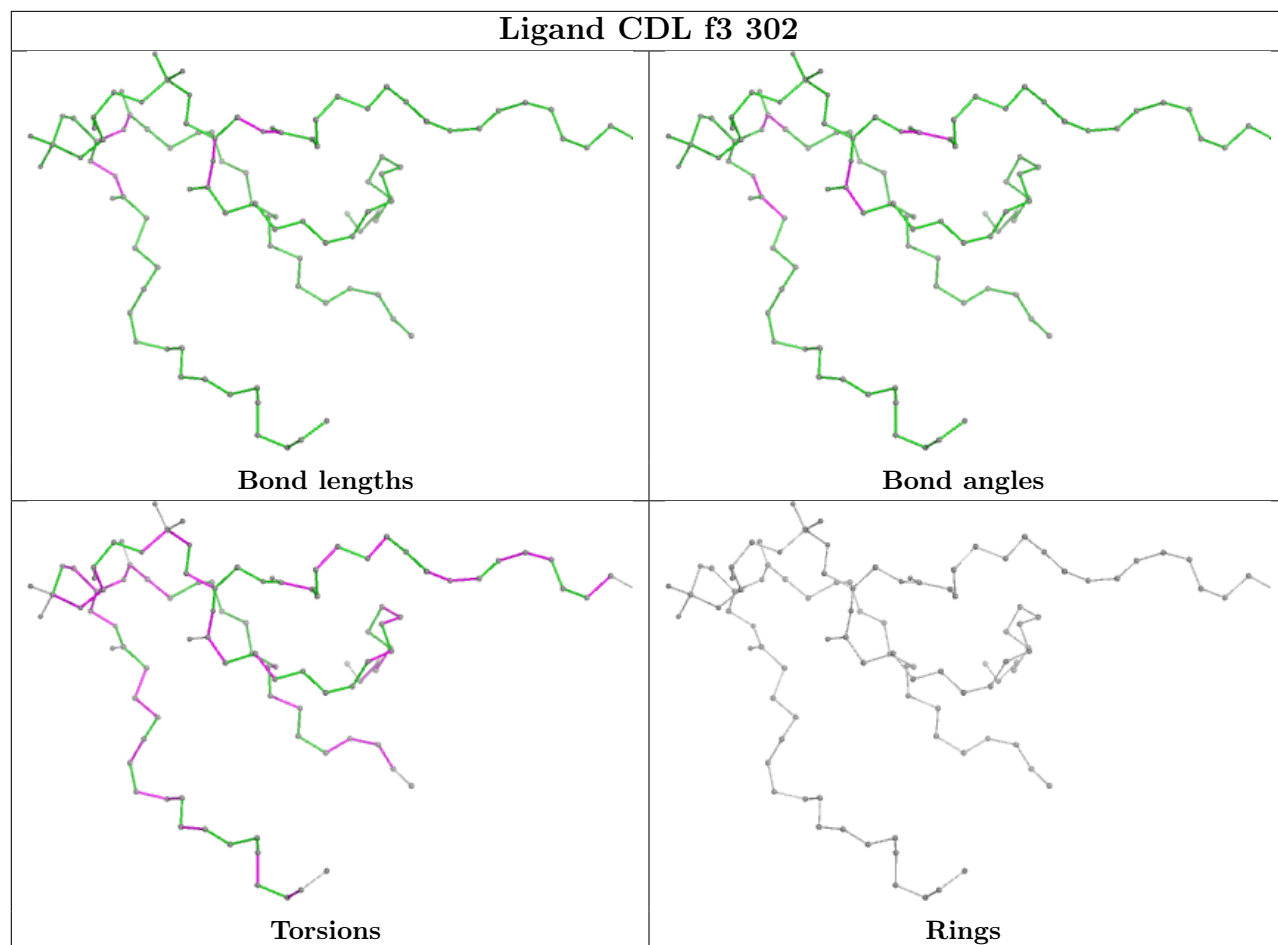


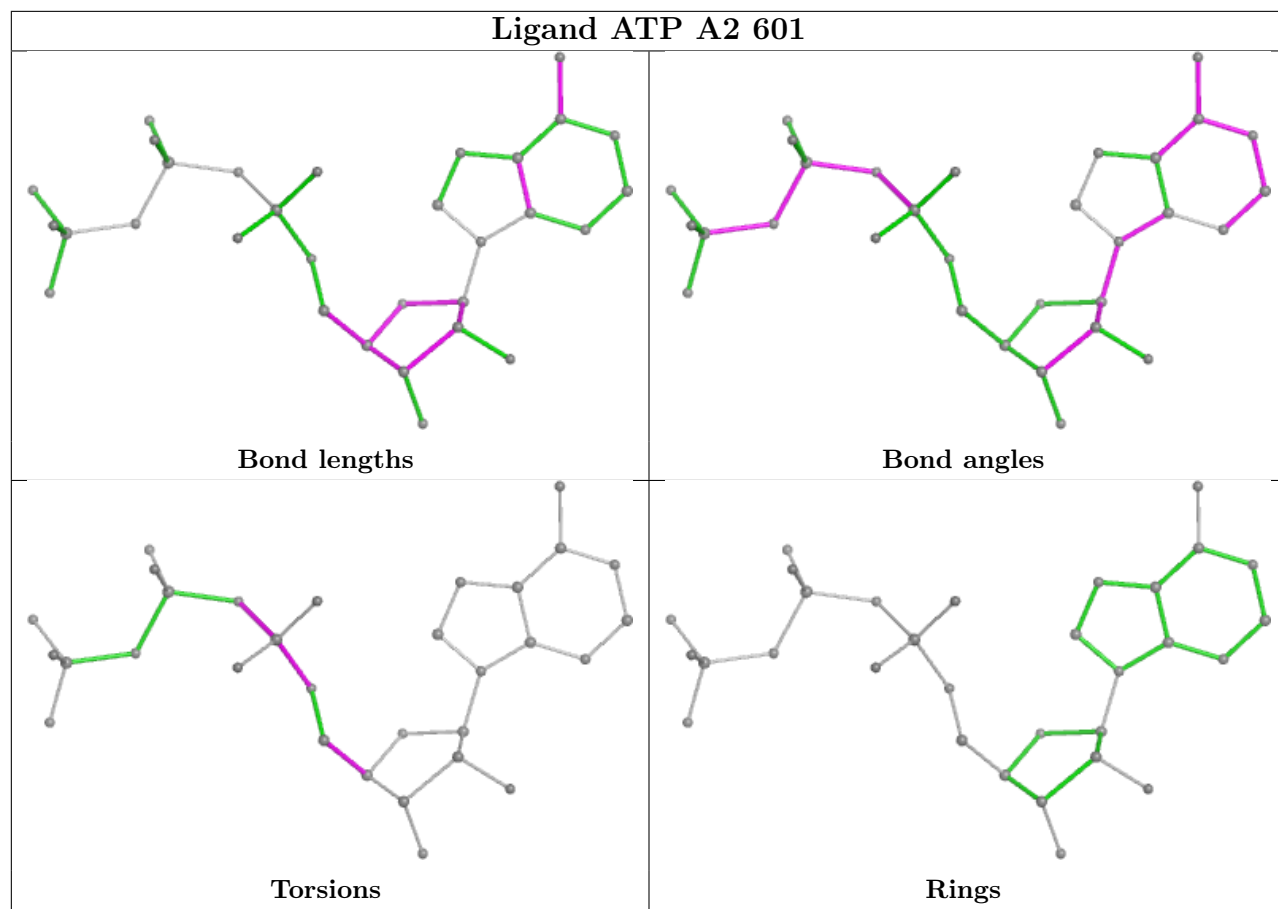


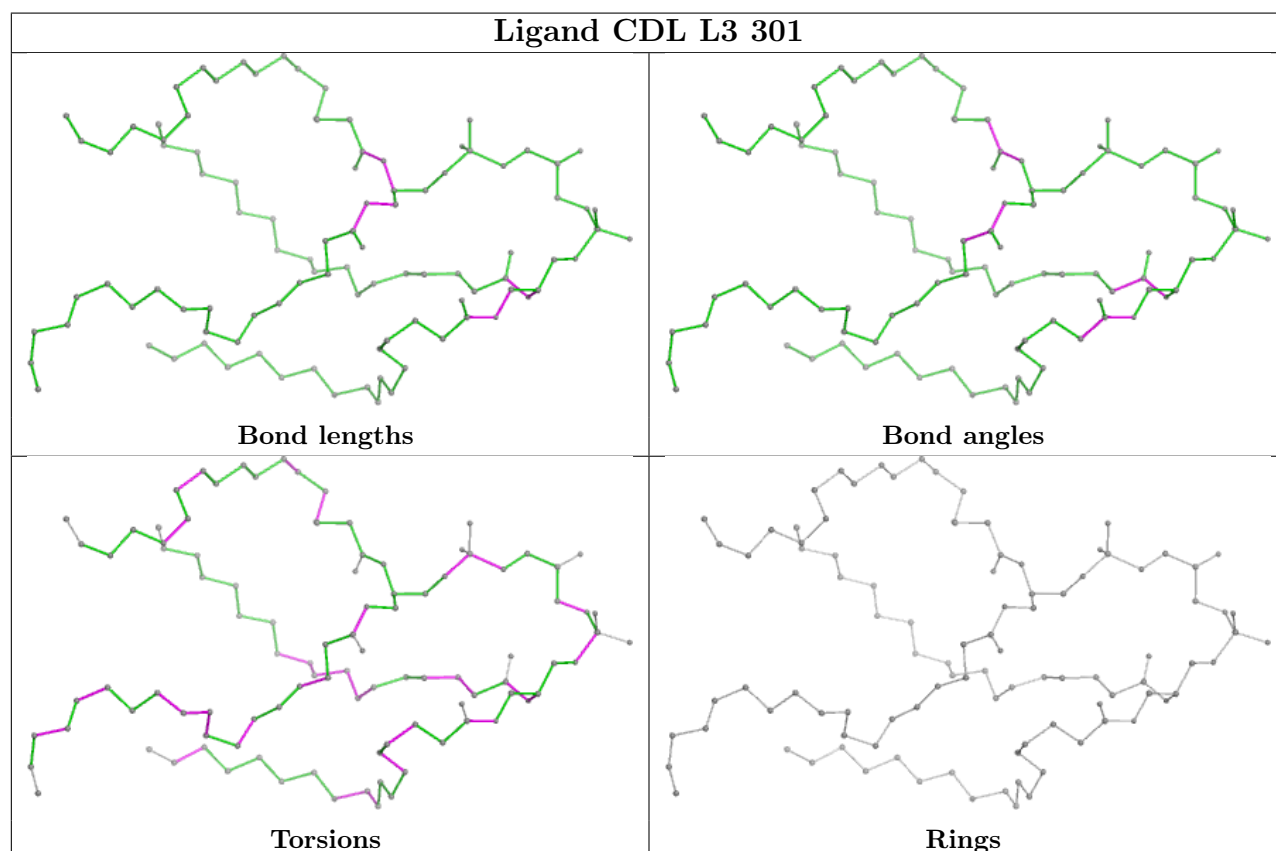
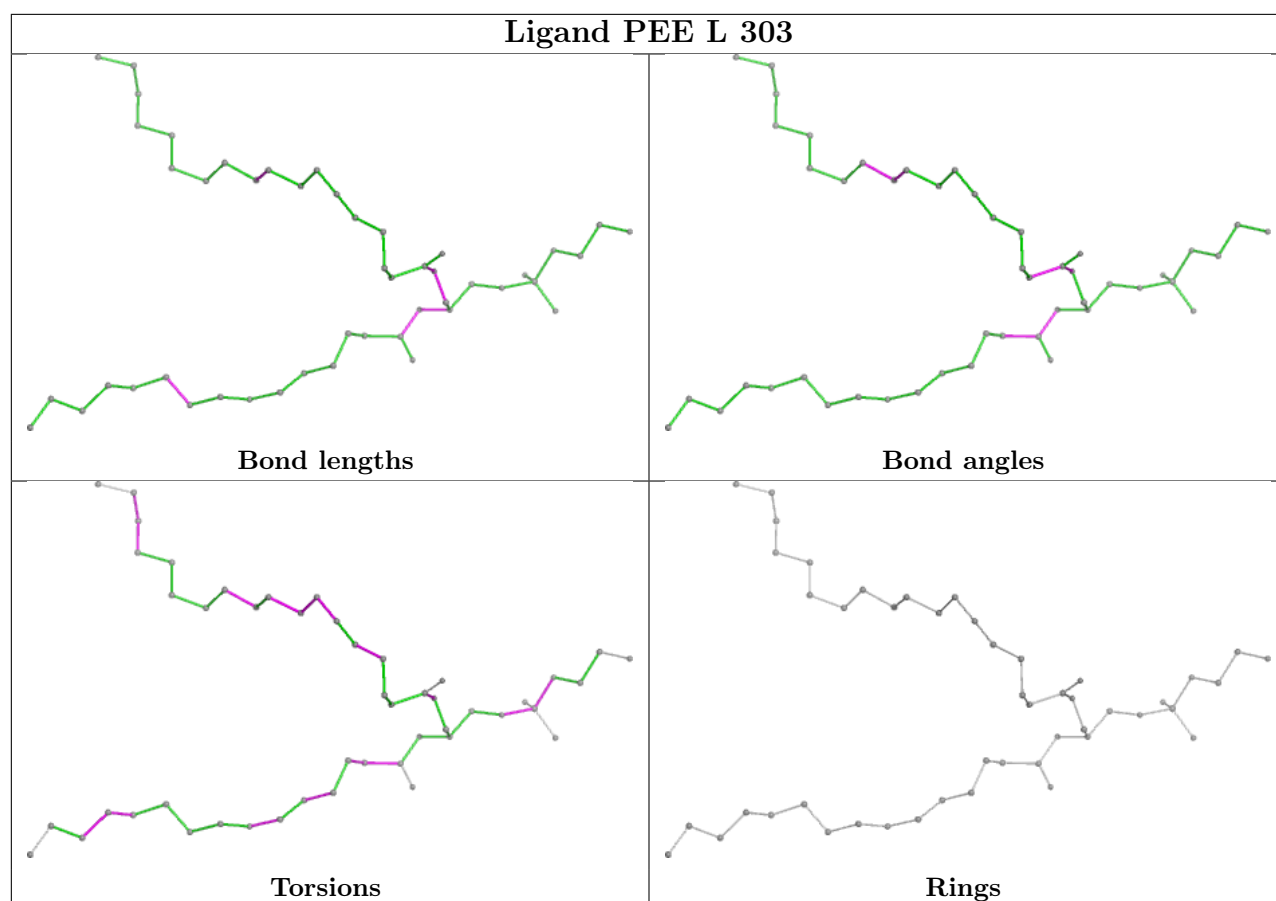


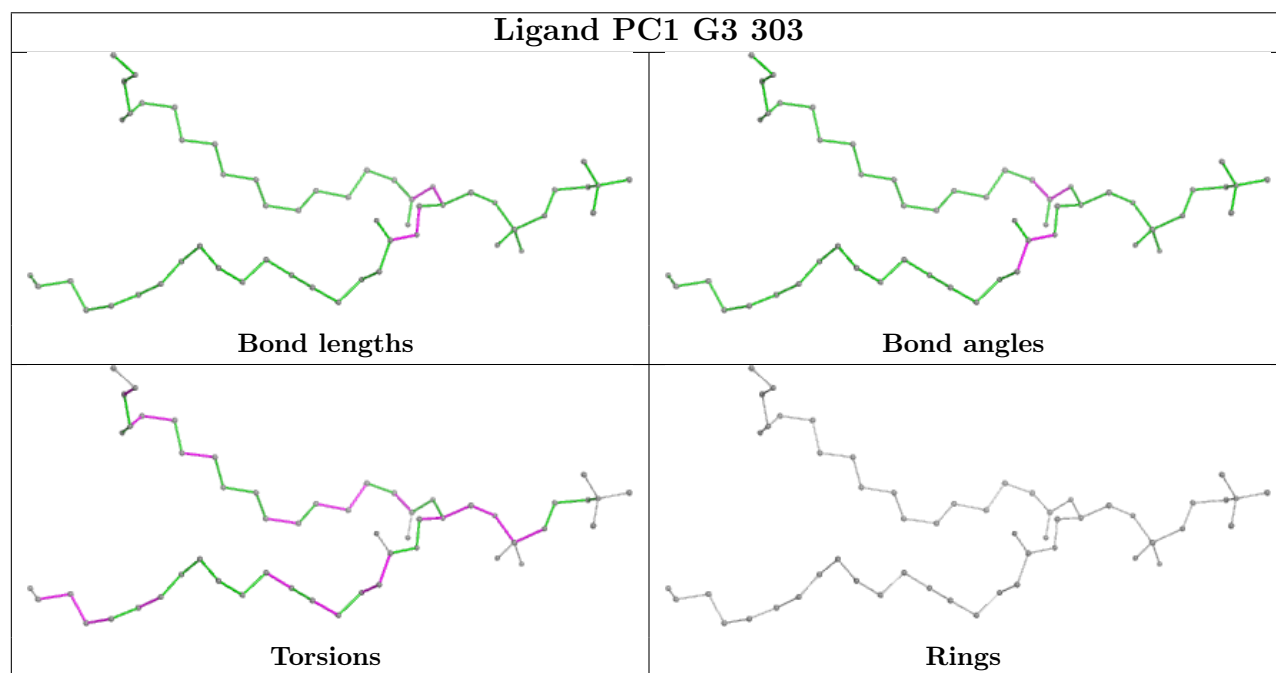
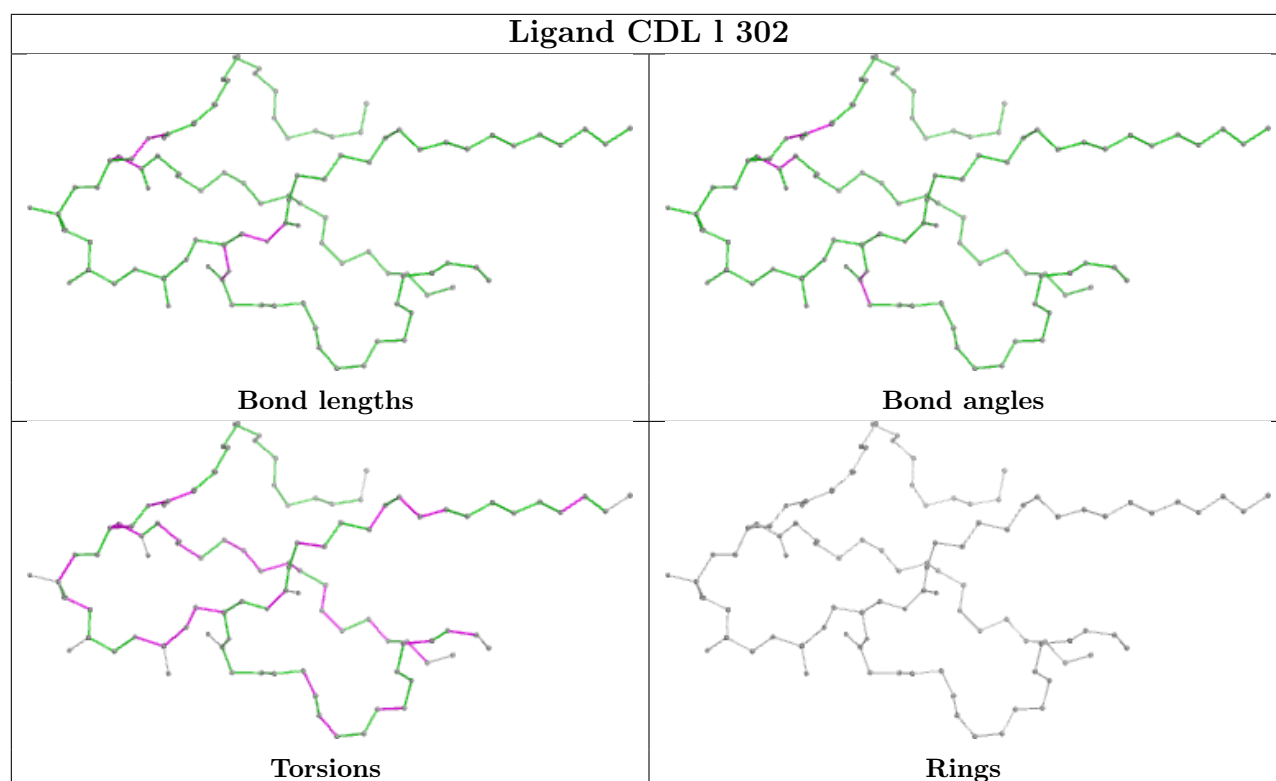


