



## Full wwPDB EM Validation Report ⓘ

Dec 31, 2024 – 10:20 PM EST

PDB ID : 8Q1Y  
EMDB ID : EMD-18068  
Title : Outward-facing, open2 proteoliposome complex I at 2.6 Å, after deactivation treatment. Initially purified in LMNG.  
Authors : Grba, D.N.; Hirst, J.  
Deposited on : 2023-08-01  
Resolution : 2.60 Å(reported)  
Based on initial model : 7QSN

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

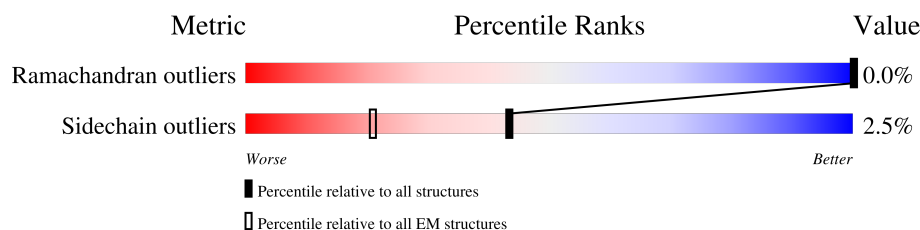
EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.60 Å.

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



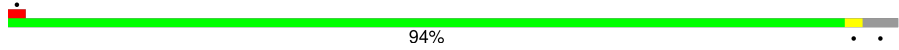
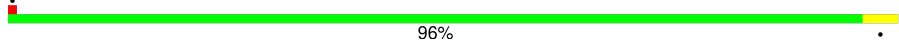
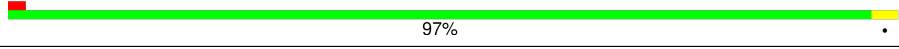
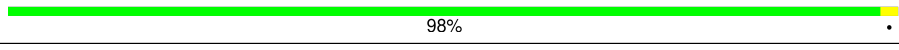
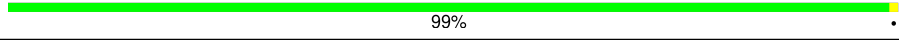
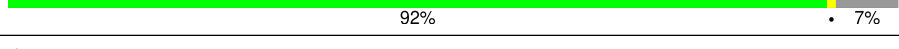
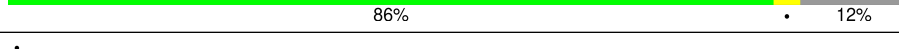
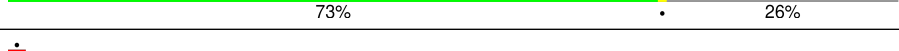
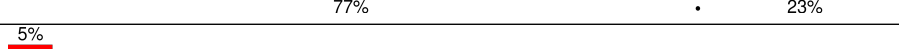
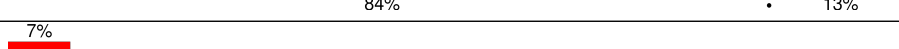
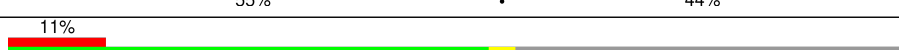

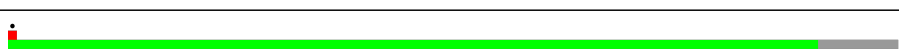
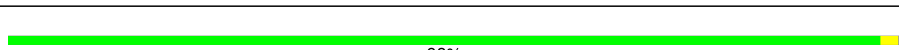
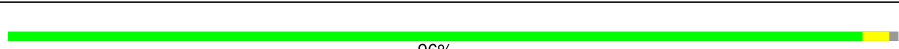
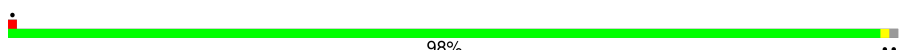