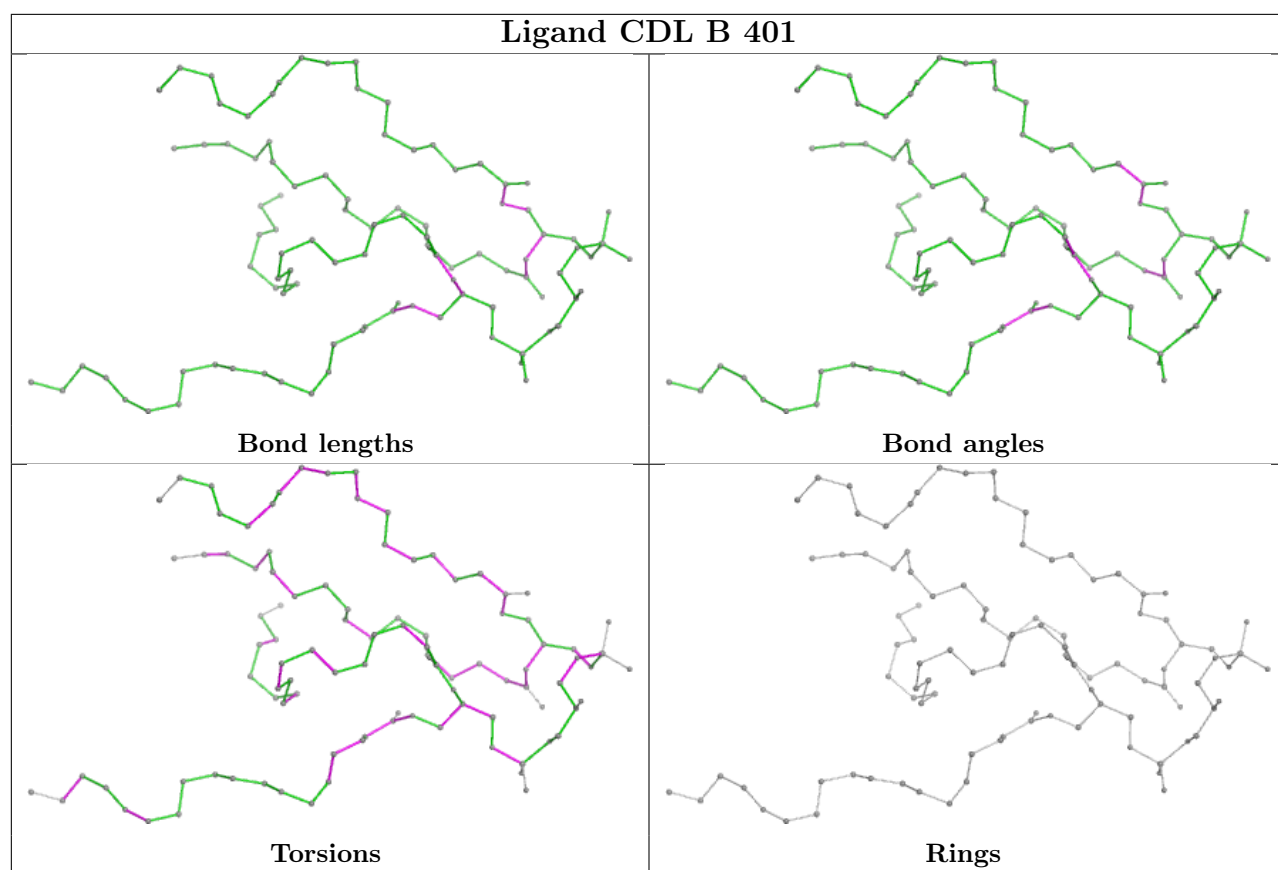


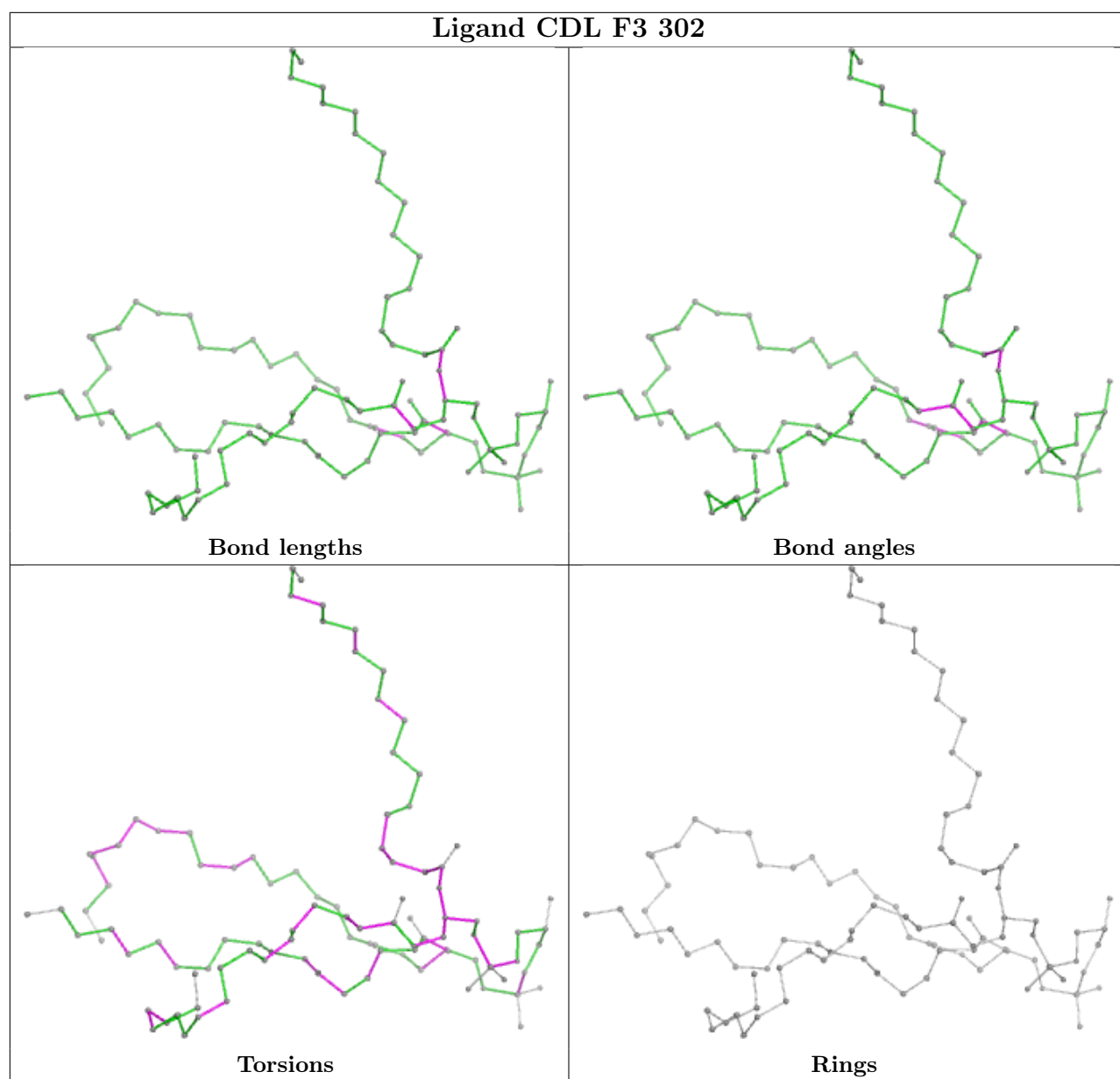


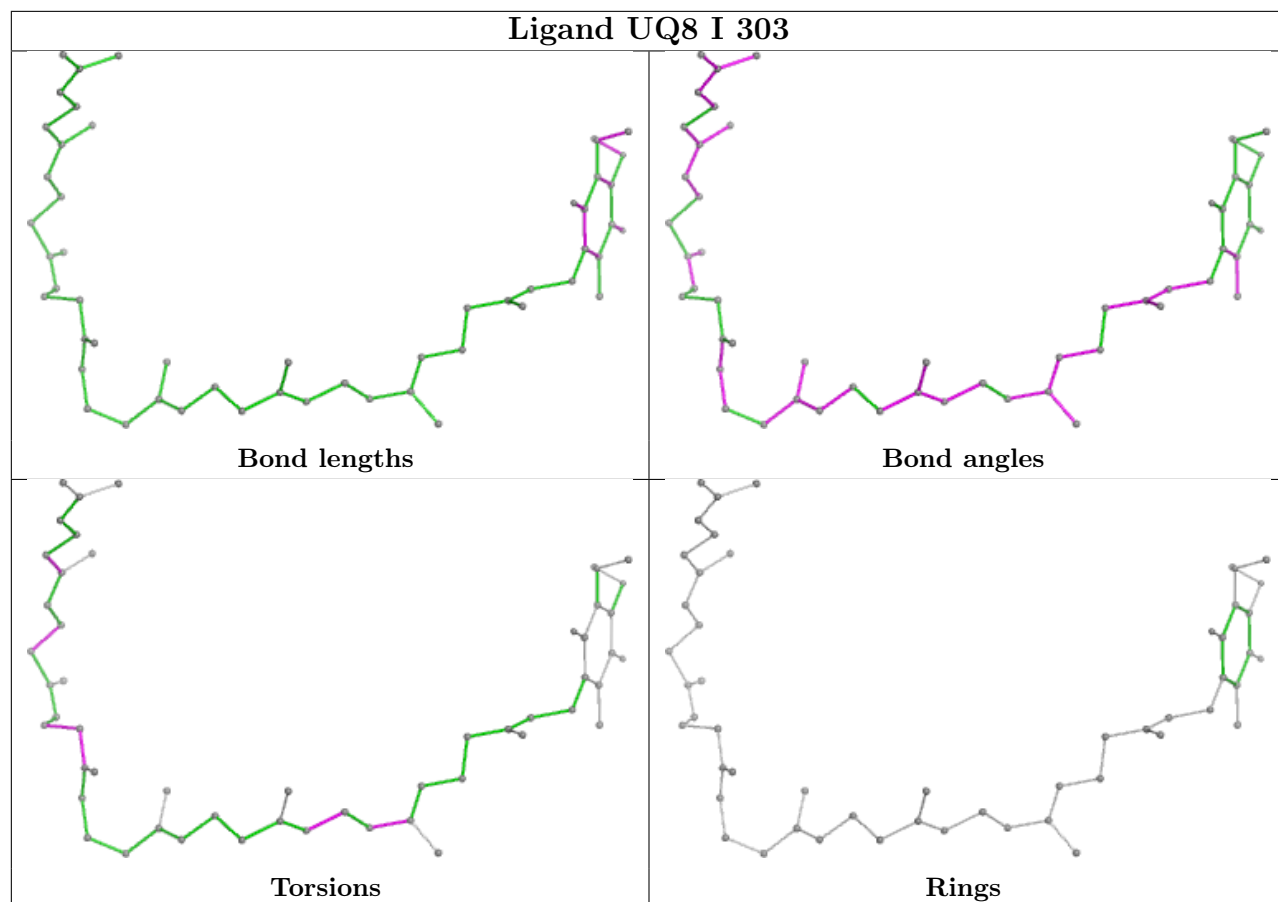


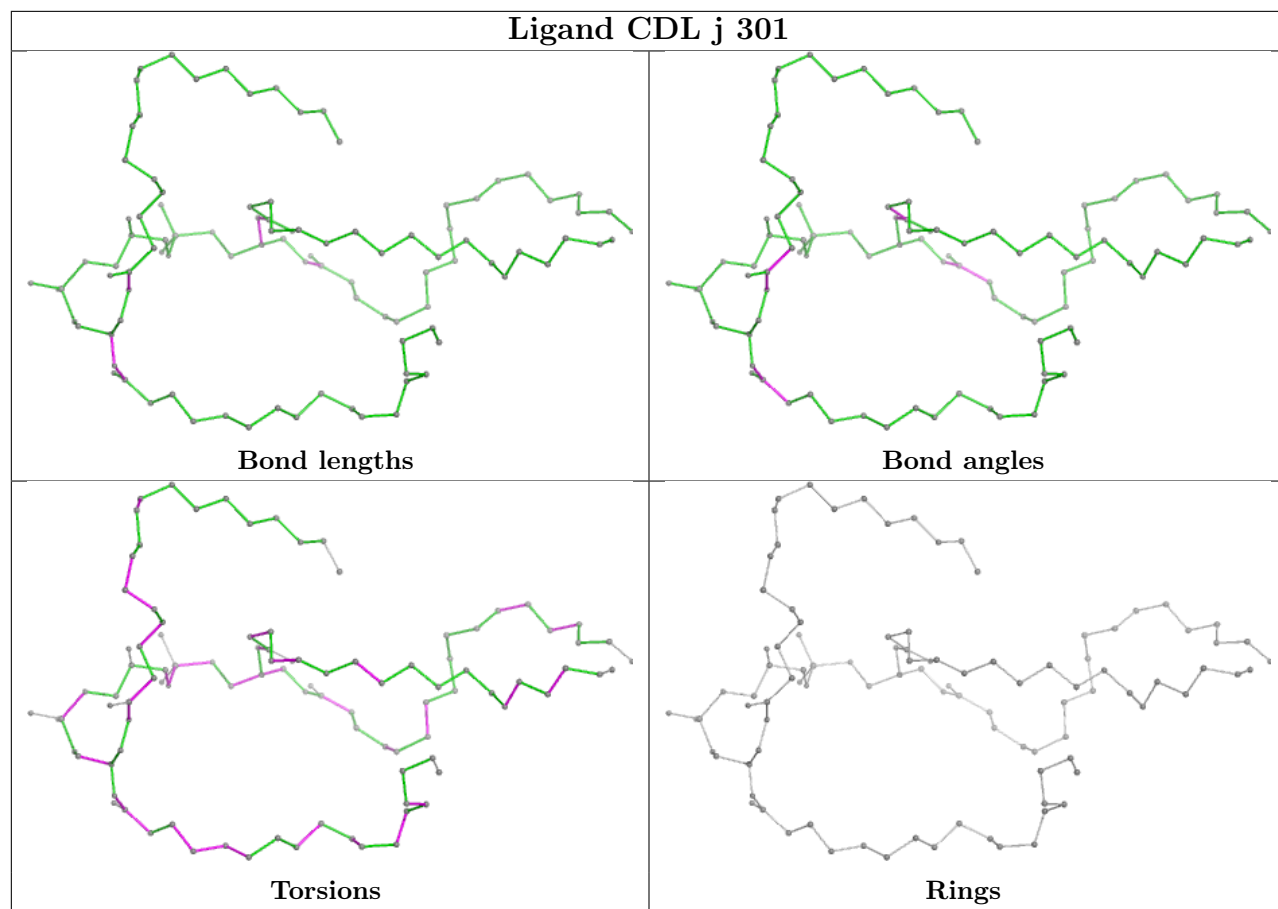


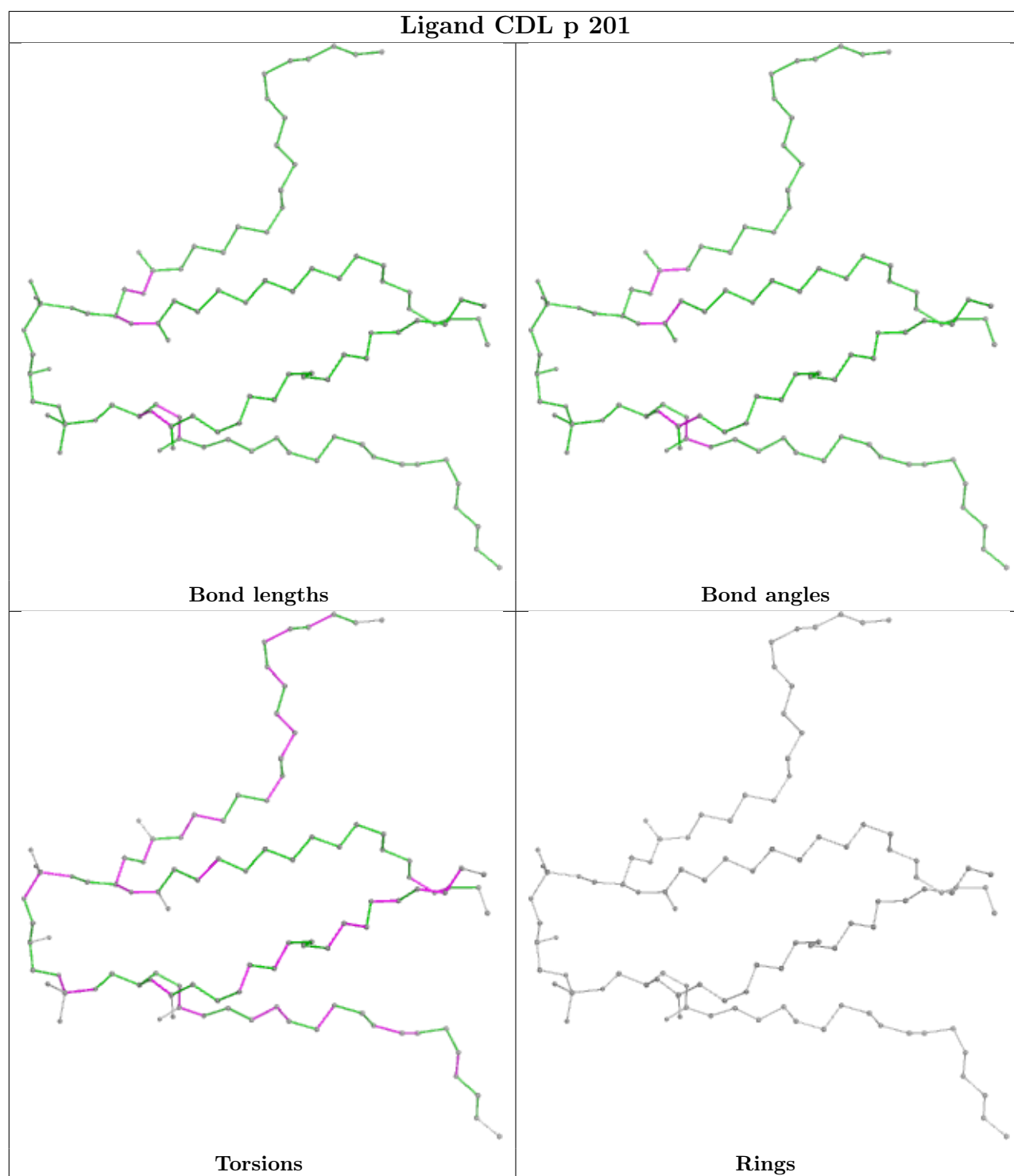


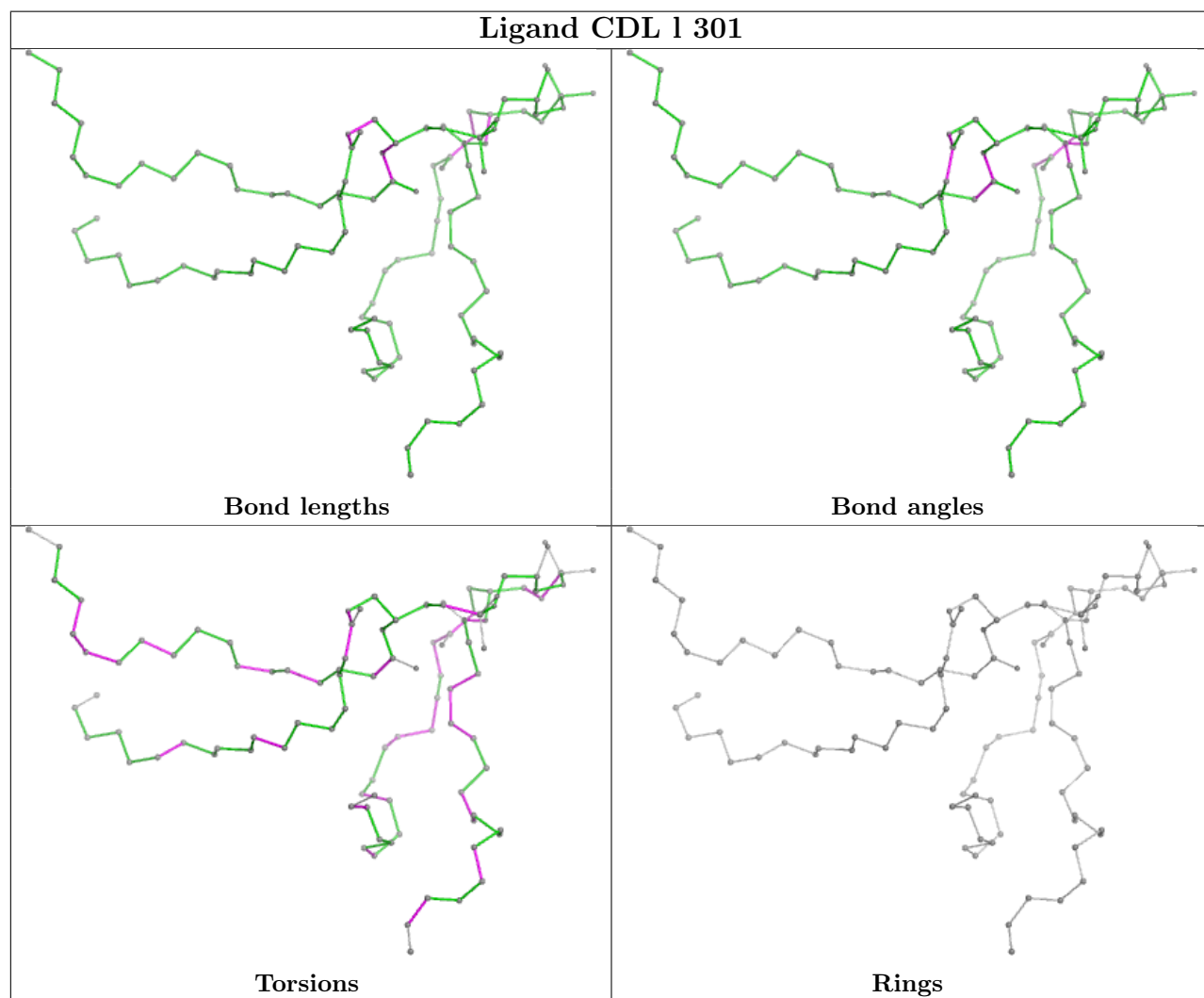
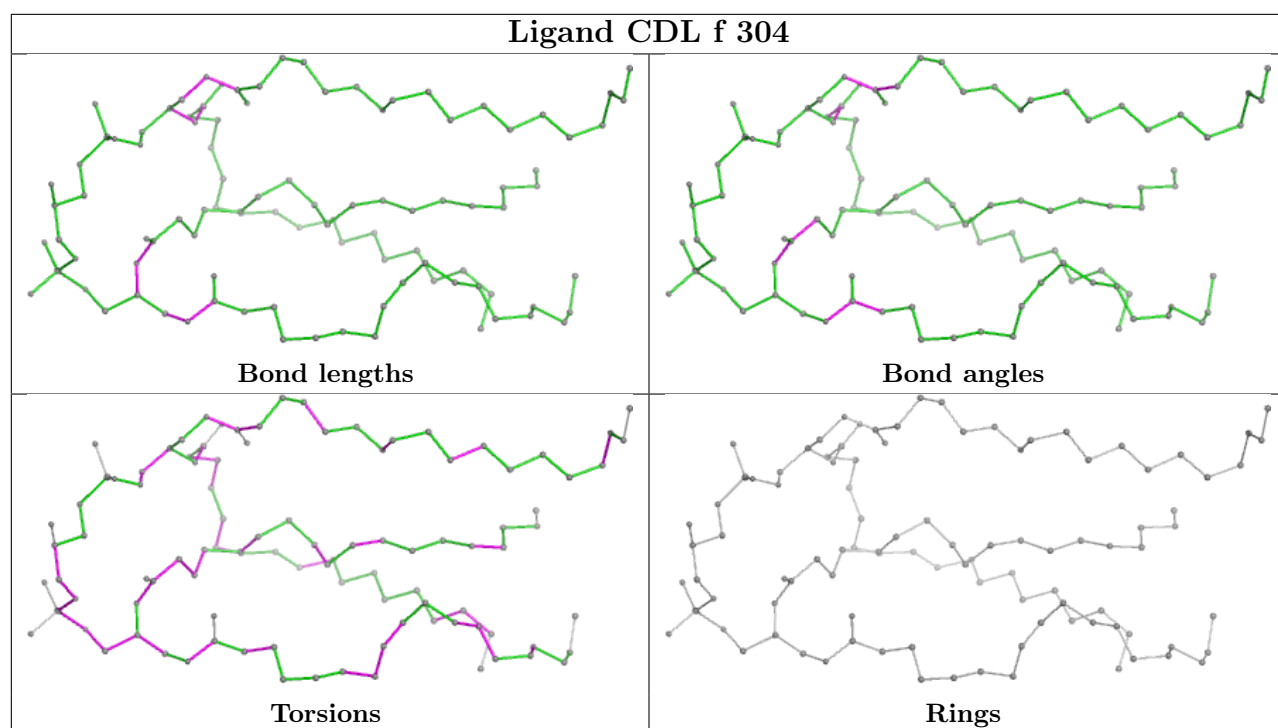


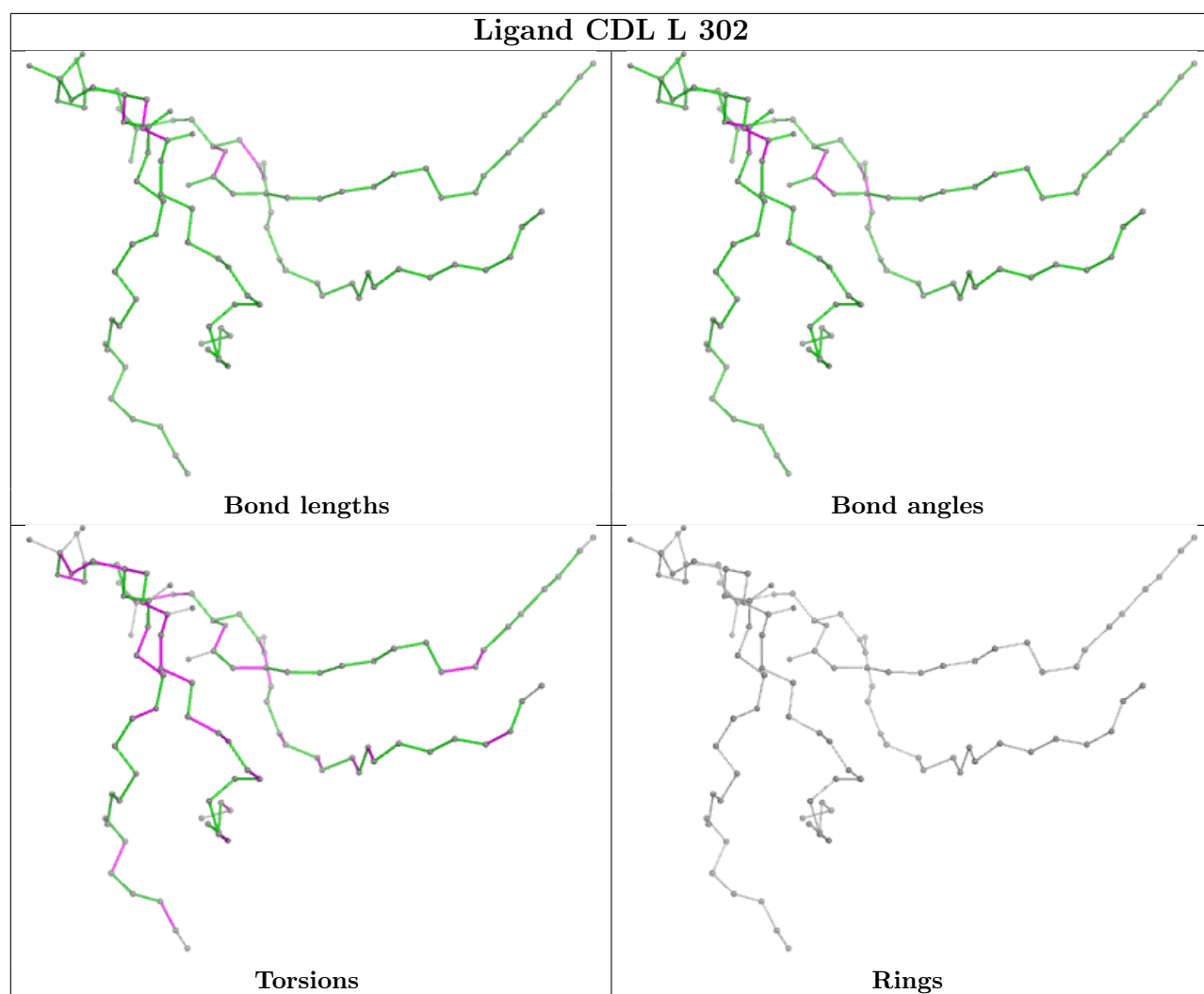


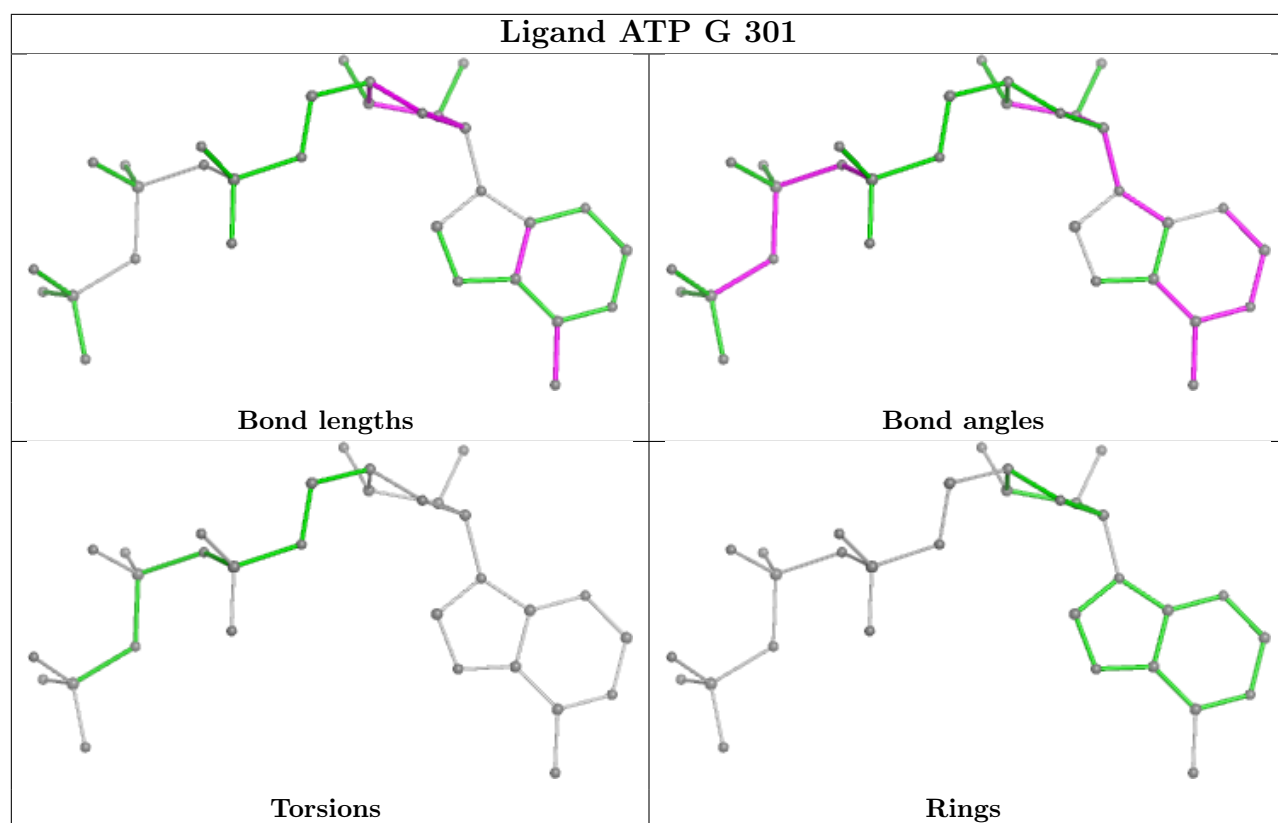


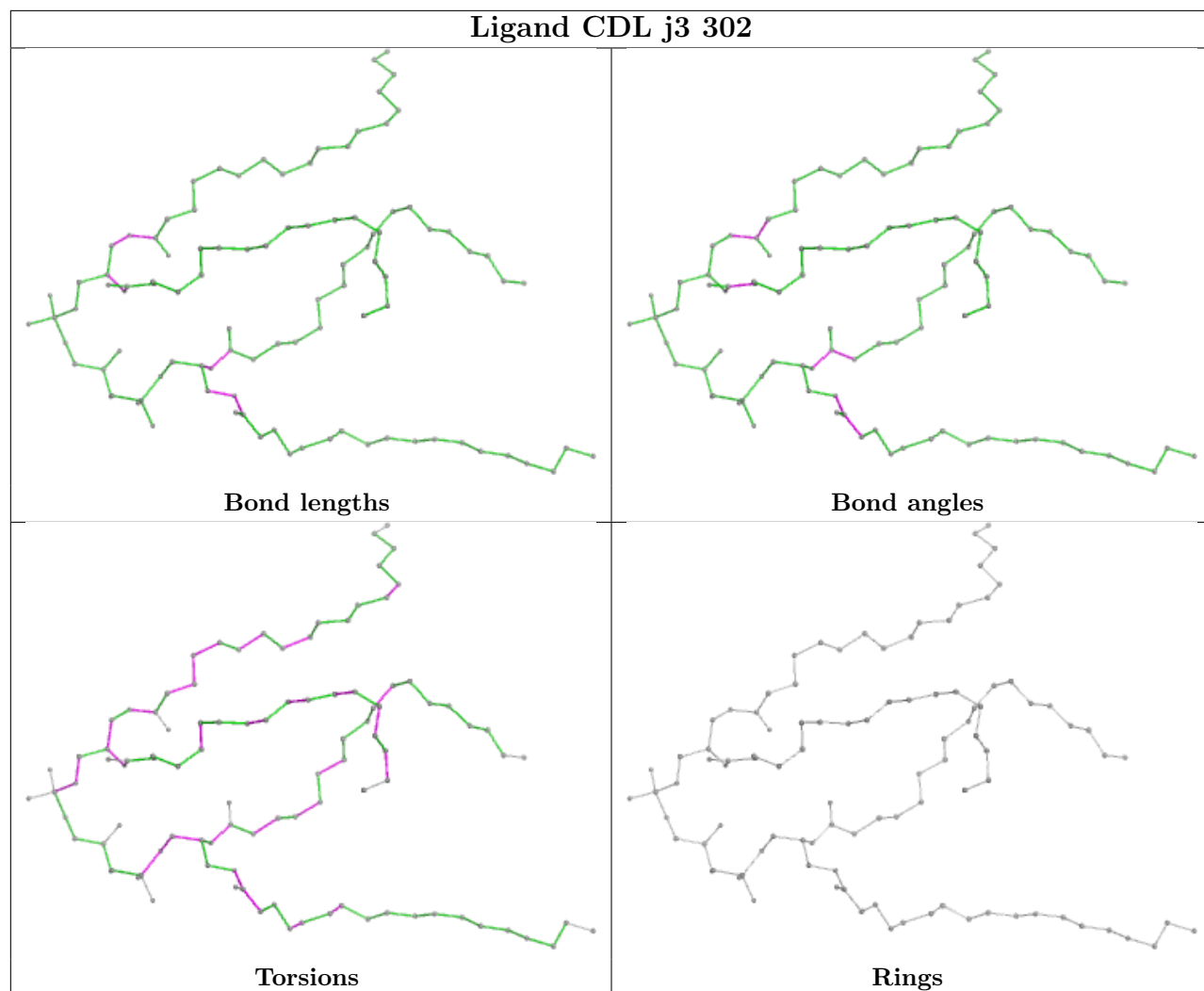


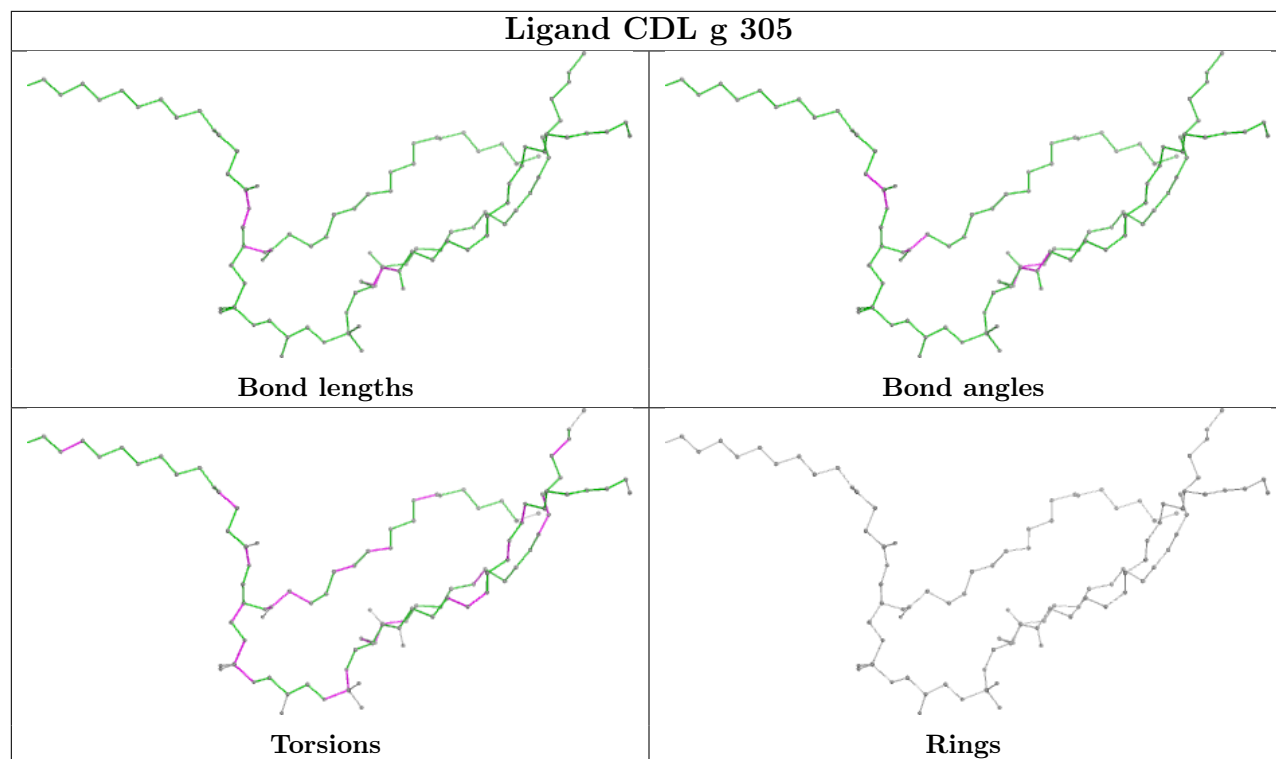




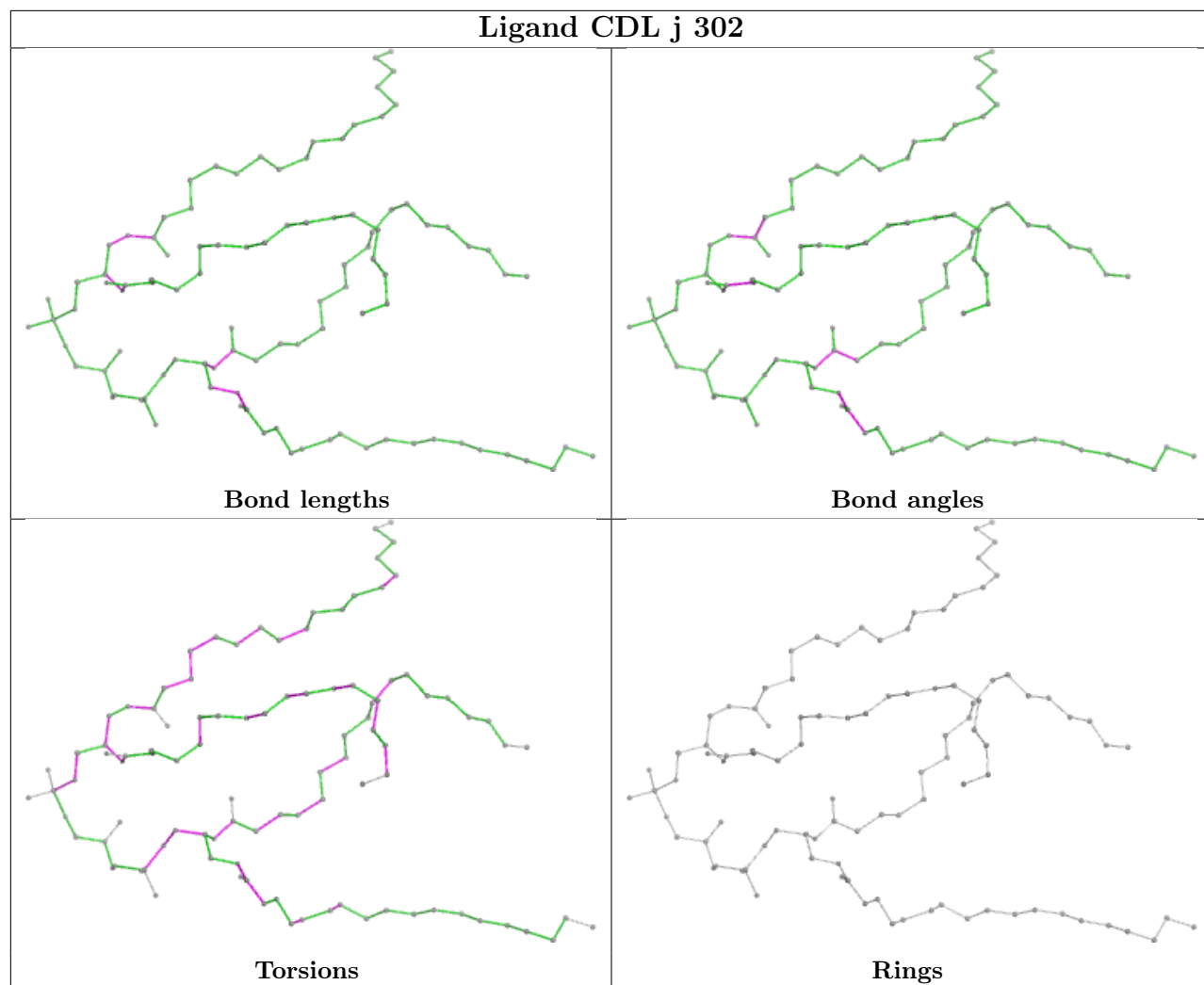


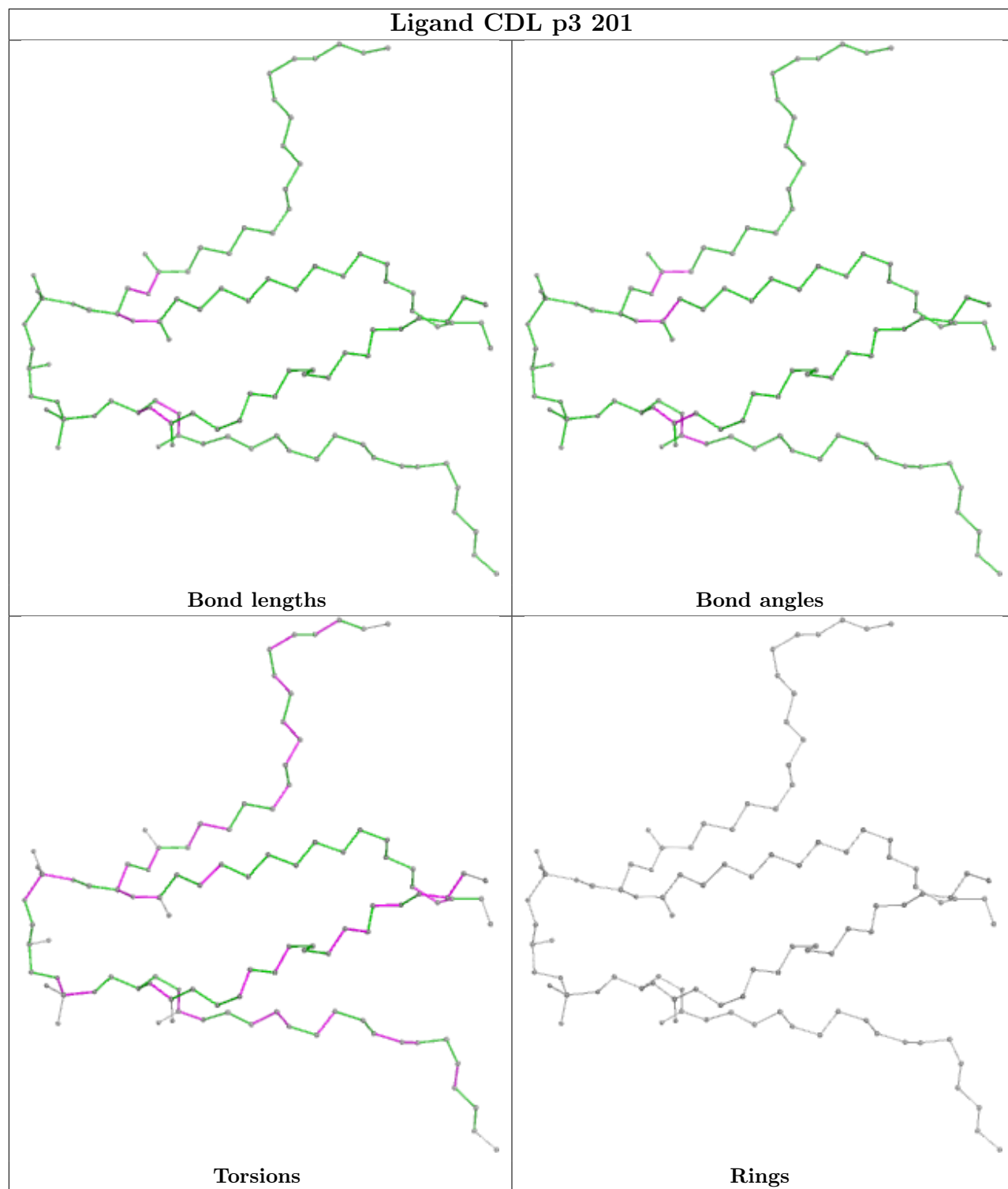


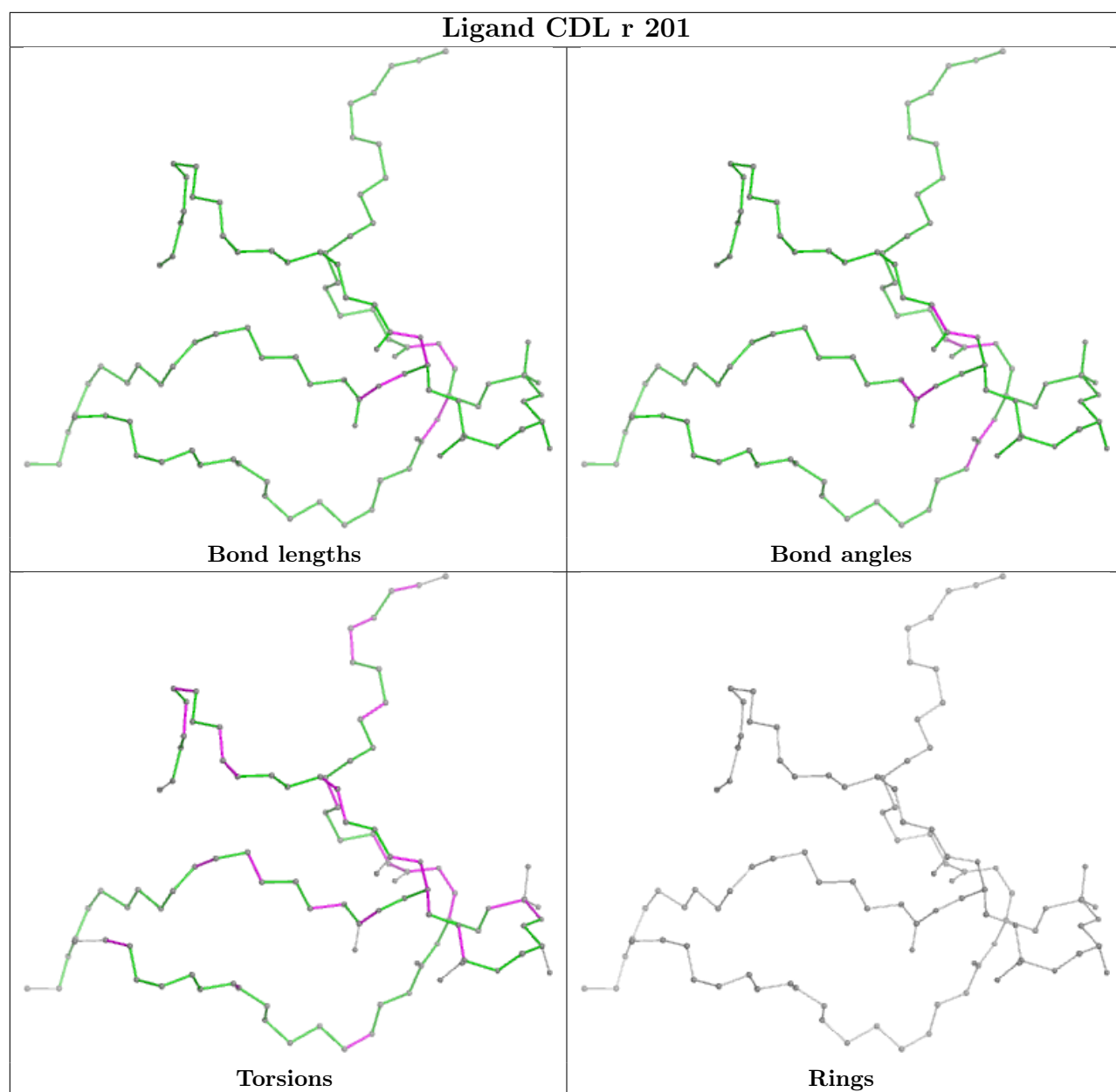




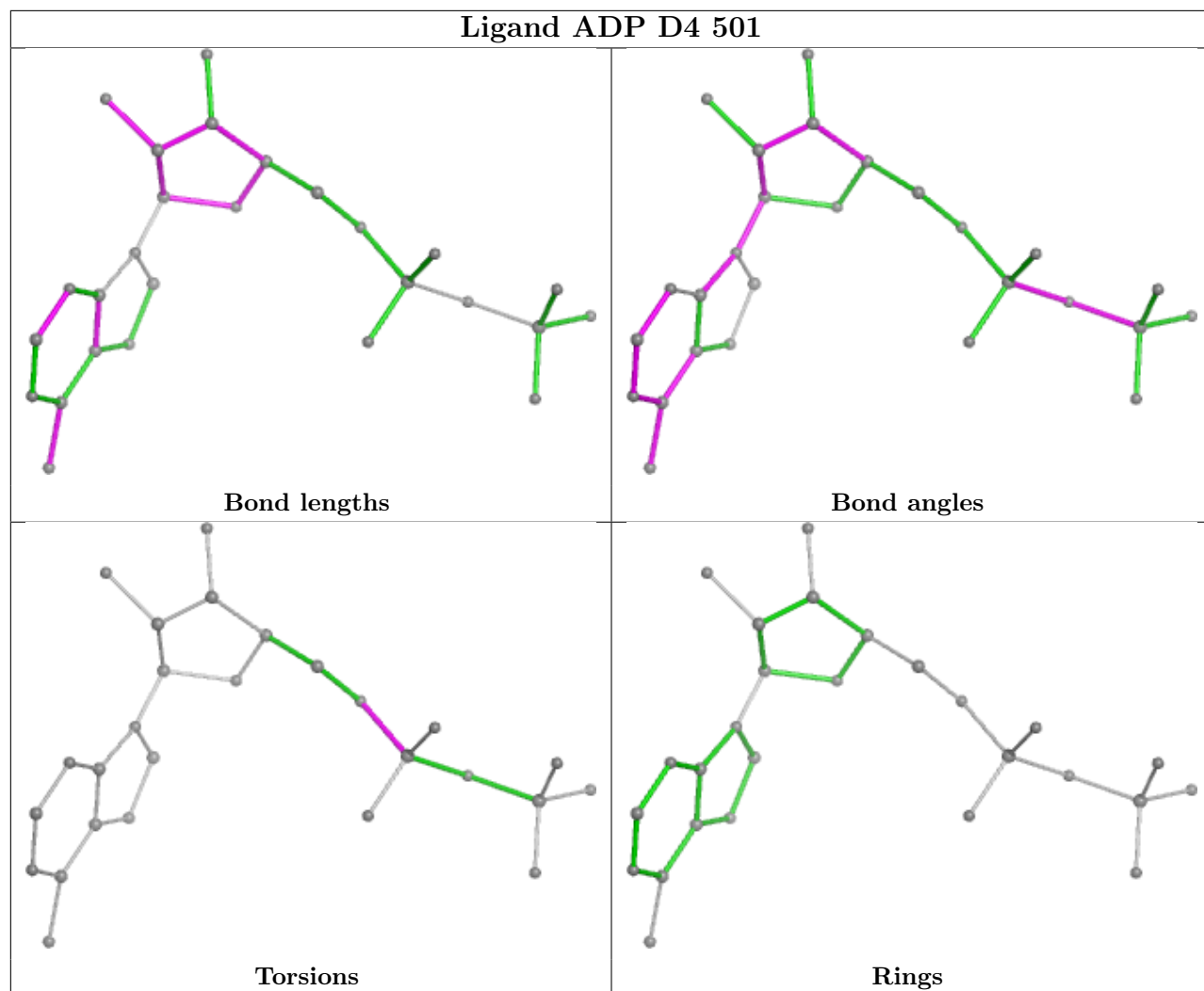
Ligand CDL j 302

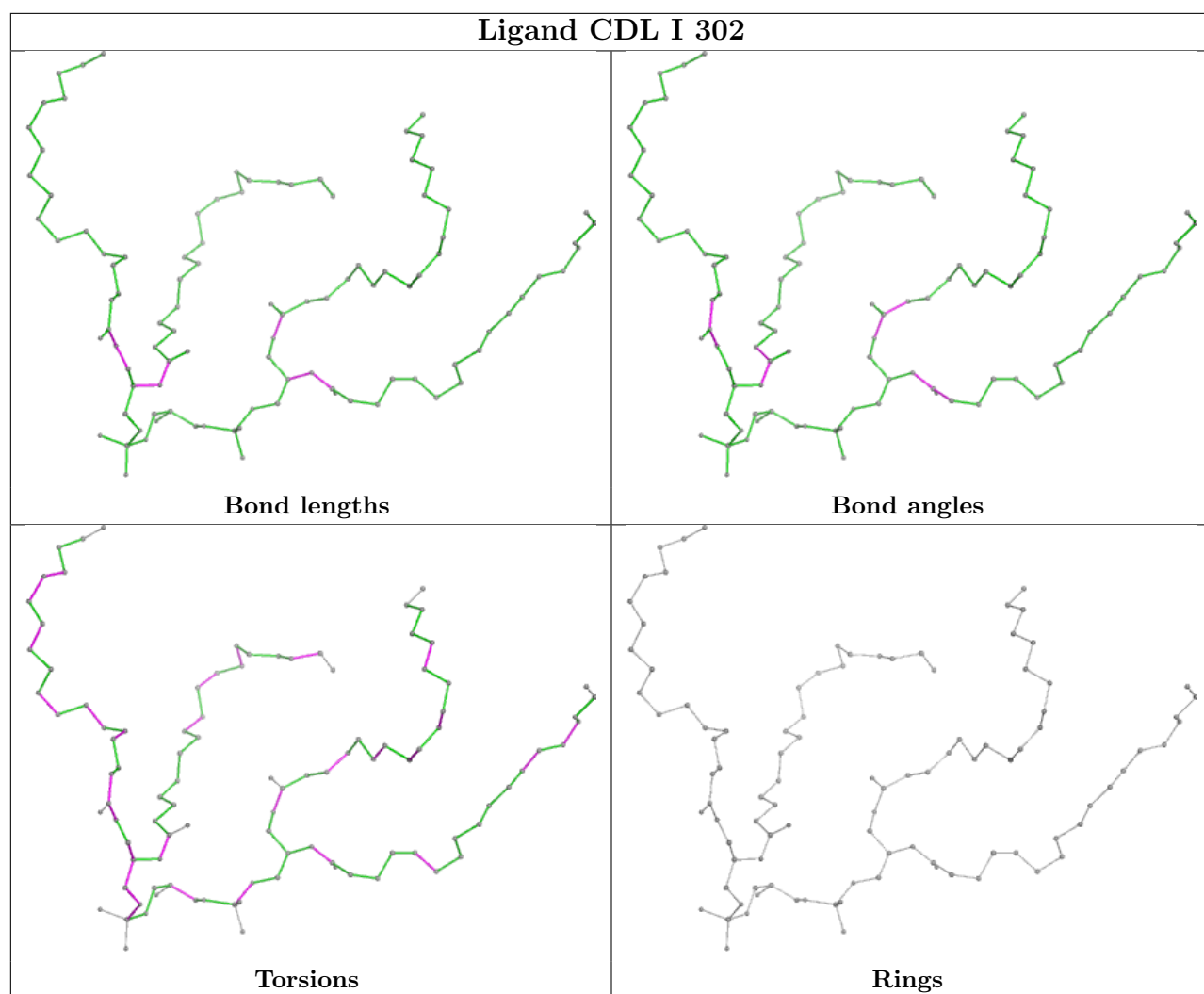