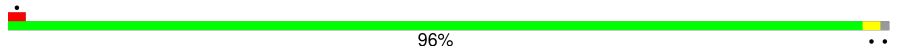

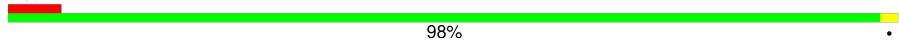
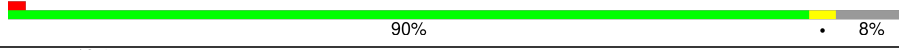
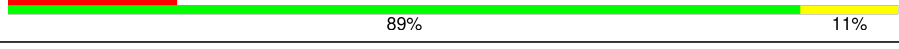



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Ramachandran outliers | 207382                      | 16835                       |
| Sidechain outliers    | 206894                      | 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 115    |                  |
| 2   | B     | 216    |                  |
| 3   | C     | 266    |                  |
| 4   | D     | 463    |                  |
| 5   | E     | 249    |                  |
| 6   | F     | 464    |                  |
| 7   | G     | 727    |                  |
| 8   | H     | 318    |                  |
| 9   | I     | 212    |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 10  | J     | 175    |    |
| 11  | K     | 98     |    |
| 12  | L     | 606    |    |
| 13  | M     | 459    |    |
| 14  | N     | 347    |    |
| 15  | O     | 343    |    |
| 16  | P     | 380    |    |
| 17  | Q     | 175    |    |
| 18  | R     | 124    |    |
| 19  | S     | 99     |    |
| 20  | T     | 156    |    |
| 20  | U     | 156    |  |
| 21  | V     | 116    |  |
| 22  | W     | 128    |  |
| 23  | X     | 172    |  |
| 24  | Y     | 141    |  |
| 25  | Z     | 144    |  |
| 26  | a     | 70     |  |
| 27  | b     | 84     |  |
| 28  | c     | 76     |  |
| 29  | d     | 120    |  |
| 30  | e     | 106    |  |
| 31  | f     | 57     |  |
| 32  | g     | 154    |  |
| 33  | h     | 189    |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 34  | i     | 128    |                  |
| 35  | j     | 108    |                  |
| 36  | k     | 98     |                  |
| 37  | l     | 186    |                  |
| 38  | m     | 129    |                  |
| 39  | n     | 179    |                  |
| 40  | o     | 137    |                  |
| 41  | p     | 176    |                  |
| 42  | q     | 145    |                  |
| 43  | r     | 113    |                  |
| 44  | s     | 109    |                  |

## 2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 69324 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | A     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 815   | 555 | 116 | 139 | 5 |         |       |

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 2   | B     | 156      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1247  | 795 | 225 | 213 | 14 |         |       |

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | C     | 207      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1721  | 1111 | 296 | 311 | 3 |         |       |

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | D     | 417      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3364  | 2151 | 577 | 611 | 25 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| D     | 129     | ARG      | GLN    | variant | UNP P17694 |

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | E     | 214      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1659  | 1059 | 278 | 312 | 10 |         |       |

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6   | F     | 432      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3326  | 2096 | 594 | 616 | 20 |         |       |

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 7   | G     | 691      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5298  | 3318 | 925 | 1016 | 39 |         |       |

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 8   | H     | 316      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2496  | 1673 | 383 | 417 | 23 |         |       |

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 9   | I     | 176      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1414  | 889 | 243 | 270 | 12 |         |       |

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 10  | J     | 168      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1281  | 861 | 183 | 225 | 12 |         |       |

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 11  | K     | 98       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 745   | 486 | 112 | 131 | 16 |         |       |

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 12  | L     | 606      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4802  | 3195 | 737 | 827 | 43 |         |       |

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 13  | M     | 459      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3654  | 2436 | 570 | 609 | 39 |         |       |

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 14  | N     | 347      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2733  | 1817 | 416 | 457 | 43 |         |       |

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 15  | O     | 320      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2589  | 1662 | 429 | 488 | 10 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| O     | 255     | LYS      | ASN    | variant | UNP P34942 |

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 16  | P     | 335      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2689  | 1739 | 476 | 469 | 5 |         |       |

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | Q     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1049  | 659 | 188 | 199 | 3 |         |       |