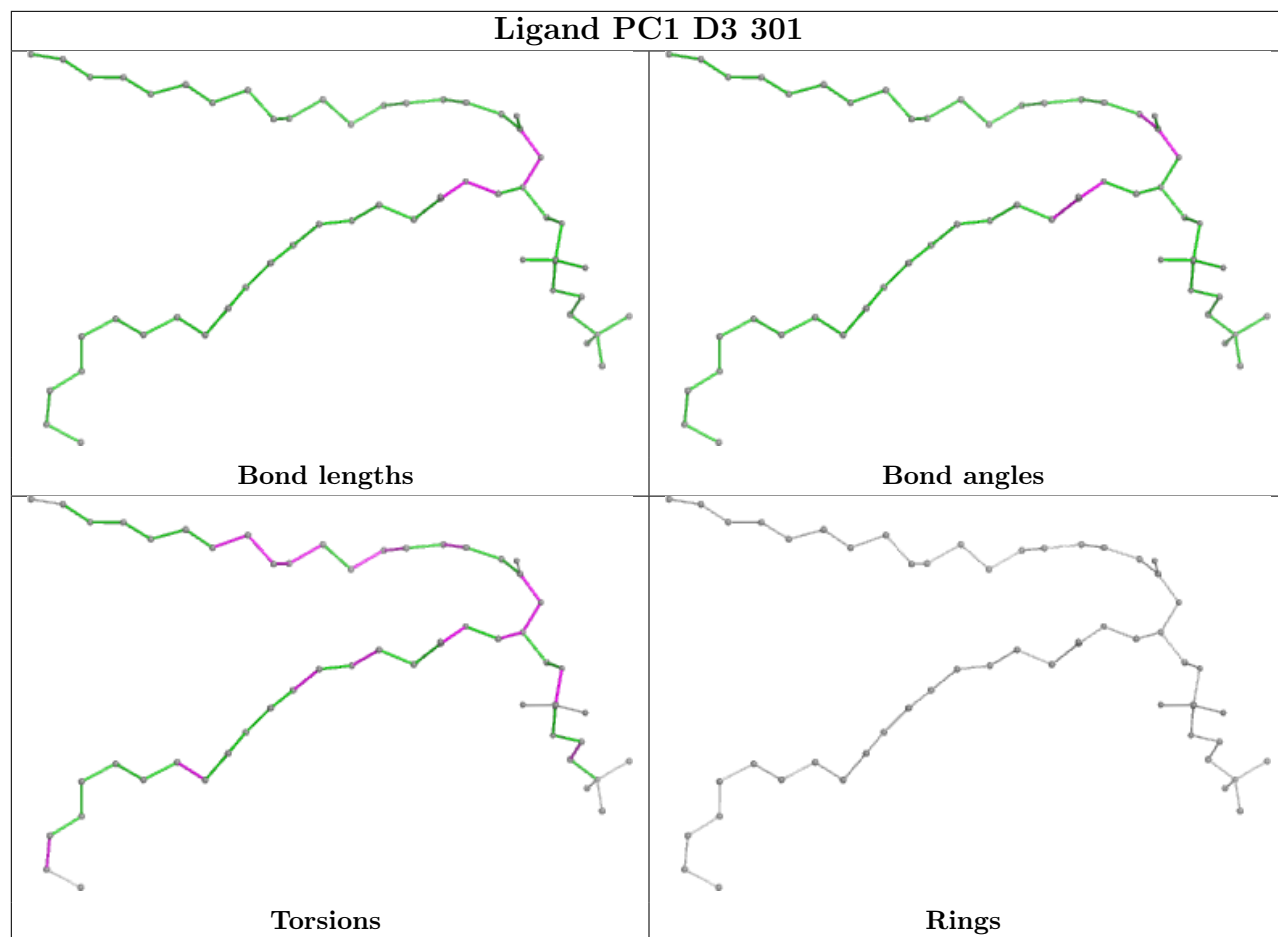


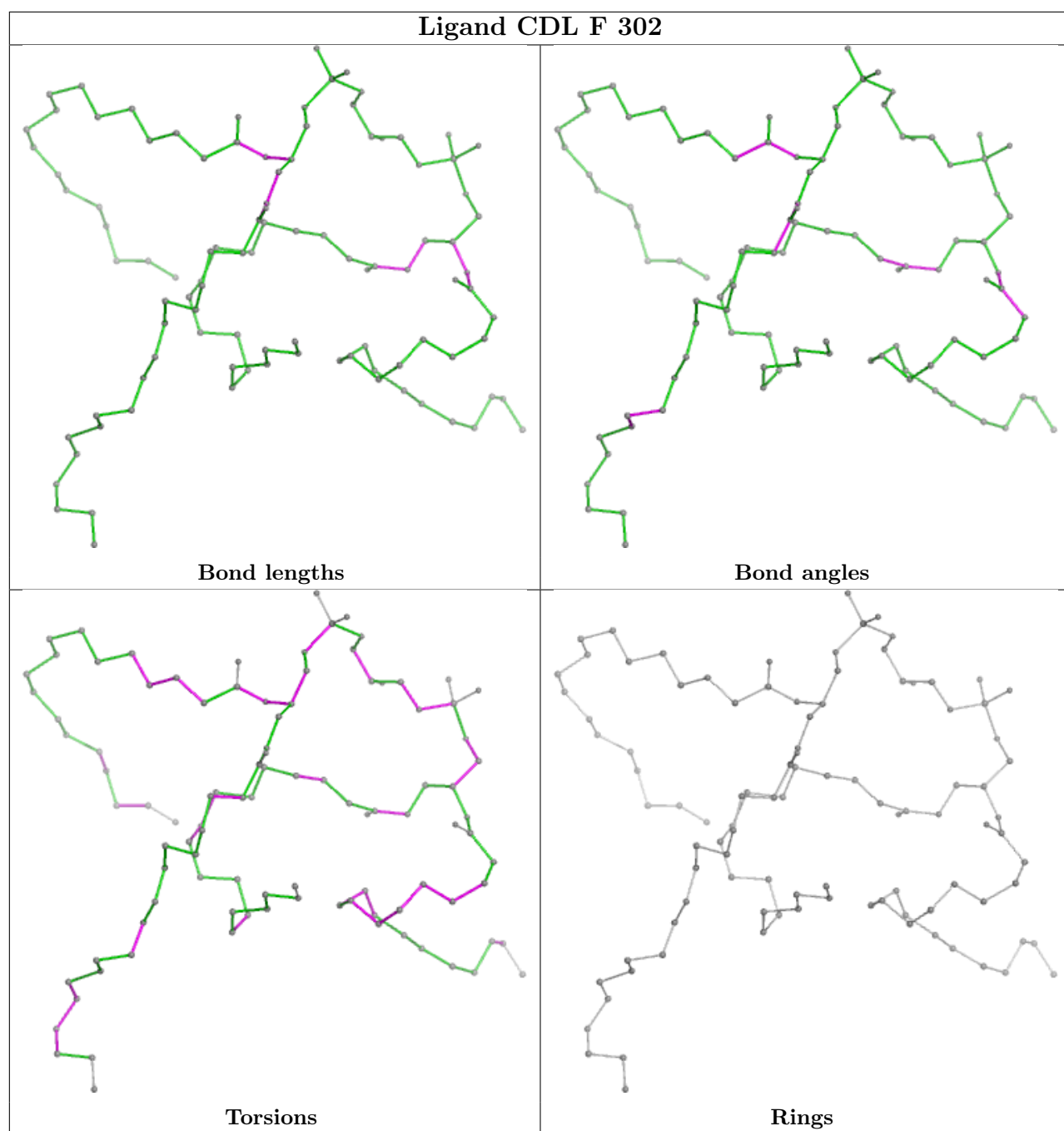


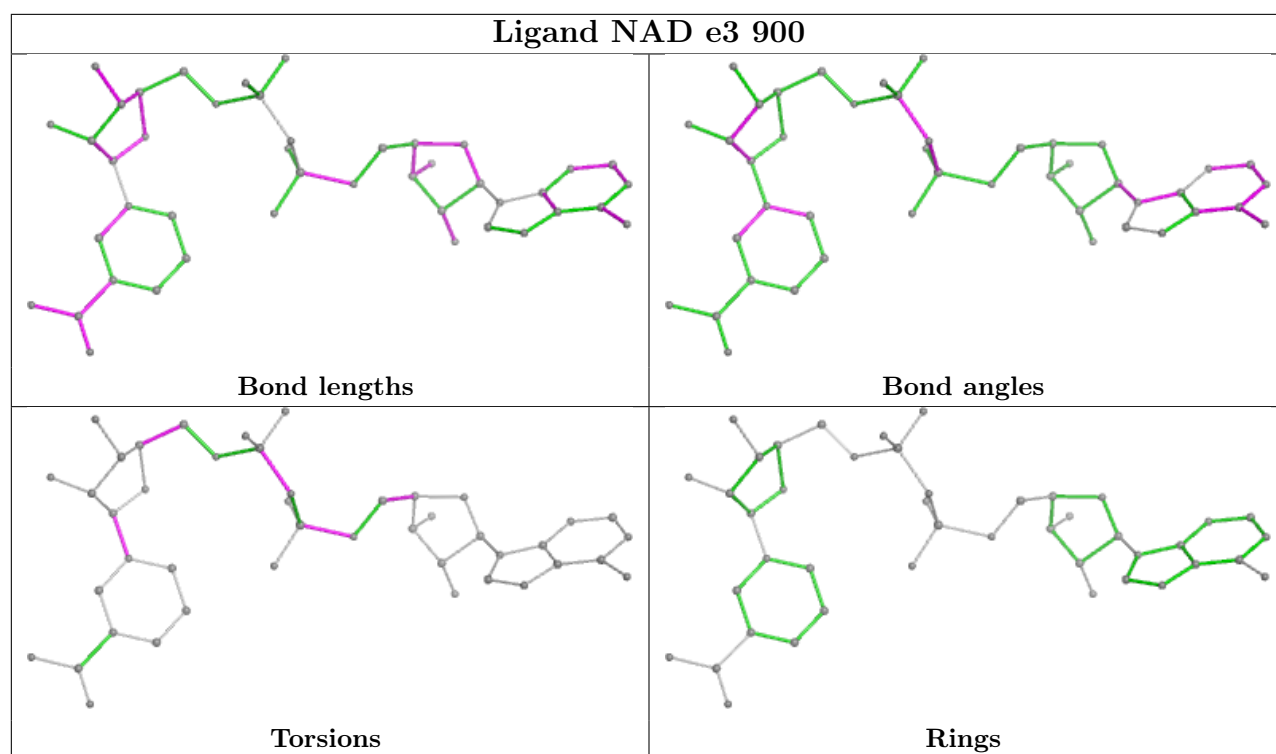
Ligand ADP D4 501



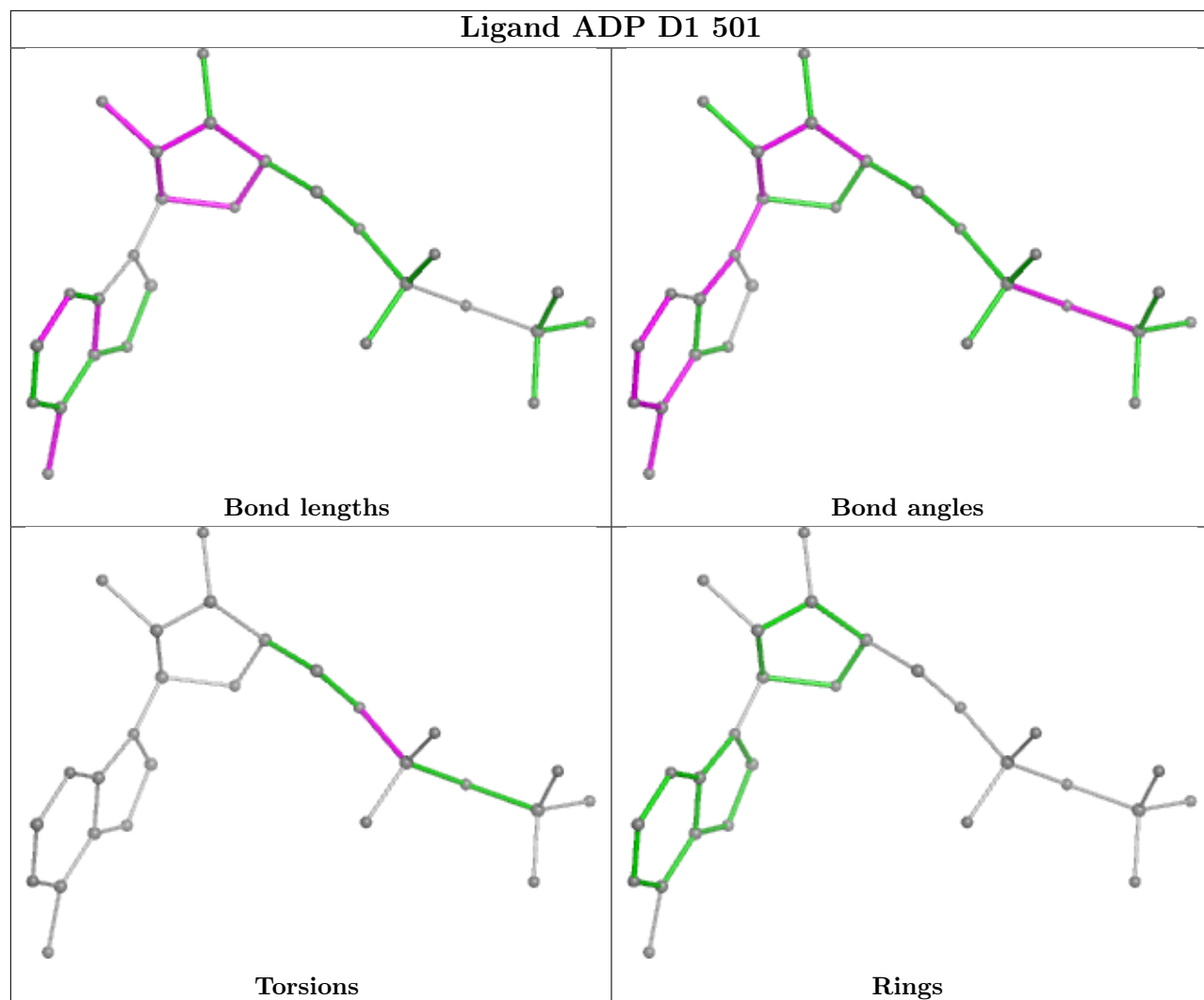




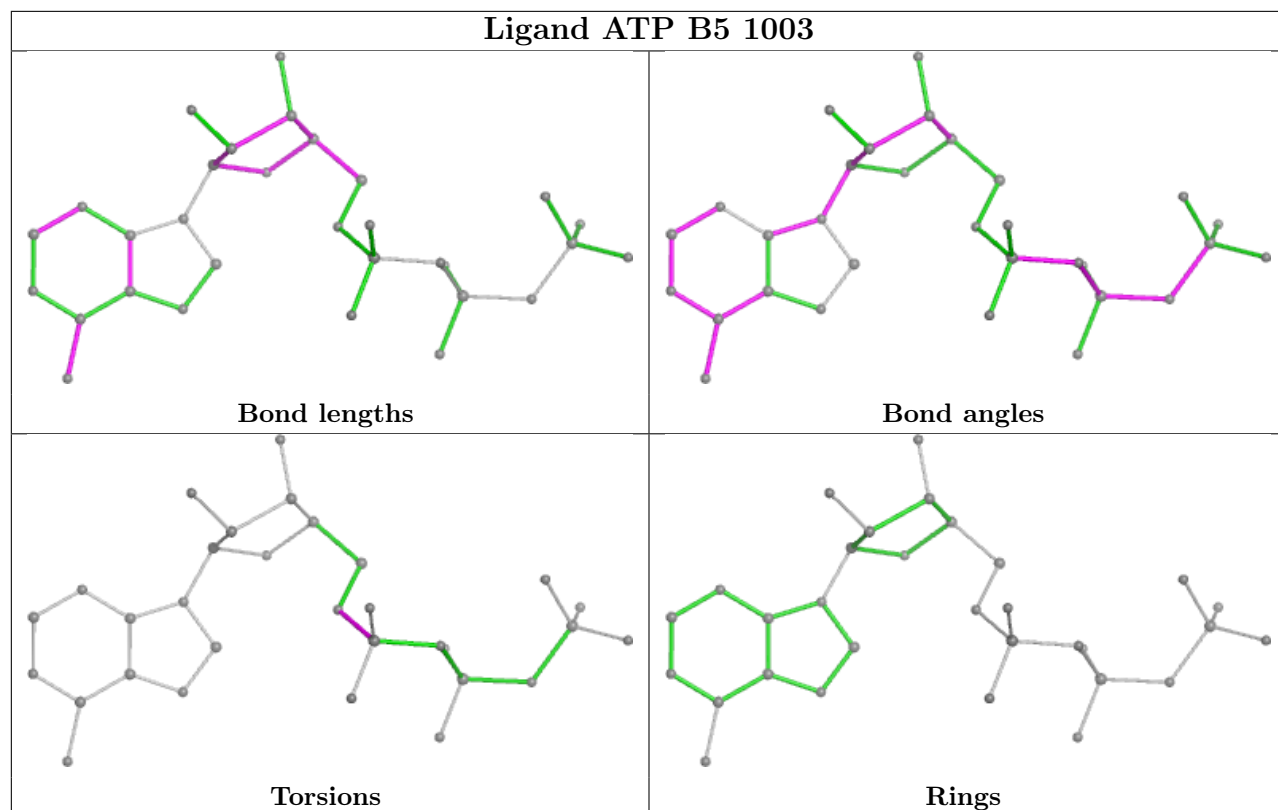




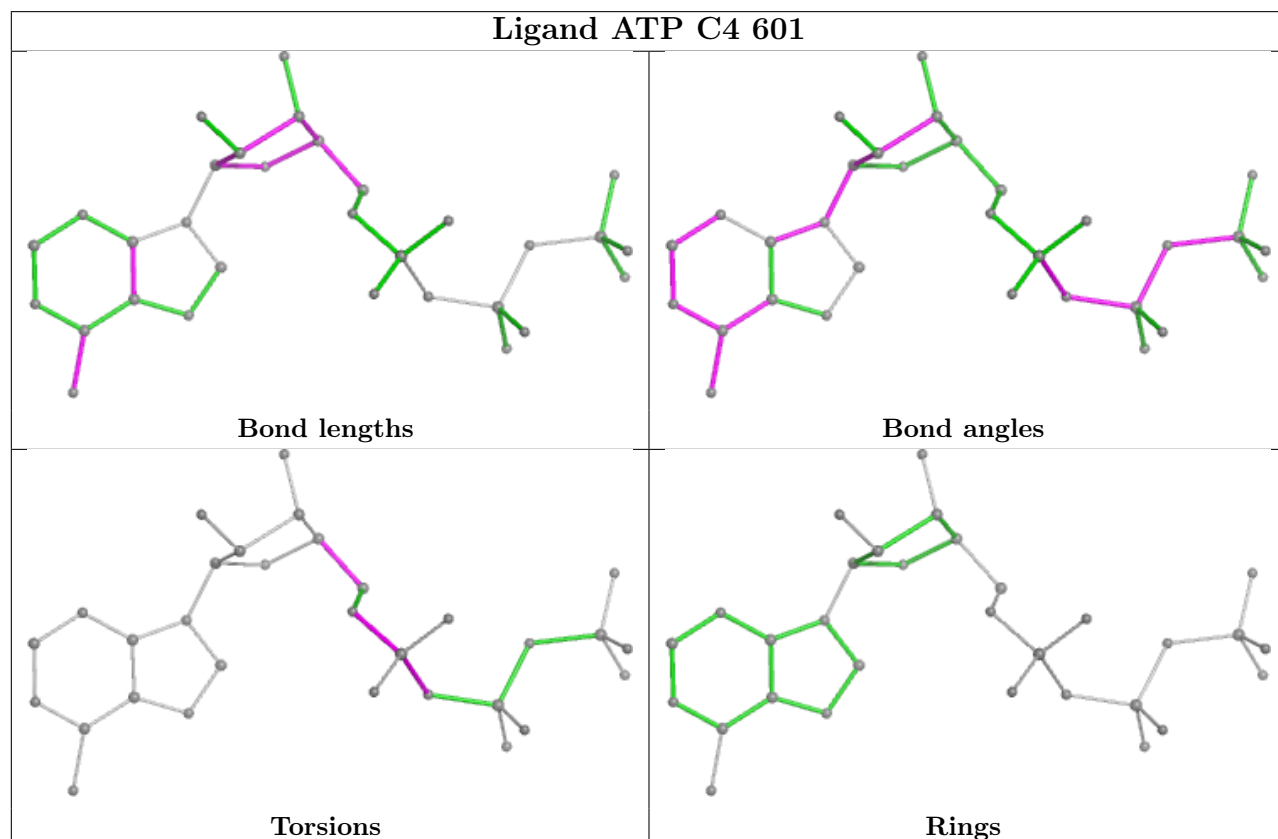
Ligand ADP D1 501

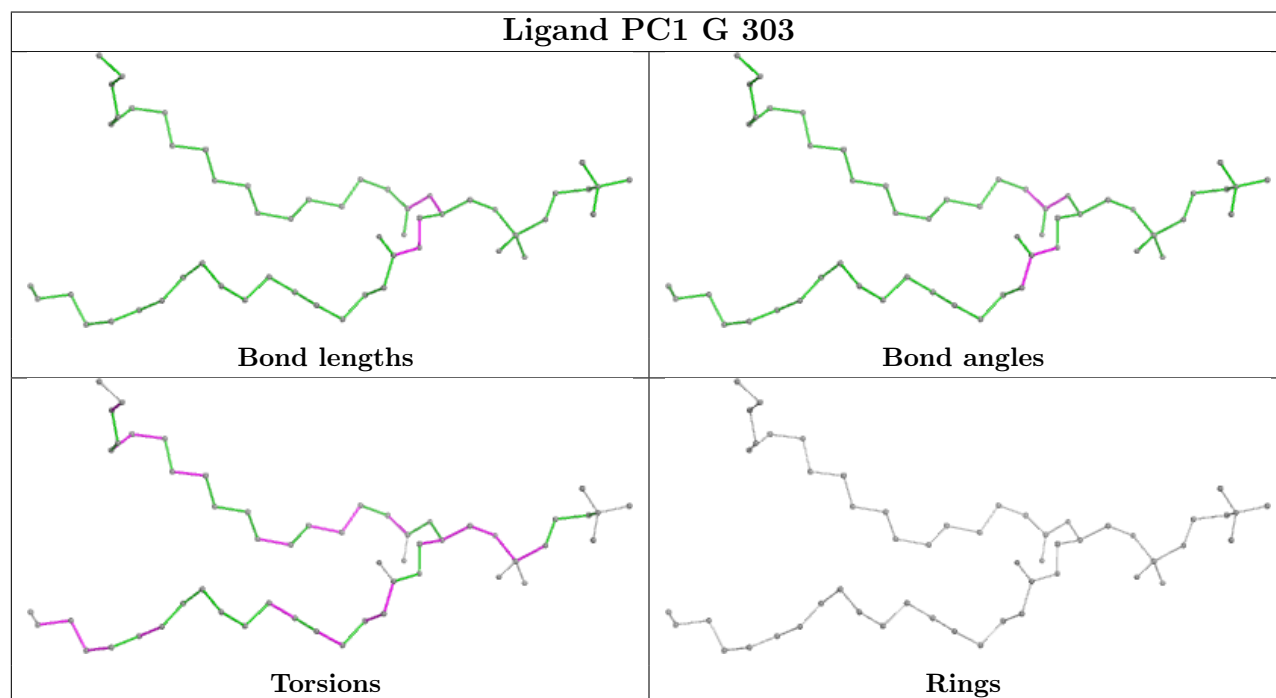
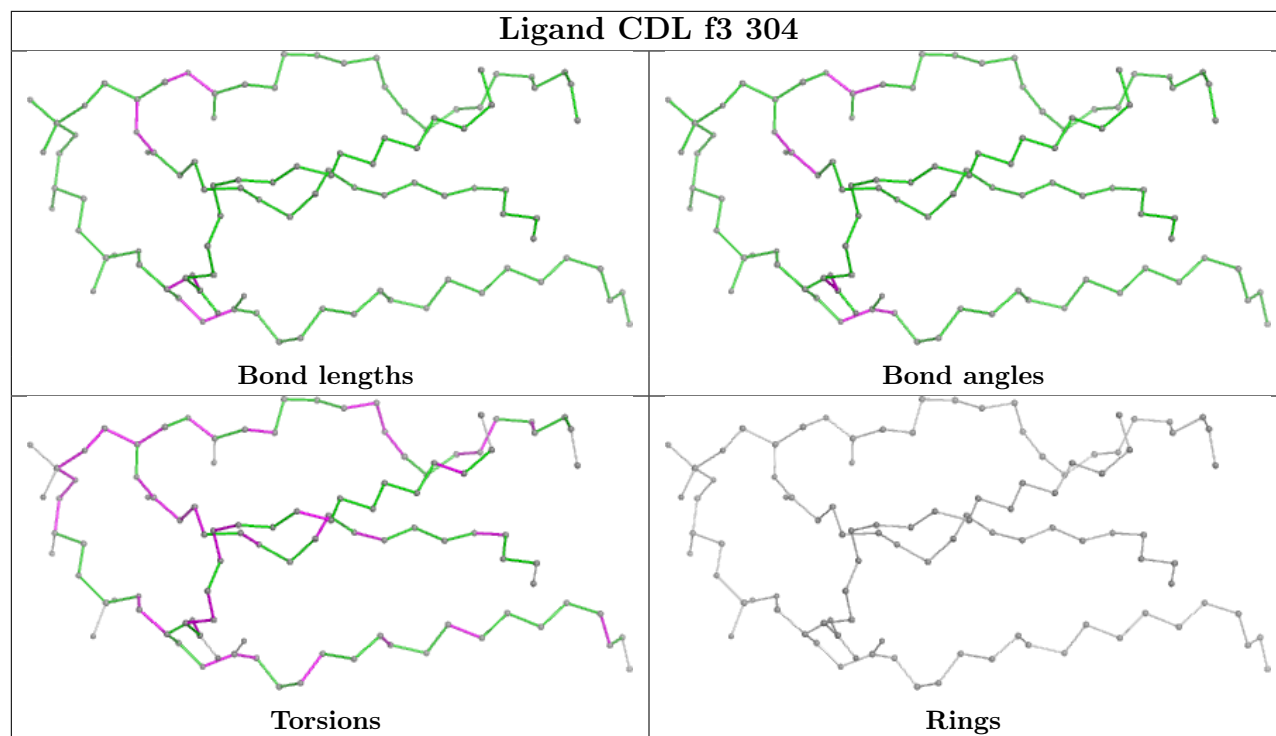


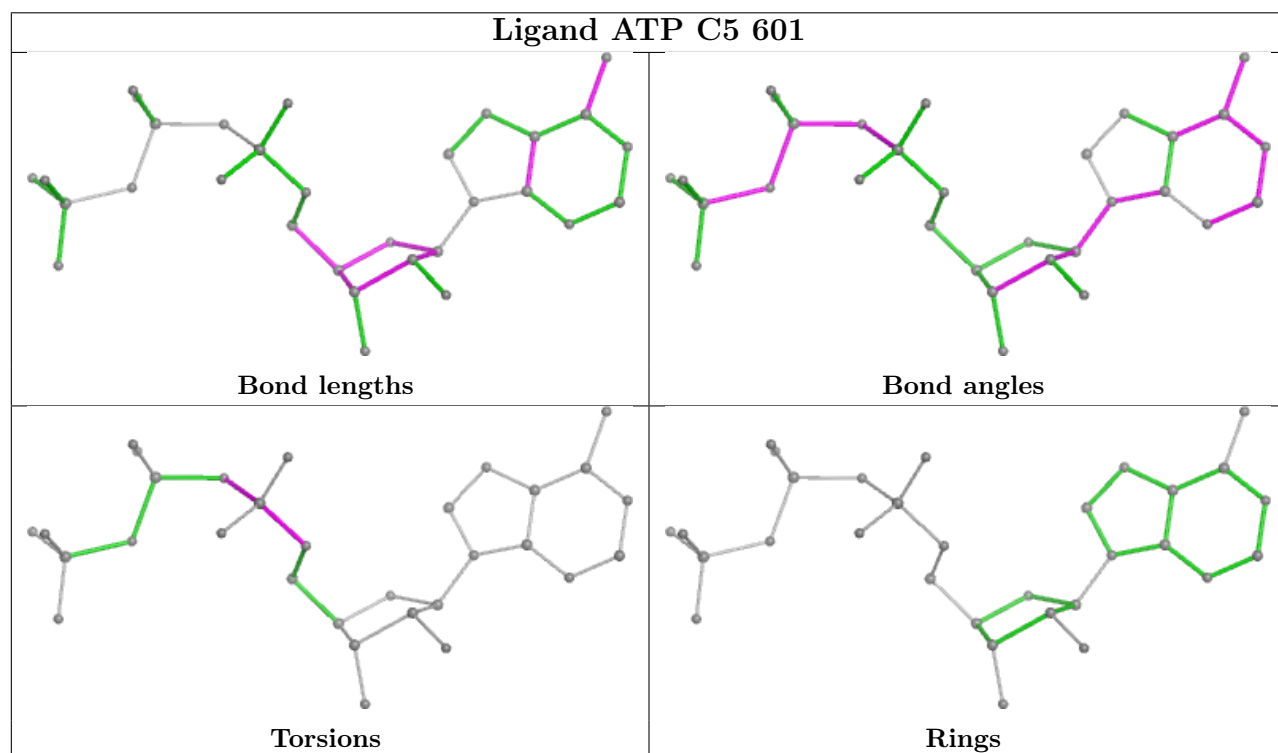
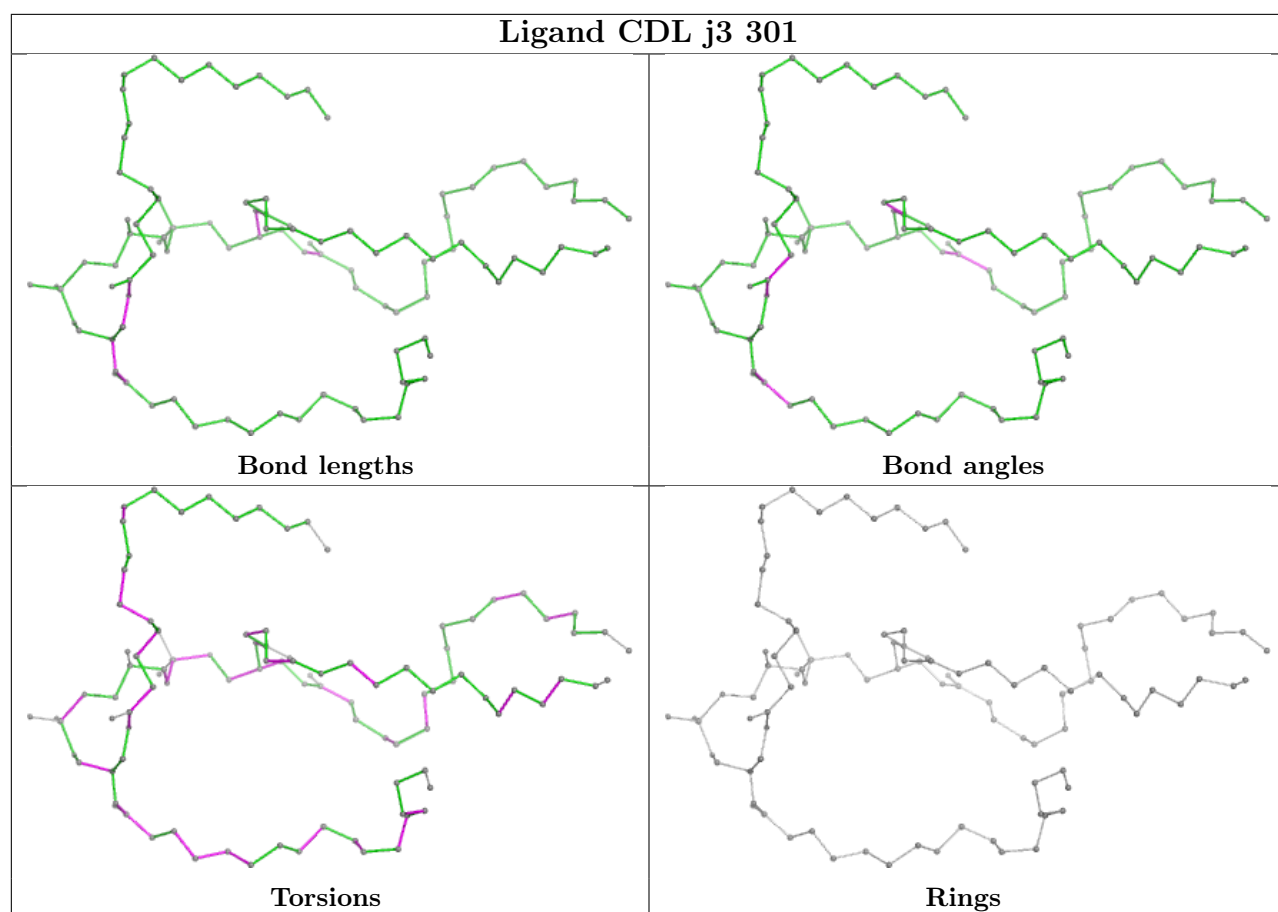
Ligand ATP B5 1003

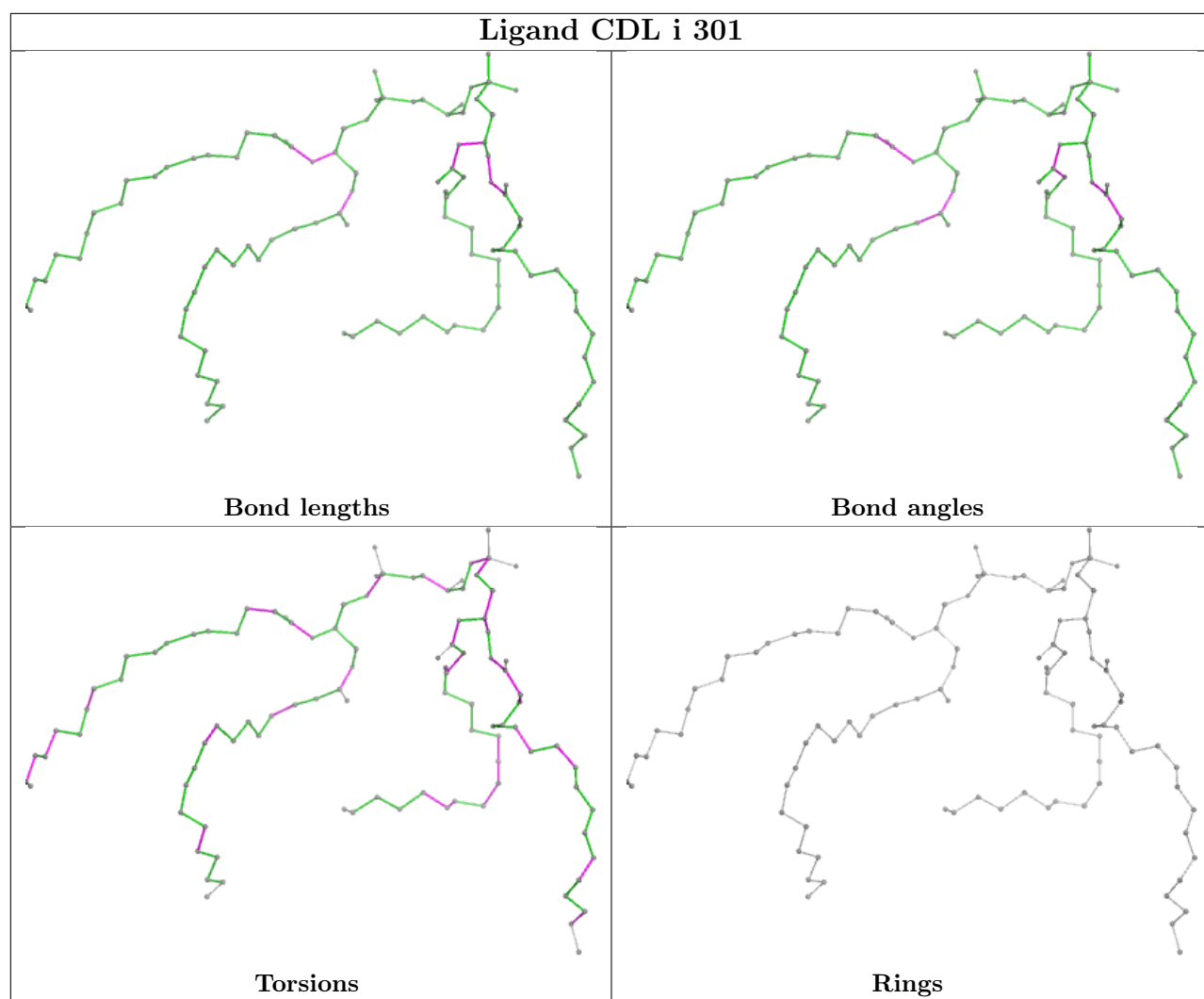


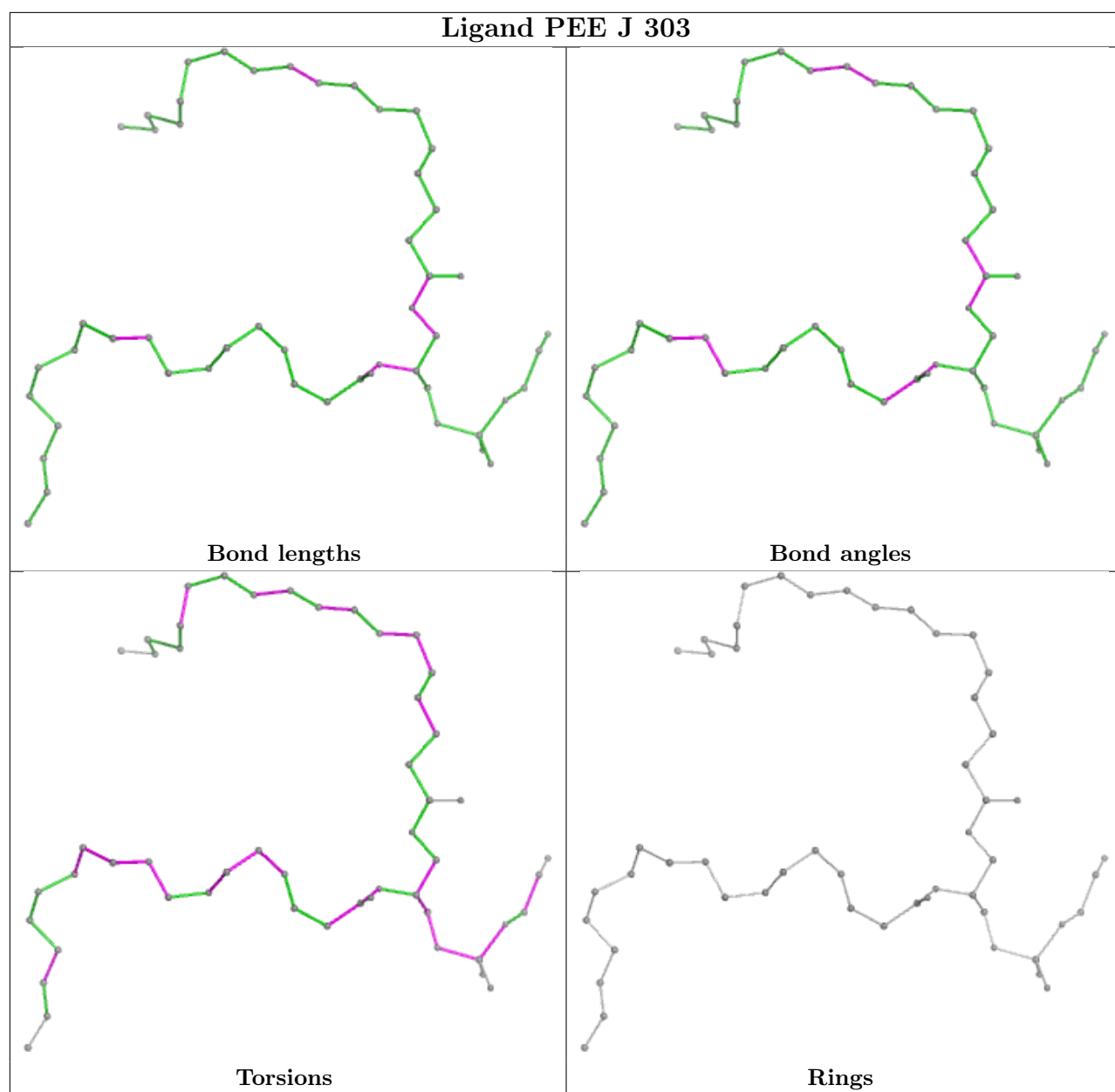
Ligand ATP C4 601

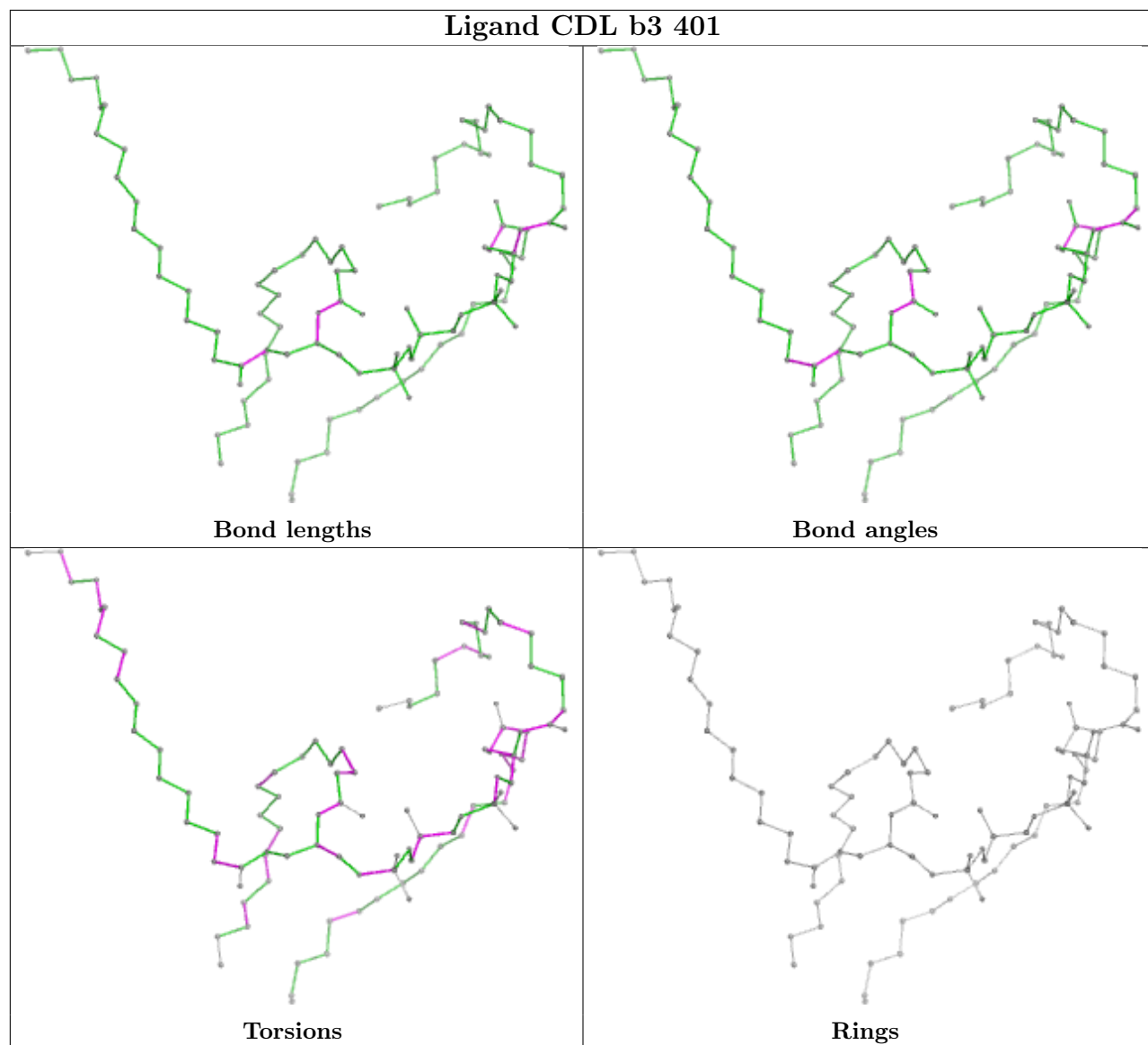


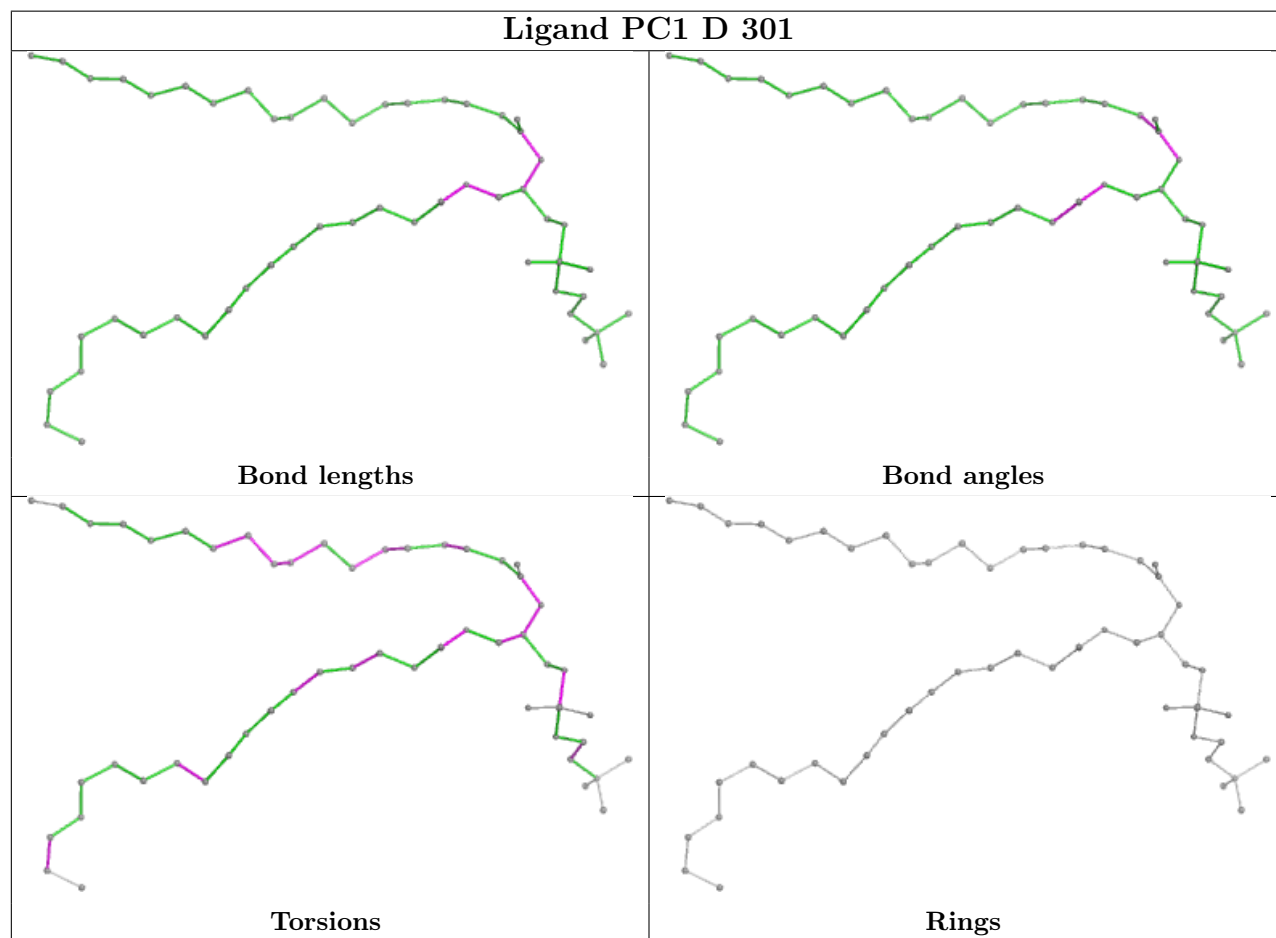
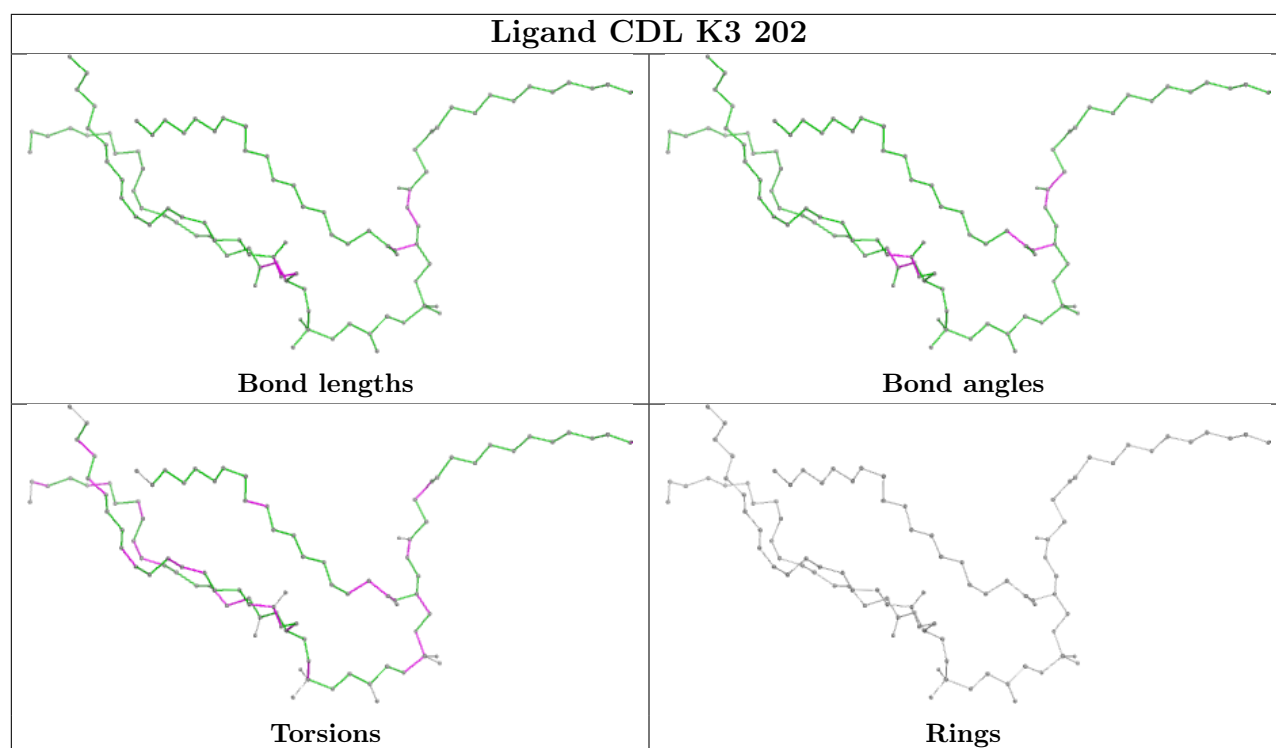


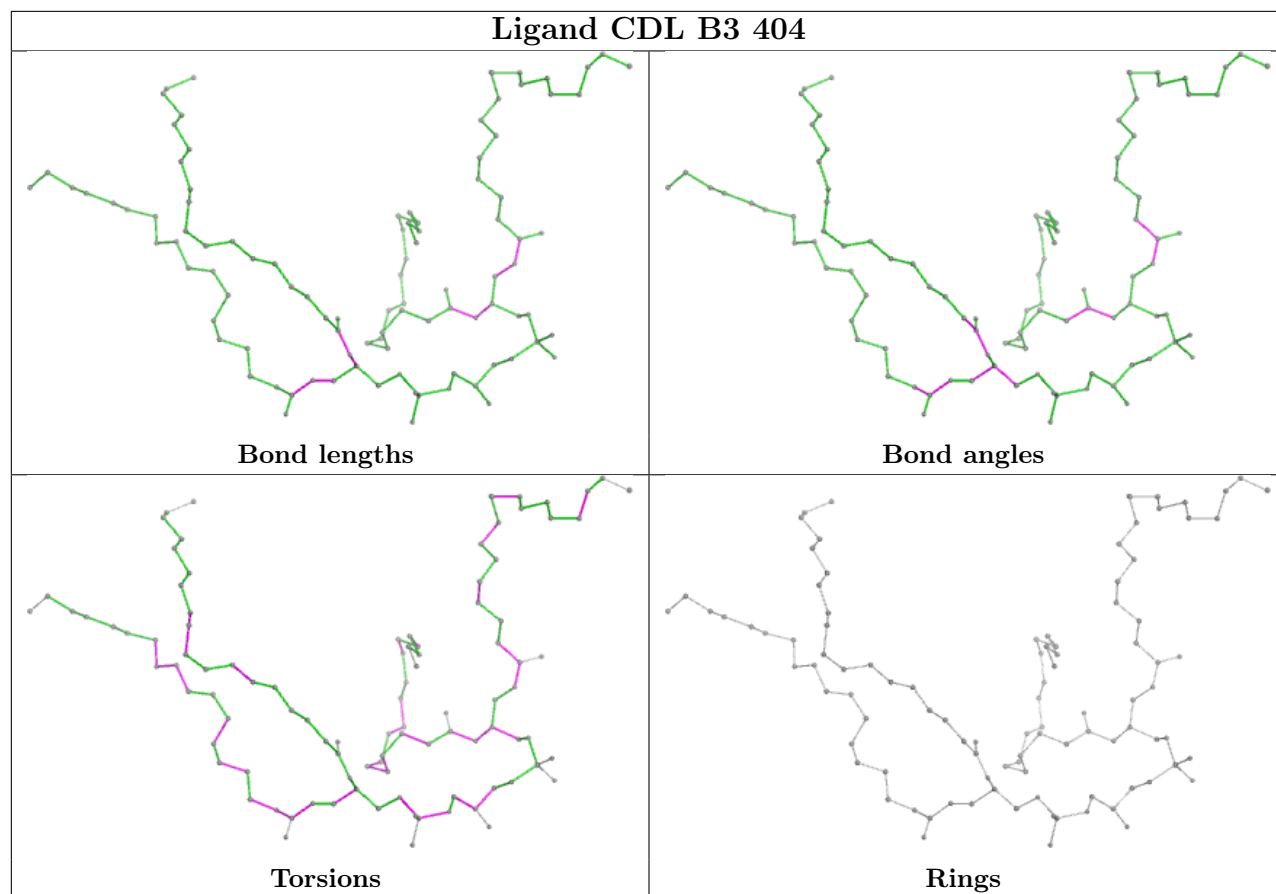


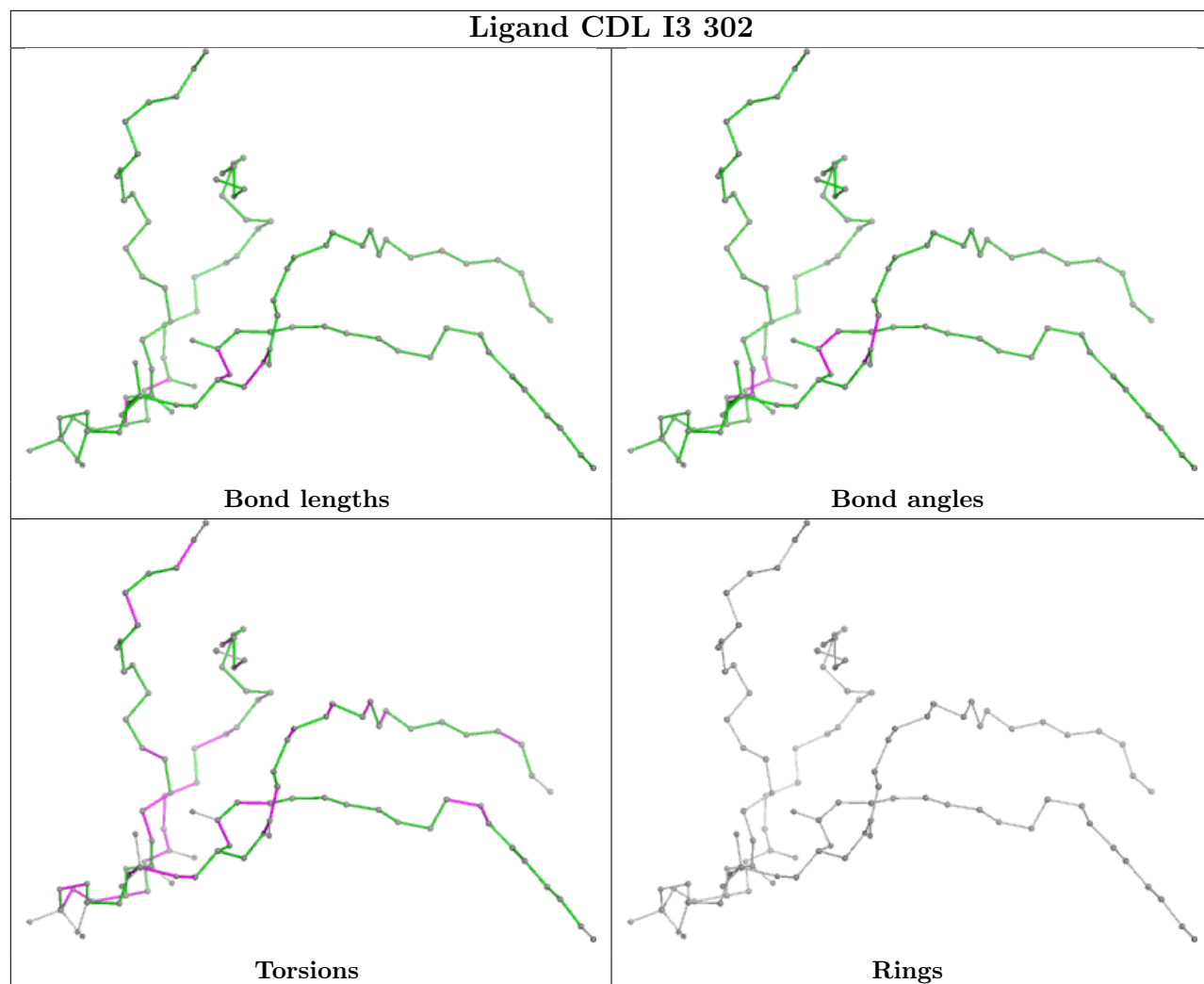


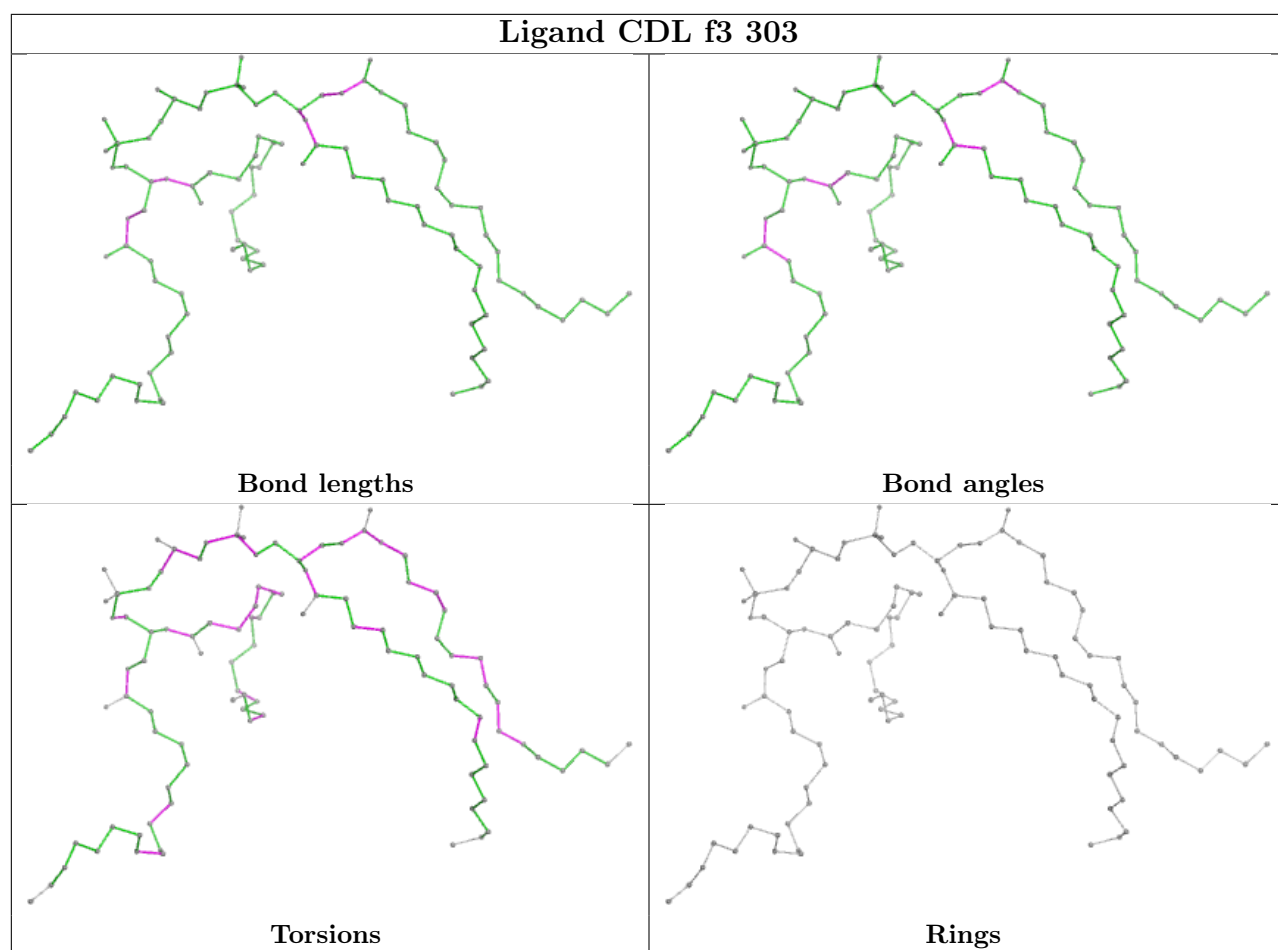


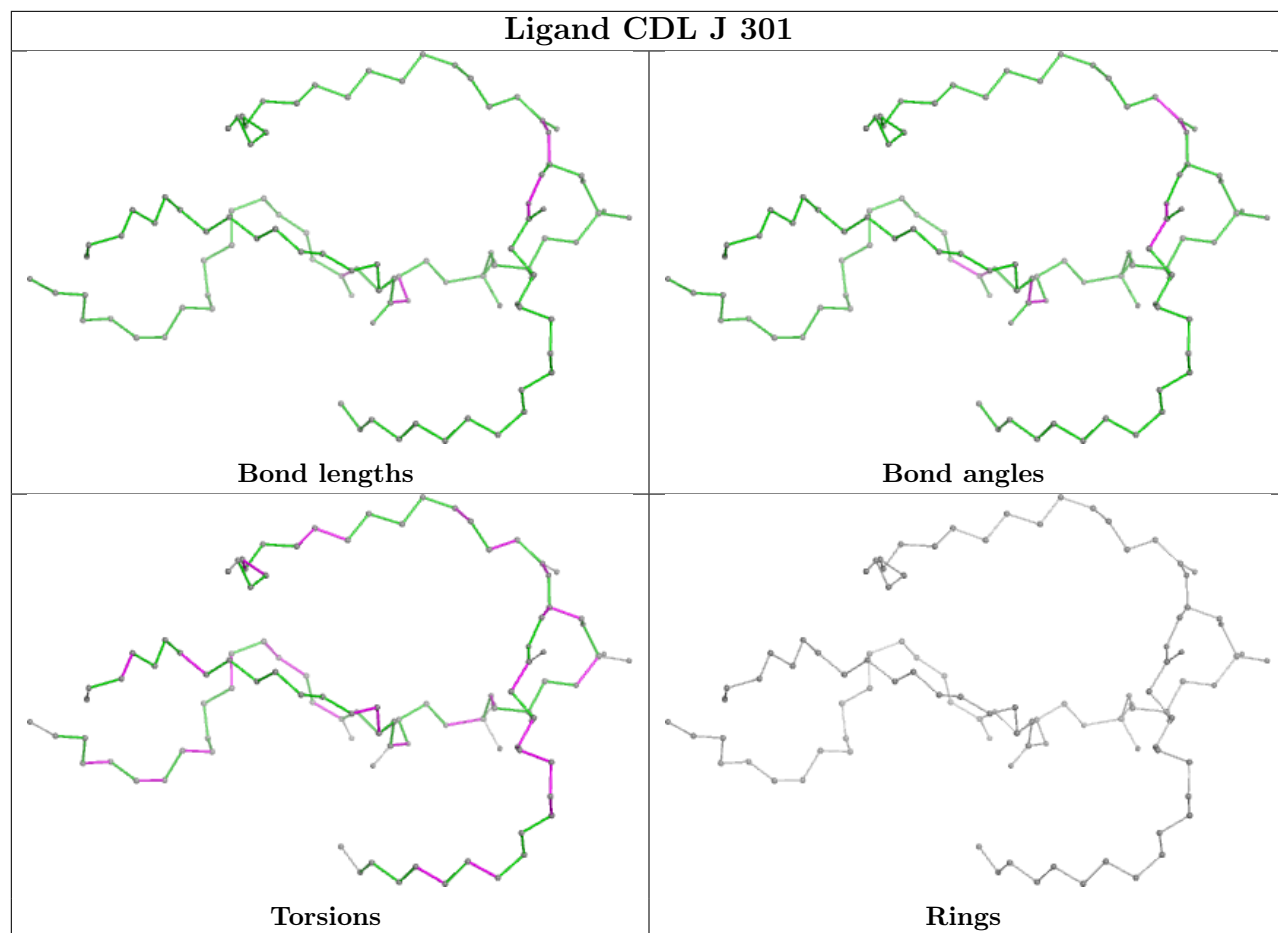


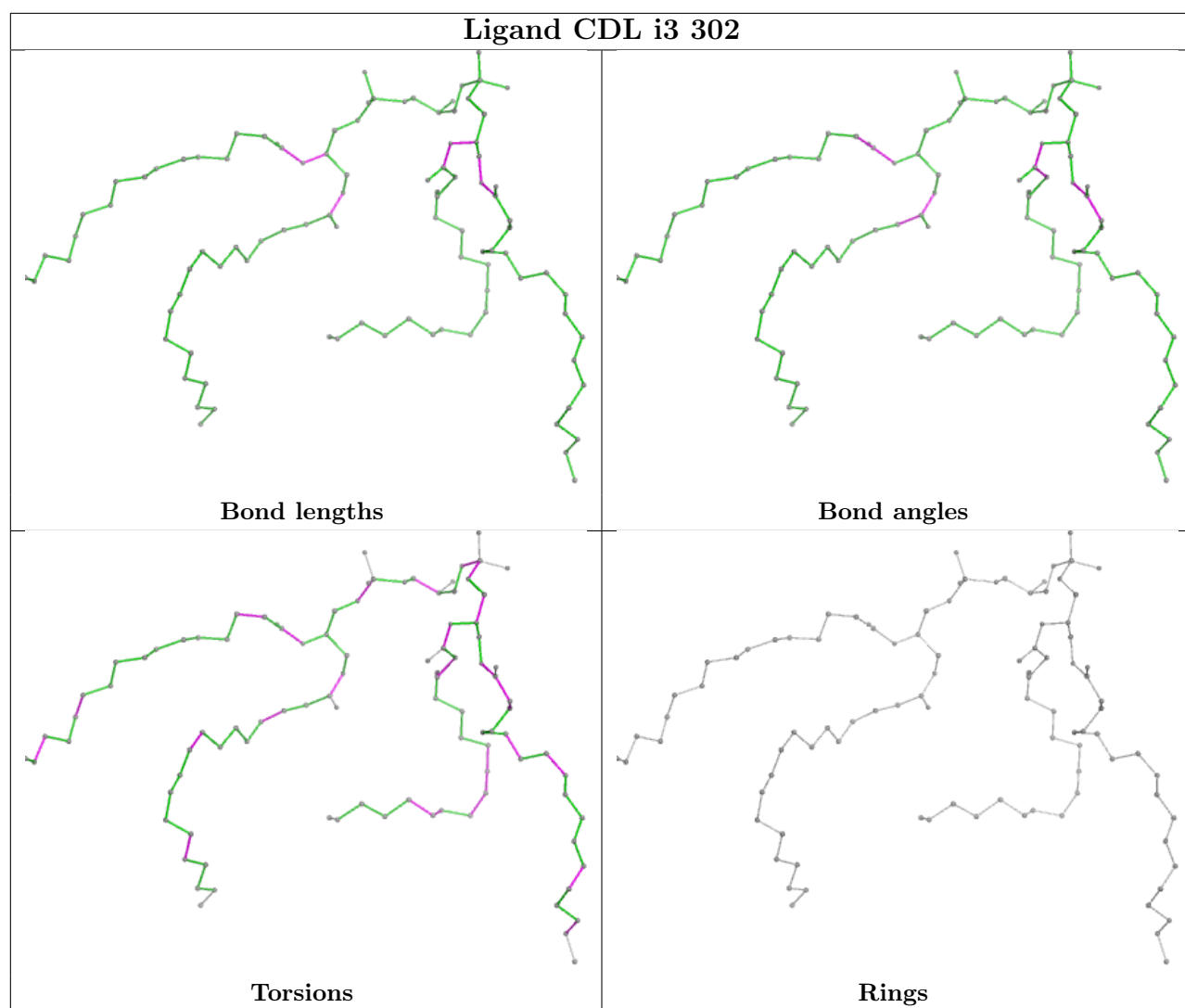


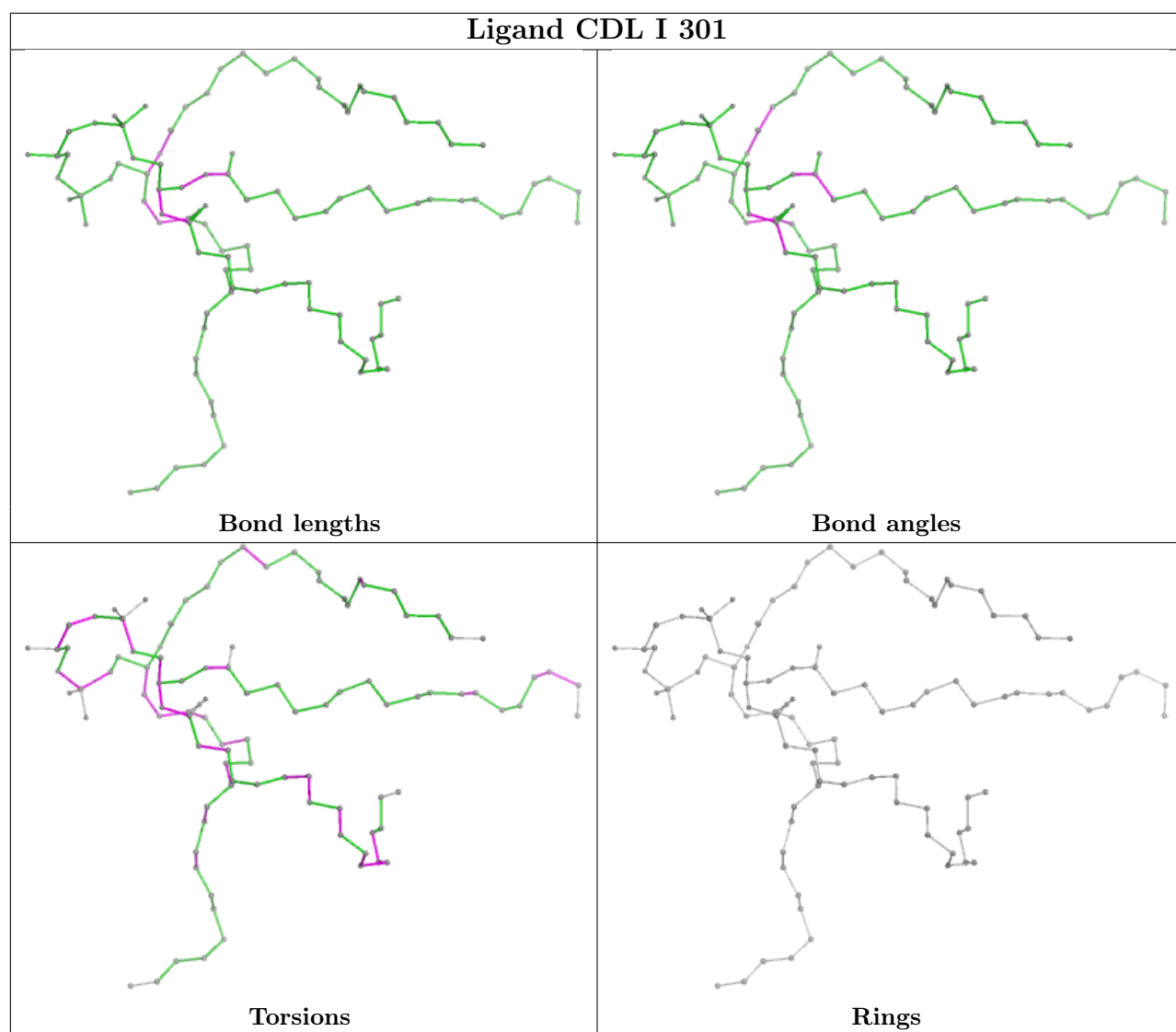


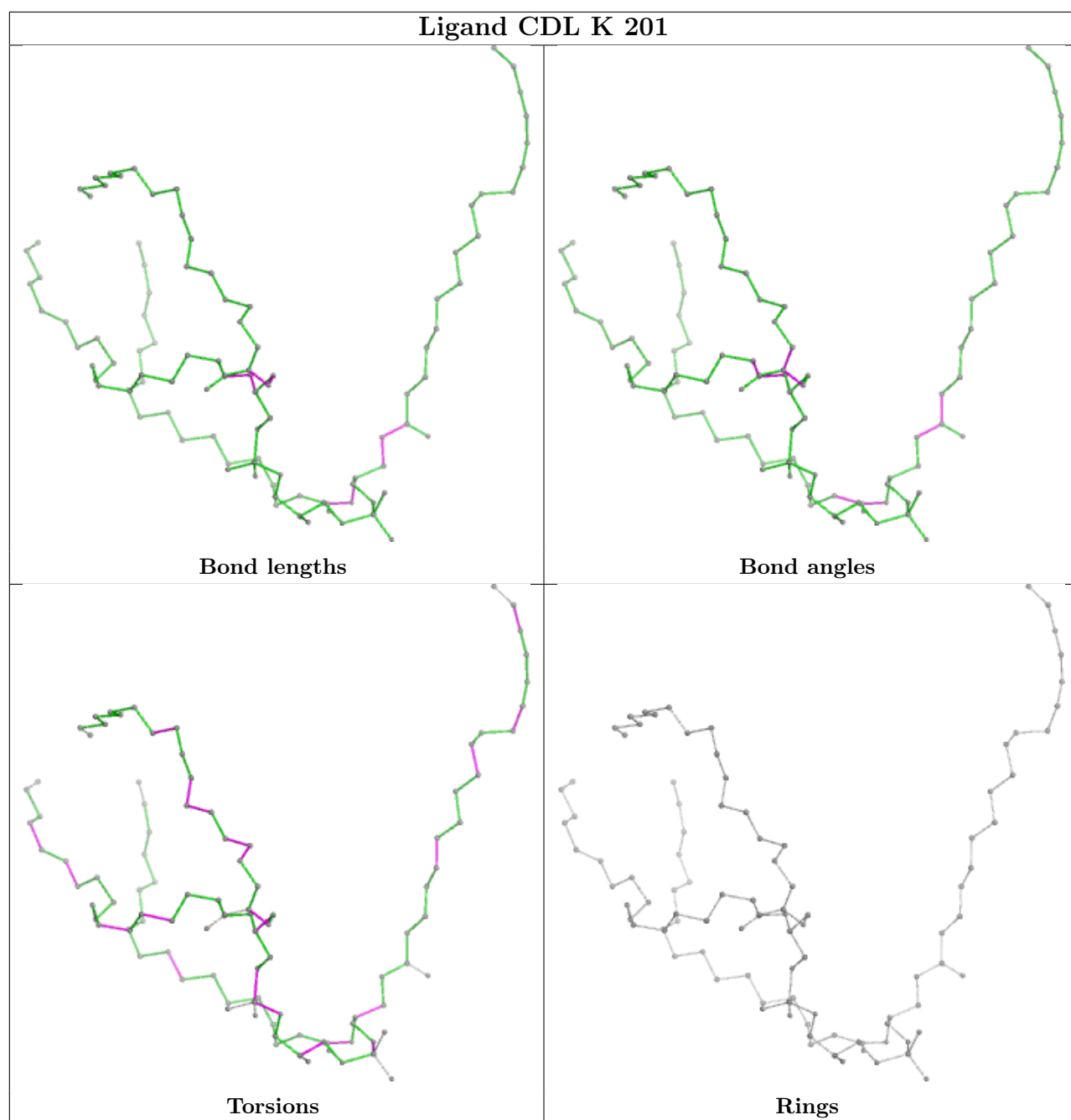


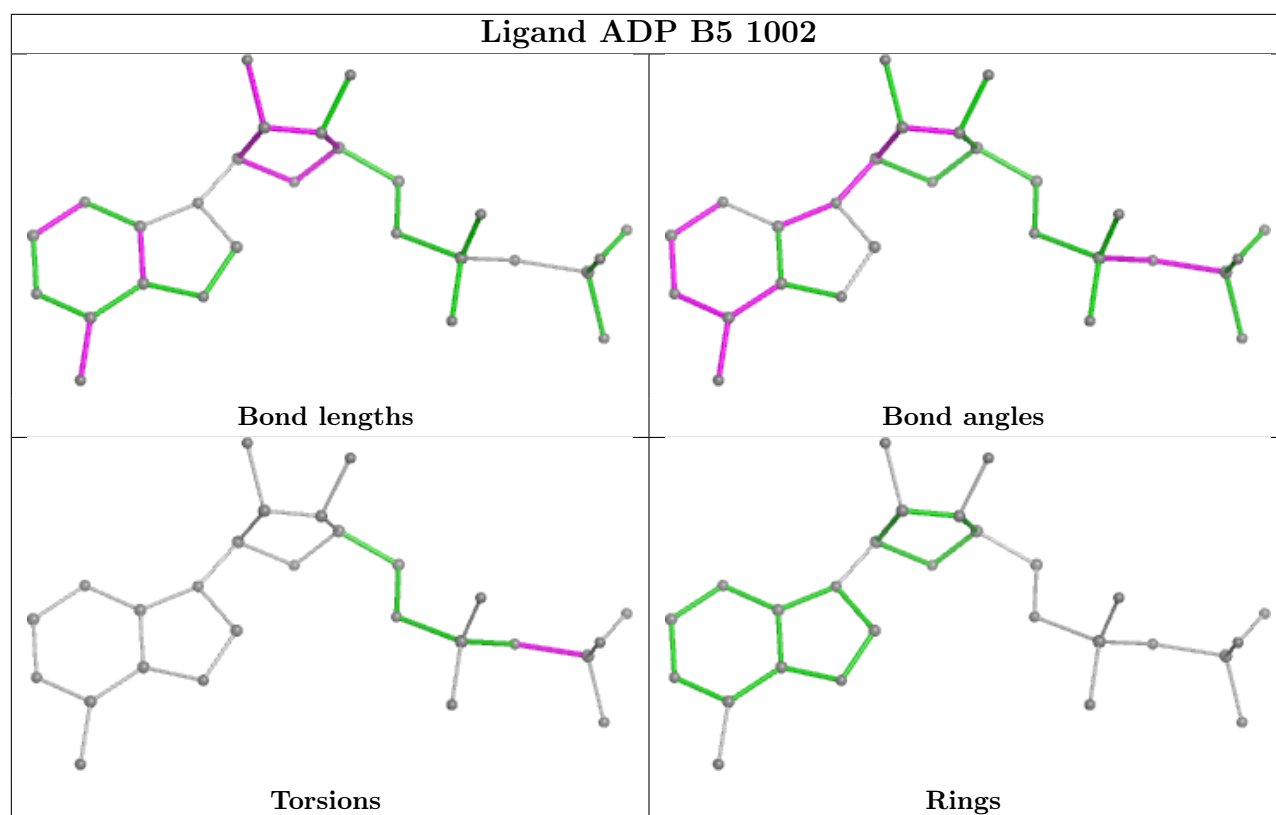


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5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

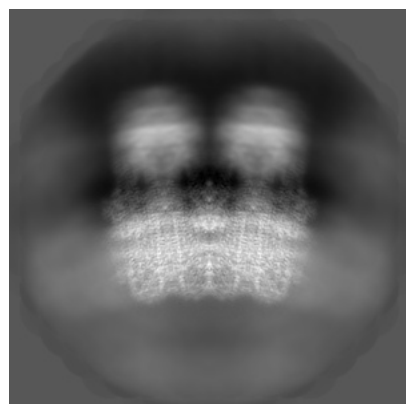
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10861. These allow visual inspection of the internal detail of the map and identification of artifacts.

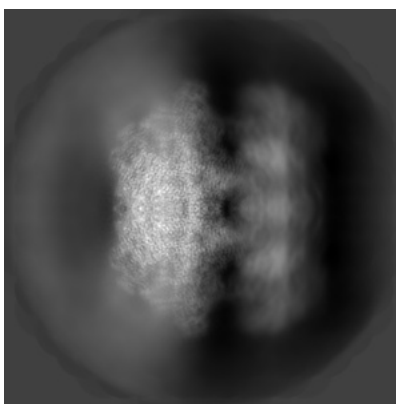
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

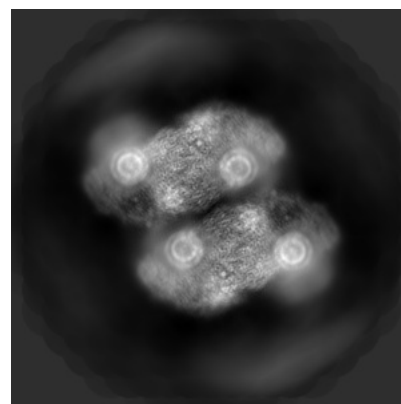
6.1.1 Primary map



X

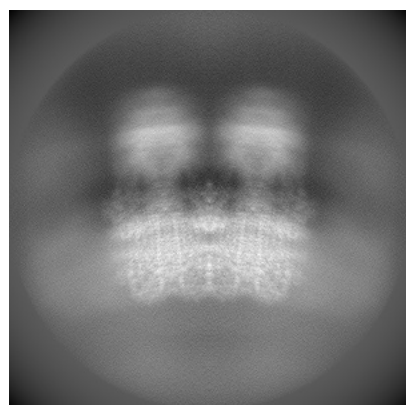


Y

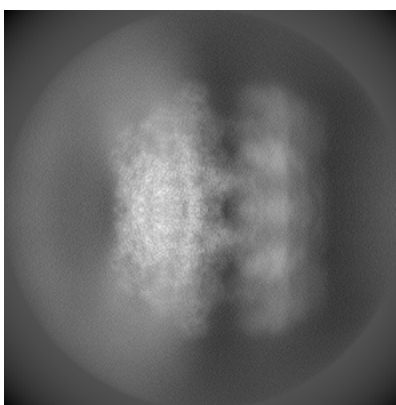


Z

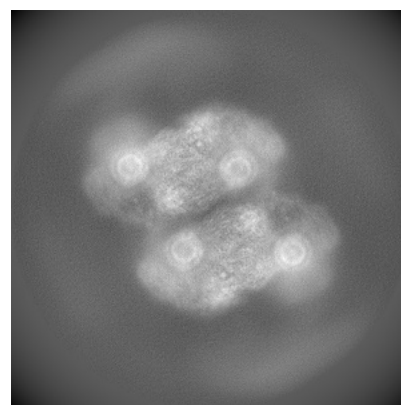
6.1.2 Raw map



X



Y

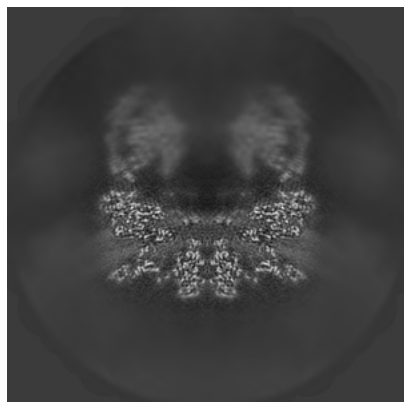


Z

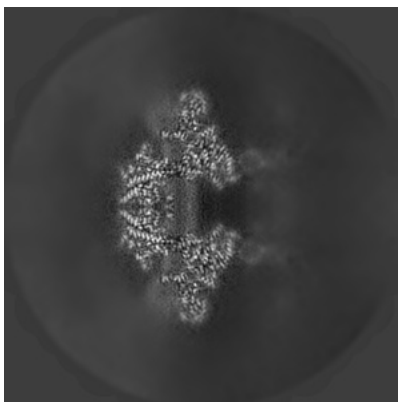
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

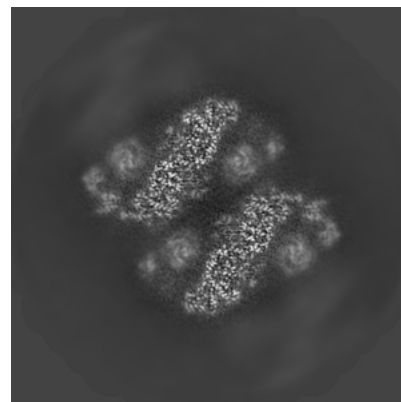
6.2.1 Primary map



X Index: 300

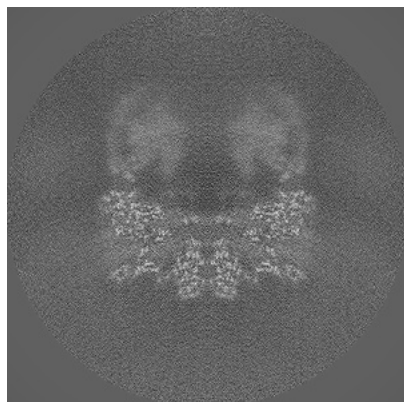


Y Index: 300

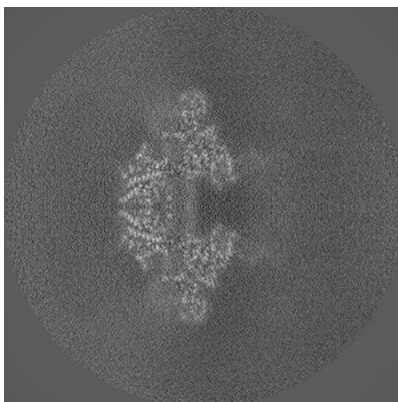


Z Index: 300

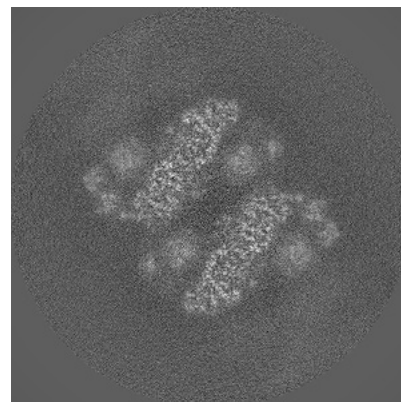
6.2.2 Raw map



X Index: 300



Y Index: 300

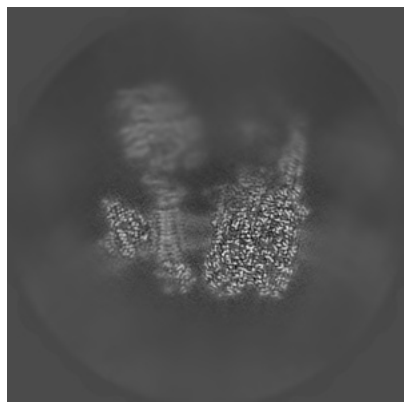


Z Index: 300

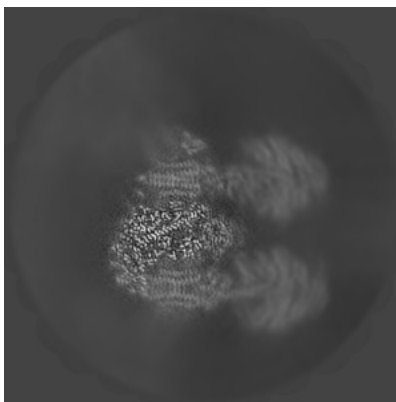
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

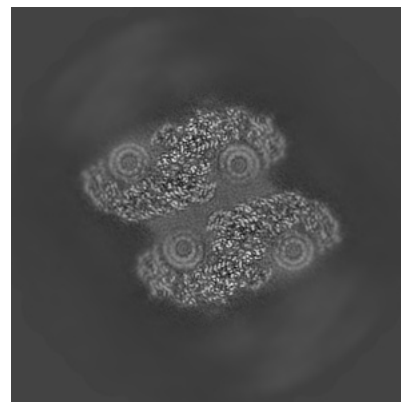
6.3.1 Primary map



X Index: 275

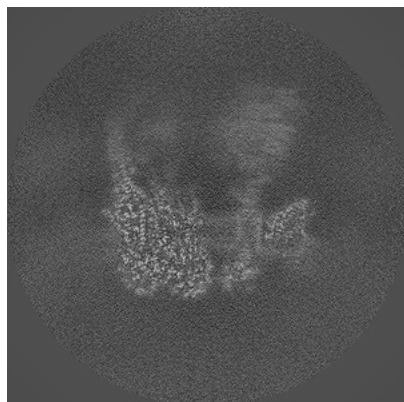


Y Index: 376

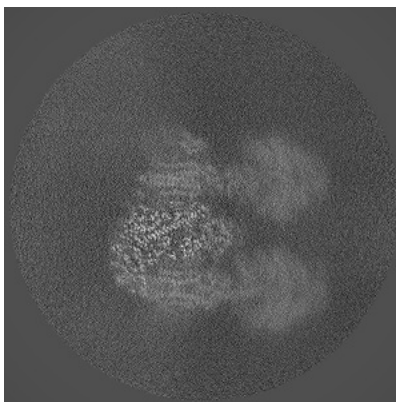


Z Index: 278

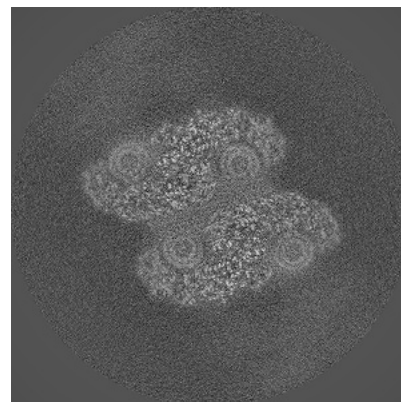
6.3.2 Raw map



X Index: 320



Y Index: 376

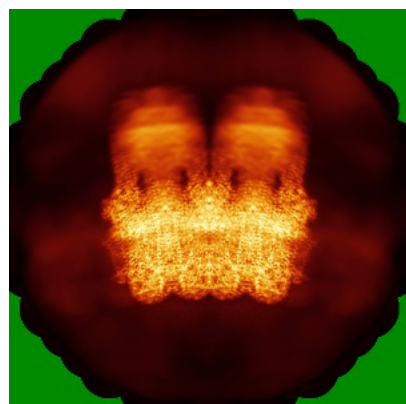


Z Index: 278

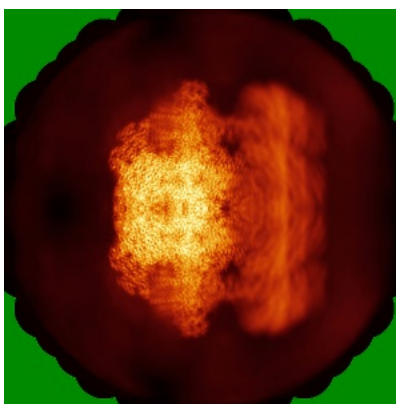
The images above show the largest variance slices of the map in three orthogonal directions.

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

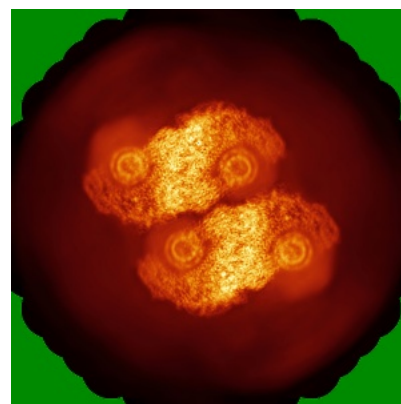
6.4.1 Primary map



X

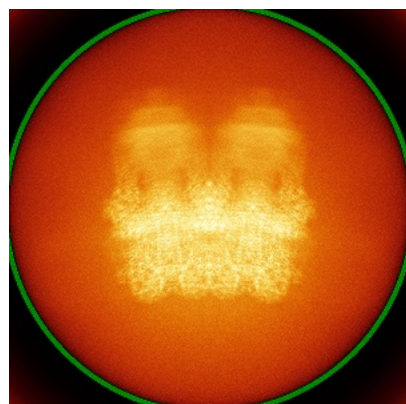


Y

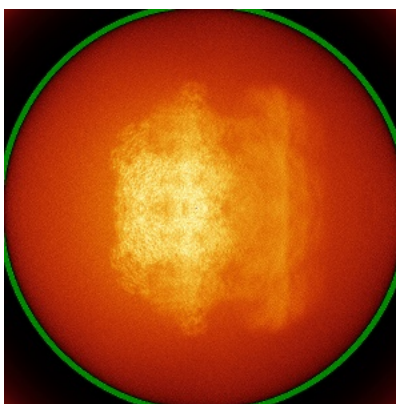


Z

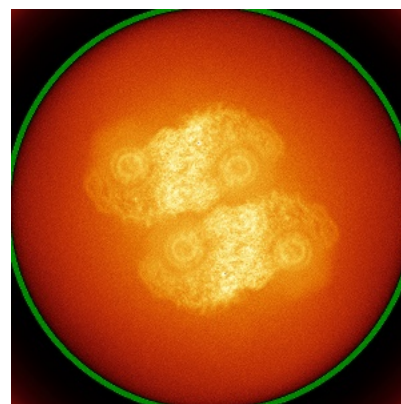
6.4.2 Raw map



X



Y



Z

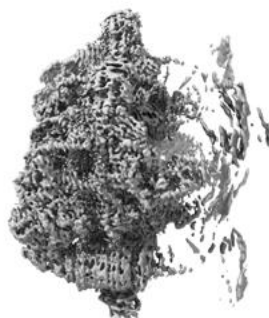
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

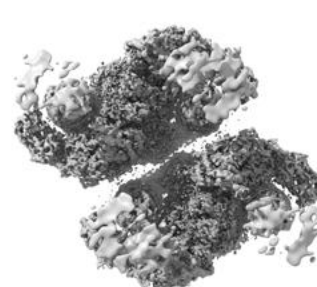
6.5.1 Primary map



X



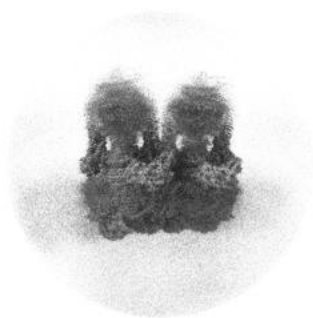
Y



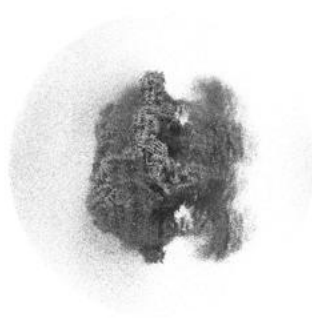
Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

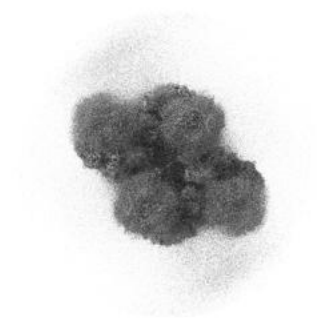
6.5.2 Raw map



X



Y



Z

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

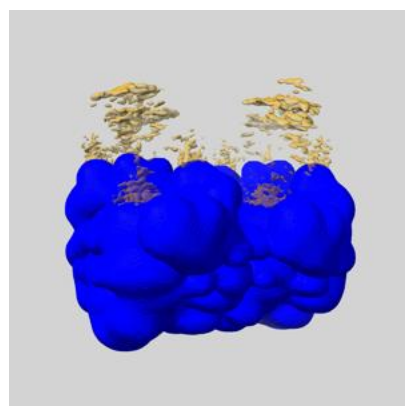
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

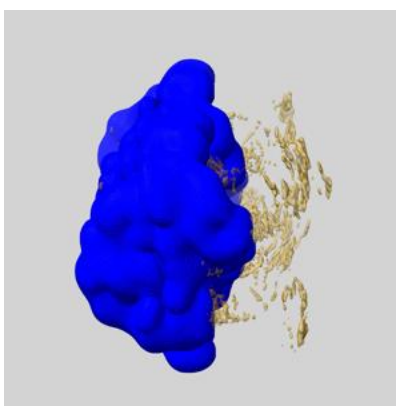
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

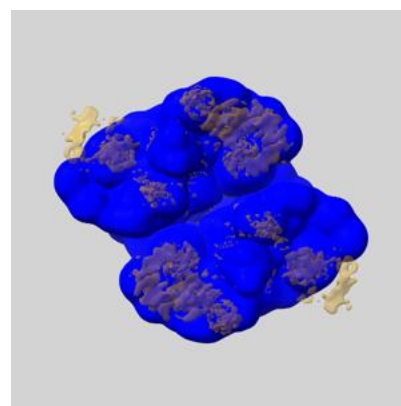
6.6.1 emd_10861_msk_1.map [i](#)



X



Y

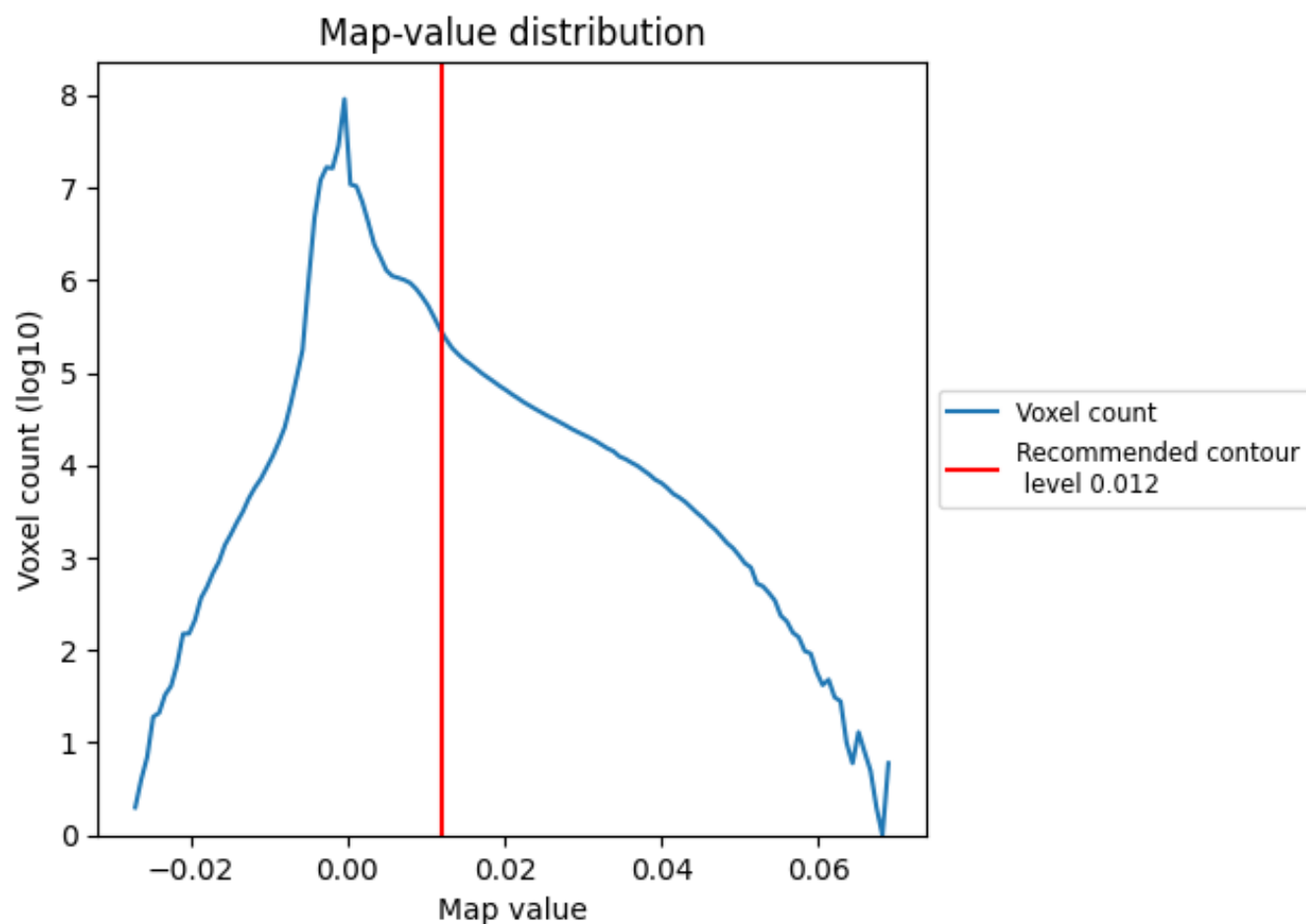


Z

7 Map analysis [i](#)

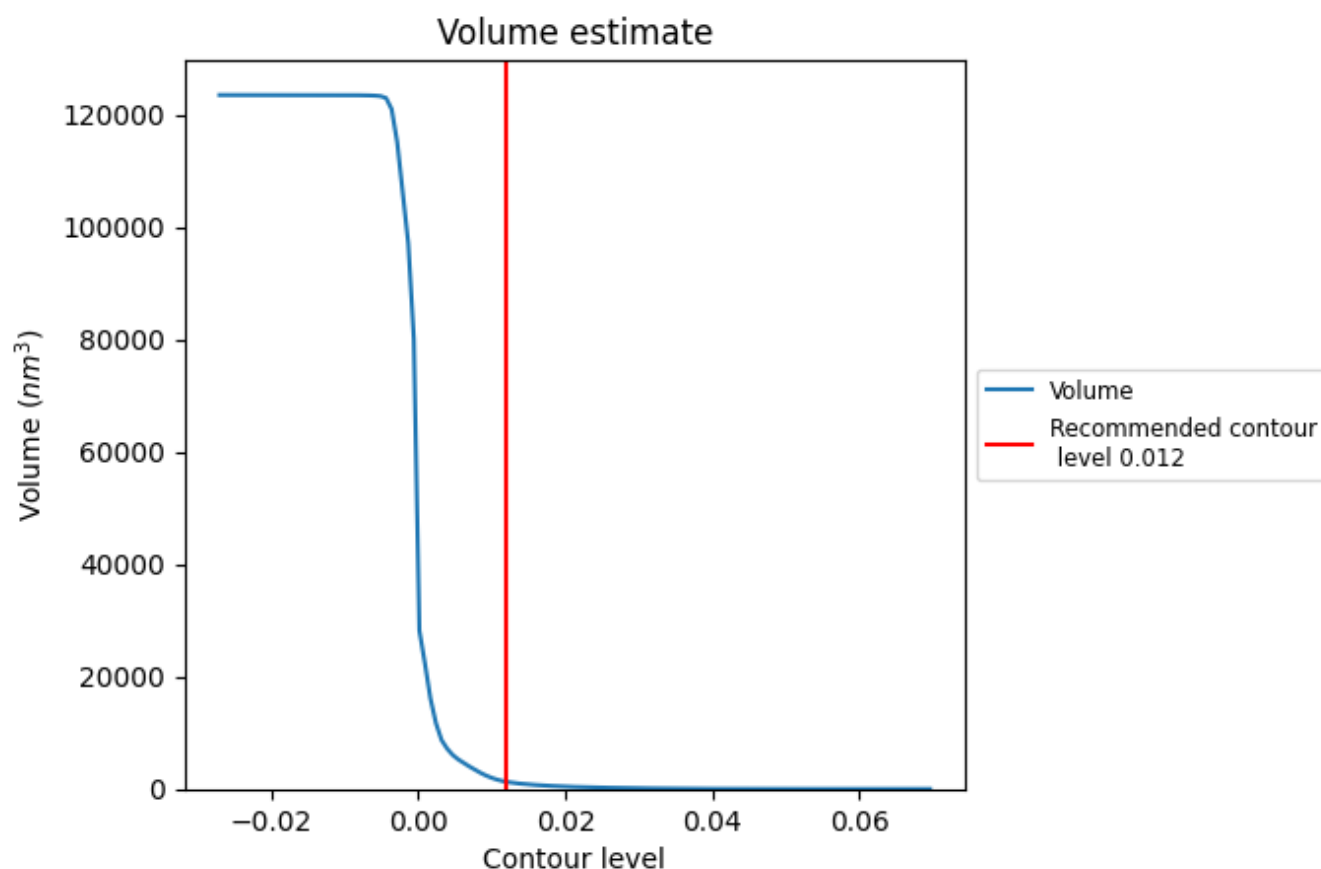
This section contains the results of statistical analysis of the map.

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.

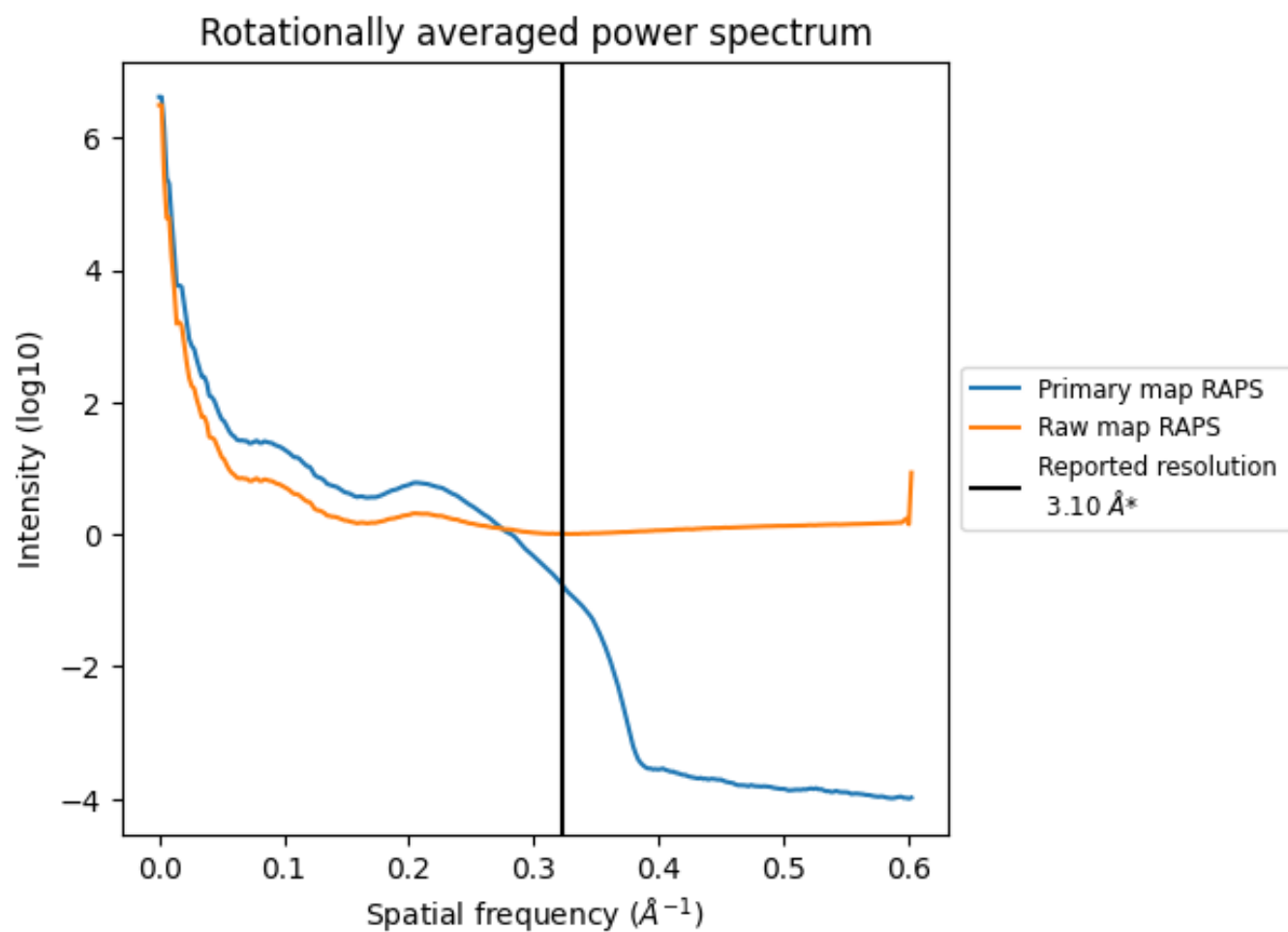
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1280 nm³; this corresponds to an approximate mass of 1157 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 ⓘ

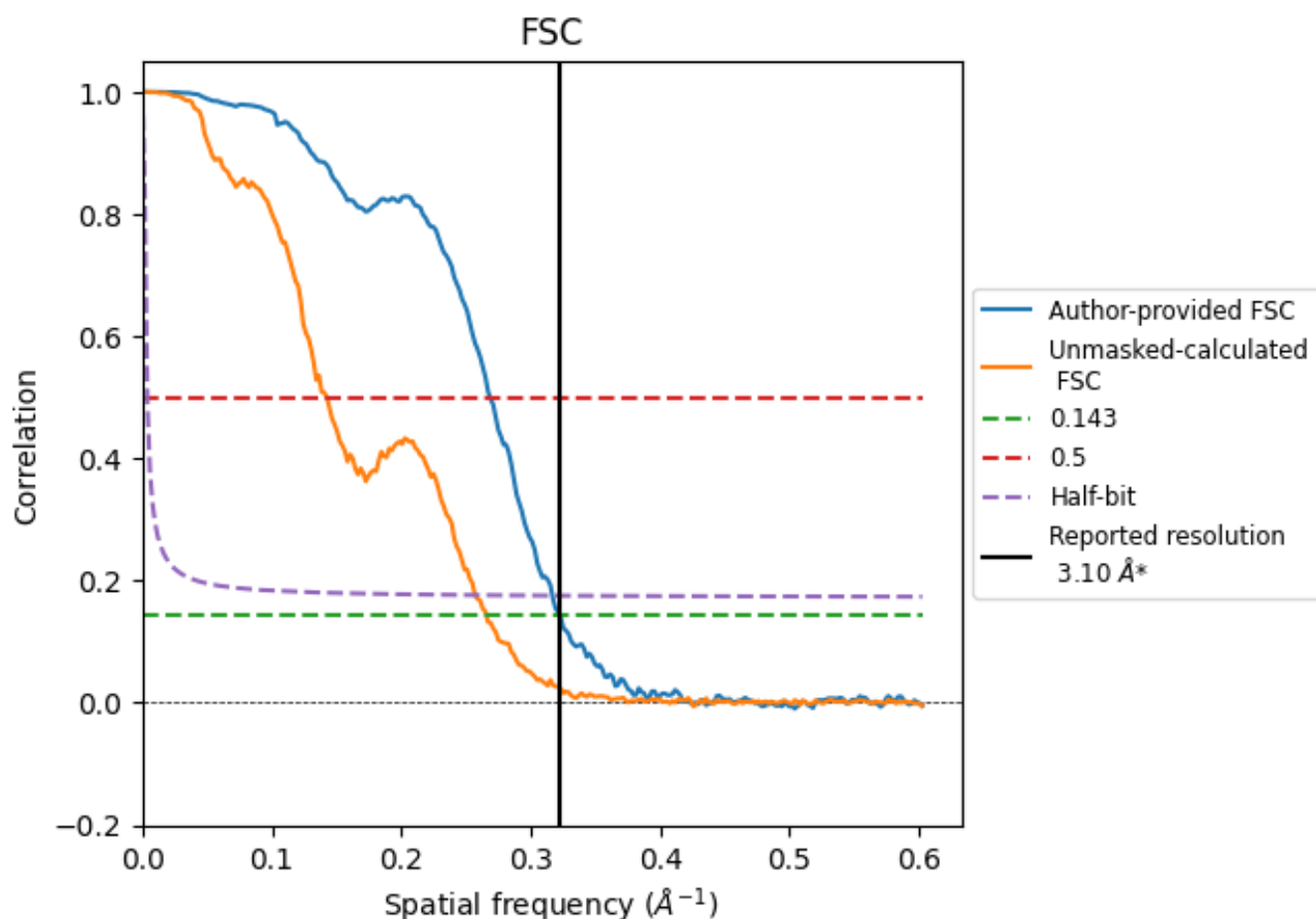


*Reported resolution corresponds to spatial frequency of 0.323 \AA^{-1}

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 0.323 \AA^{-1}

8.2 Resolution estimates [i](#)

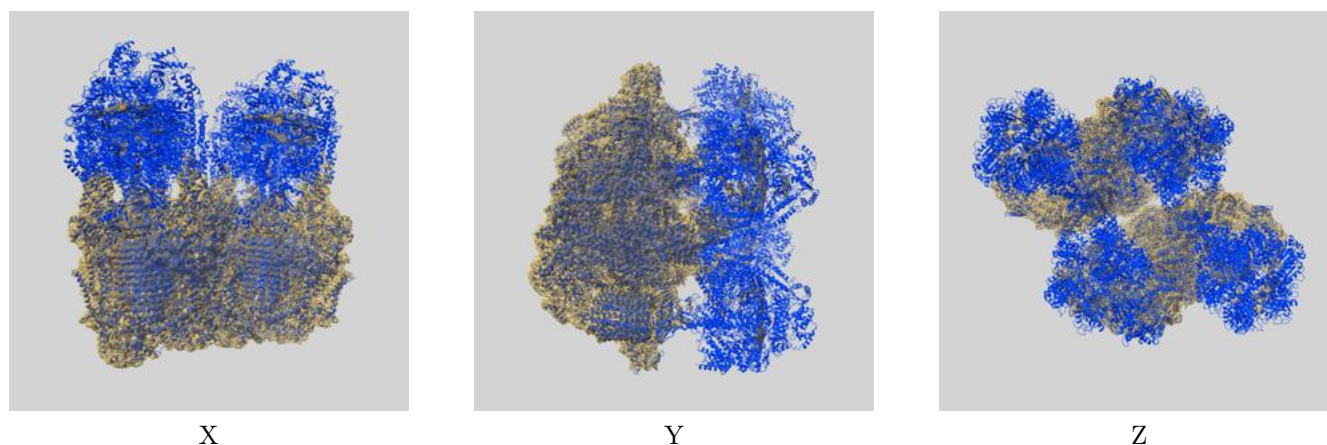
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.10 | - | - |
| Author-provided FSC curve | 3.10 | 3.72 | 3.16 |
| Unmasked-calculated* | 3.76 | 7.01 | 3.89 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.76 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

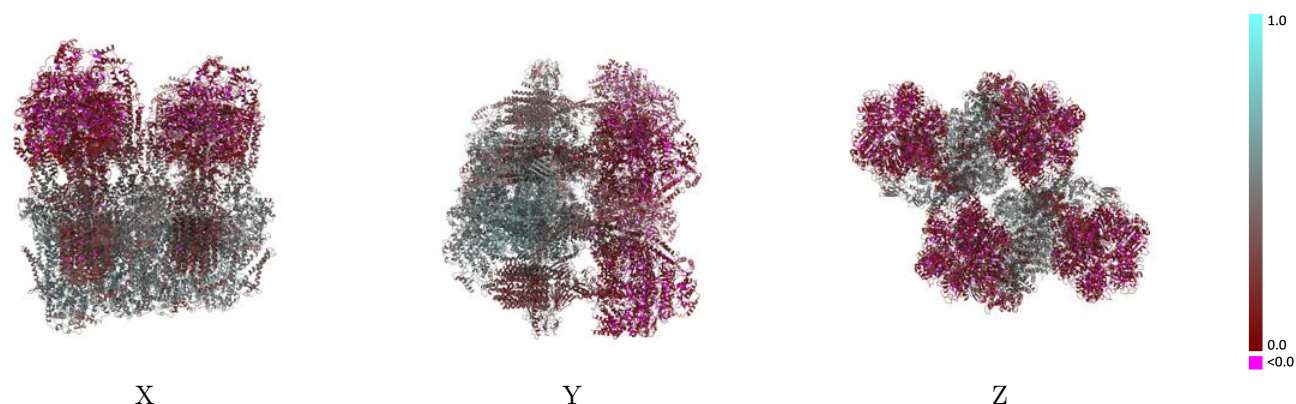
This section contains information regarding the fit between EMDB map EMD-10861 and PDB model 6YNZ. Per-residue inclusion information can be found in section [3](#) on page [32](#).

9.1 Map-model overlay [i](#)



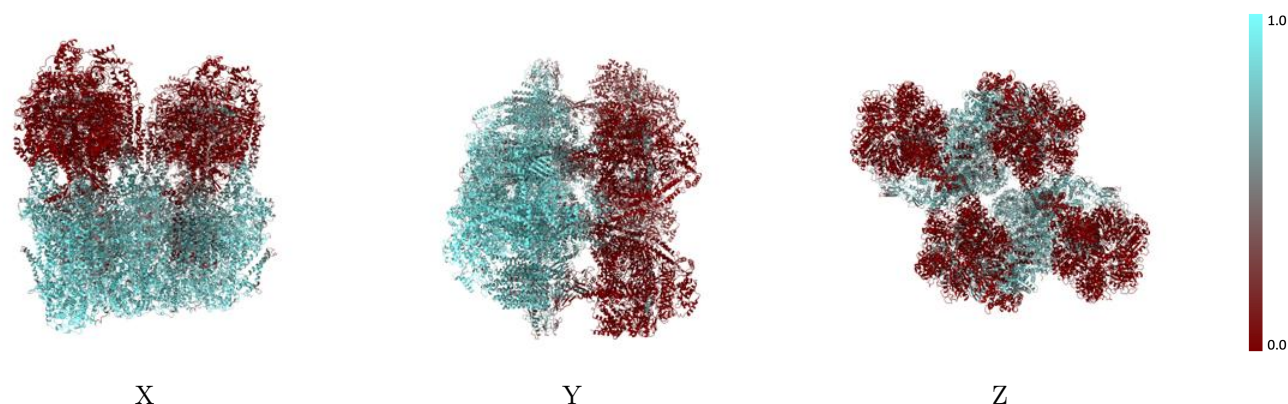
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



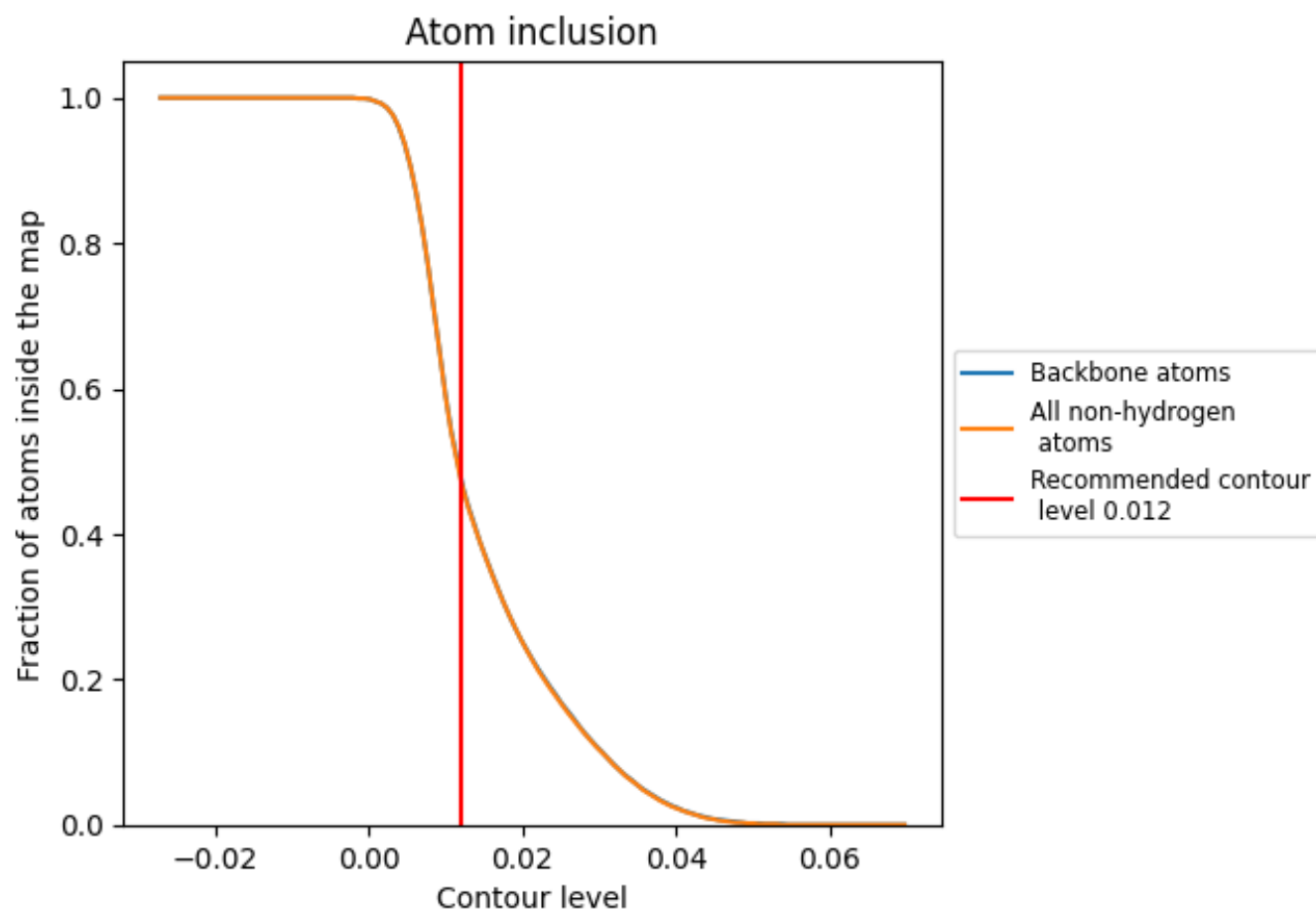
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 48% of all backbone atoms, 47% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|----------------|---------|
| All | 0.4740 | 0.3170 |
| A | 0.8900 | 0.5390 |
| A1 | 0.1400 | 0.1480 |
| A2 | 0.0490 | 0.1350 |
| A3 | 0.8860 | 0.5350 |
| A4 | 0.0500 | 0.1360 |
| A5 | 0.1440 | 0.1460 |
| B | 0.4990 | 0.3720 |
| B1 | 0.0720 | 0.1030 |
| B2 | 0.0260 | 0.0960 |
| B3 | 0.4380 | 0.3590 |
| B4 | 0.0260 | 0.0910 |
| B5 | 0.0750 | 0.1090 |
| C | 0.9210 | 0.5390 |
| C1 | 0.0110 | 0.1020 |
| C2 | 0.0100 | 0.0850 |
| C3 | 0.9010 | 0.5170 |
| C4 | 0.0100 | 0.0910 |
| C5 | 0.0110 | 0.0980 |
| D | 0.6370 | 0.4190 |
| D1 | 0.0110 | 0.1130 |
| D2 | 0.0140 | 0.1060 |
| D3 | 0.5740 | 0.4000 |
| D4 | 0.0150 | 0.1120 |
| D5 | 0.0110 | 0.1070 |
| E | 0.6940 | 0.3810 |
| E1 | 0.0850 | 0.1090 |
| E2 | 0.0070 | 0.0990 |
| E3 | 0.5910 | 0.3760 |
| E4 | 0.0060 | 0.0930 |
| E5 | 0.0840 | 0.1120 |
| F | 0.8620 | 0.5330 |
| F1 | 0.0330 | 0.1050 |
| F2 | 0.0300 | 0.0930 |
| F3 | 0.8620 | 0.5410 |























































































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| Chain | Atom inclusion | Q-score |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| F4 |  0.0270 |  0.0900 |
| F5 |  0.0340 |  0.1070 |
| G |  0.8260 |  0.4910 |
| G1 |  0.0000 |  0.1100 |
| G2 |  0.0000 |  0.1040 |
| G3 |  0.7570 |  0.4600 |
| G4 |  0.0000 |  0.1020 |
| G5 |  0.0000 |  0.1110 |
| H |  0.8440 |  0.4920 |
| H1 |  0.7070 |  0.3200 |
| H2 |  0.7480 |  0.3540 |
| H3 |  0.7470 |  0.4600 |
| H4 |  0.7370 |  0.3510 |
| H5 |  0.7070 |  0.3140 |
| I |  0.8520 |  0.5090 |
| I1 |  0.6670 |  0.3080 |
| I2 |  0.7480 |  0.3210 |
| I3 |  0.7920 |  0.4940 |
| I4 |  0.7480 |  0.3170 |
| I5 |  0.6640 |  0.3040 |
| J |  0.8320 |  0.4970 |
| J1 |  0.5780 |  0.3010 |
| J2 |  0.7500 |  0.3050 |
| J3 |  0.8030 |  0.4820 |
| J4 |  0.7420 |  0.3020 |
| J5 |  0.5730 |  0.3020 |
| K |  0.7860 |  0.4370 |
| K1 |  0.5560 |  0.2960 |
| K2 |  0.6910 |  0.2760 |
| K3 |  0.7690 |  0.4430 |
| K4 |  0.6960 |  0.2740 |
| K5 |  0.5510 |  0.2980 |
| L |  0.8910 |  0.5260 |
| L1 |  0.5580 |  0.3000 |
| L2 |  0.7080 |  0.2540 |
| L3 |  0.8580 |  0.5160 |
| L4 |  0.7000 |  0.2520 |
| L5 |  0.5730 |  0.3000 |
| M |  0.9330 |  0.5270 |
| M1 |  0.6370 |  0.2900 |
| M2 |  0.7510 |  0.2800 |
| M3 |  0.9140 |  0.5170 |





















































































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| Chain | Atom inclusion | Q-score |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| M4 |  0.7580 |  0.2820 |
| M5 |  0.6350 |  0.2930 |
| N |  0.9300 |  0.5530 |
| N1 |  0.6210 |  0.2830 |
| N2 |  0.7460 |  0.2890 |
| N3 |  0.9090 |  0.5410 |
| N4 |  0.7530 |  0.2920 |
| N5 |  0.6230 |  0.2860 |
| O |  0.8700 |  0.4970 |
| O1 |  0.6400 |  0.2950 |
| O2 |  0.6960 |  0.2760 |
| O3 |  0.8960 |  0.4930 |
| O4 |  0.6920 |  0.2730 |
| O5 |  0.6420 |  0.2900 |
| P |  0.7080 |  0.4440 |
| P1 |  0.6820 |  0.3080 |
| P2 |  0.6800 |  0.3040 |
| P3 |  0.7280 |  0.4340 |
| P4 |  0.6780 |  0.3030 |
| P5 |  0.6890 |  0.3090 |
| Q |  0.7870 |  0.4740 |
| Q1 |  0.6800 |  0.3010 |
| Q2 |  0.7120 |  0.3370 |
| Q3 |  0.6750 |  0.4400 |
| Q4 |  0.7190 |  0.3330 |
| Q5 |  0.6670 |  0.3010 |
| R |  0.8680 |  0.5130 |
| R3 |  0.8260 |  0.5040 |
| S |  0.7340 |  0.4300 |
| S3 |  0.6440 |  0.4040 |
| a |  0.8850 |  0.5360 |
| a3 |  0.8680 |  0.5290 |
| b |  0.4400 |  0.3580 |
| b3 |  0.5050 |  0.3720 |
| c |  0.8960 |  0.5180 |
| c3 |  0.9180 |  0.5400 |
| d |  0.5720 |  0.3980 |
| d1 |  0.2940 |  0.2560 |
| d2 |  0.3590 |  0.2310 |
| d3 |  0.6370 |  0.4210 |
| d4 |  0.3510 |  0.2340 |
| d5 |  0.2900 |  0.2610 |





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| Chain | Atom inclusion | Q-score |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| e |  0.5840 |  0.3730 |
| e1 |  0.2350 |  0.2080 |
| e2 |  0.2600 |  0.2250 |
| e3 |  0.6960 |  0.3810 |
| e4 |  0.2630 |  0.2310 |
| e5 |  0.2270 |  0.2020 |
| f |  0.7670 |  0.5250 |
| f3 |  0.8120 |  0.5360 |
| g |  0.7460 |  0.4620 |
| g1 |  0.1590 |  0.2070 |
| g2 |  0.1950 |  0.2080 |
| g3 |  0.8180 |  0.4890 |
| g4 |  0.1970 |  0.2050 |
| g5 |  0.1610 |  0.2050 |
| h |  0.7220 |  0.4690 |
| h3 |  0.8190 |  0.5010 |
| i |  0.8250 |  0.4940 |
| i1 |  0.0400 |  0.1780 |
| i2 |  0.0700 |  0.1820 |
| i3 |  0.8470 |  0.5160 |
| i4 |  0.0910 |  0.2000 |
| i5 |  0.0300 |  0.1910 |
| j |  0.8010 |  0.4810 |
| j3 |  0.8380 |  0.4910 |
| k |  0.7840 |  0.4400 |
| k3 |  0.7920 |  0.4370 |
| l |  0.8520 |  0.5170 |
| l3 |  0.8930 |  0.5230 |
| m |  0.9040 |  0.5140 |
| m3 |  0.9320 |  0.5230 |
| n |  0.9070 |  0.5410 |
| n3 |  0.9280 |  0.5530 |
| o |  0.8960 |  0.4970 |
| o3 |  0.8580 |  0.4950 |
| p |  0.7170 |  0.4310 |
| p3 |  0.7090 |  0.4430 |
| q |  0.6780 |  0.4440 |
| q3 |  0.7860 |  0.4720 |
| r |  0.7860 |  0.4940 |
| r3 |  0.8700 |  0.5200 |
| s |  0.5440 |  0.3940 |
| s3 |  0.7000 |  0.4300 |

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| Chain | Atom inclusion | Q-score |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| t |  0.5330 |  0.3790 |
| t3 |  0.6050 |  0.4000 |