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | R     | 96       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 740   | 454 | 140 | 143 | 3 |         |       |

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | S     | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 691   | 434 | 129 | 126 | 2 |         |       |

- Molecule 20 is a protein called Acyl carrier protein, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | T     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 707   | 454 | 104 | 144 | 5 |         |       |
| 20  | U     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 707   | 454 | 104 | 144 | 5 |         |       |

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | V     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 923   | 597 | 156 | 167 | 3 |         |       |

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | W     | 116      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 982   | 628 | 182 | 168 | 4 |         |       |

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 8.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 23  | X     | 171      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1402  | 887 | 253 | 252 | 10 |         |       |

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 11.



| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | Y     | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1030  | 657 | 176 | 191 | 6 |         |       |

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | Z     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1157  | 743 | 202 | 203 | 9 |         |       |

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 26  | a     | 70       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 569   | 365 | 104 | 95 | 5 |         |       |

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | b     | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 654   | 427 | 109 | 116 | 2 |         |       |

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 28  | c     | 49       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 414   | 273 | 70 | 71 |         |       |

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | d     | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 999   | 650 | 172 | 172 | 5 |         |       |

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | e     | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 825   | 521 | 157 | 141 | 6 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 31  | f     | 57       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 492   | 322 | 86 | 82 | 2 |         |       |

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | g     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 846   | 544 | 140 | 158 | 4 |         |       |

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | h     | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1154  | 759 | 196 | 197 | 2 |         |       |

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | i     | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1097  | 722 | 191 | 183 | 1 |         |       |

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 35  | j     | 71       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 597   | 390 | 99 | 107 | 1 |         |       |

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | k     | 81       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 653   | 427 | 110 | 114 | 2 |         |       |

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | l     | 156      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1314  | 850 | 216 | 240 | 8 |         |       |

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | m     | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1070  | 686 | 188 | 196 |   |         |       |

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | n     | 171      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1487  | 952 | 272 | 256 | 7 |         |       |

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | o     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1048  | 653 | 201 | 185 | 9 |         |       |

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | p     | 174      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1458  | 913 | 269 | 268 | 8 |         |       |

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | q     | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1212  | 780 | 216 | 211 | 5 |         |       |

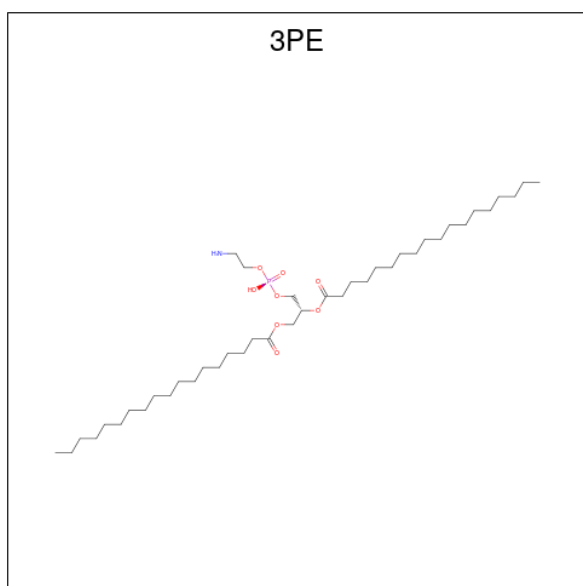
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | r     | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 776   | 490 | 144 | 139 | 3 |         |       |

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 44  | s     | 44       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 371   | 233 | 66 | 71 | 1 |         |       |

- Molecule 45 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ).



| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 45  | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 43    | 33 | 1 | 8 | 1 |         |
| 45  | H     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 36    | 26 | 1 | 8 | 1 |         |
| 45  | I     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 37    | 27 | 1 | 8 | 1 |         |
| 45  | J     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 31    | 21 | 1 | 8 | 1 |         |
| 45  | J     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 36    | 26 | 1 | 8 | 1 |         |
| 45  | K     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 44    | 34 | 1 | 8 | 1 |         |
| 45  | L     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |

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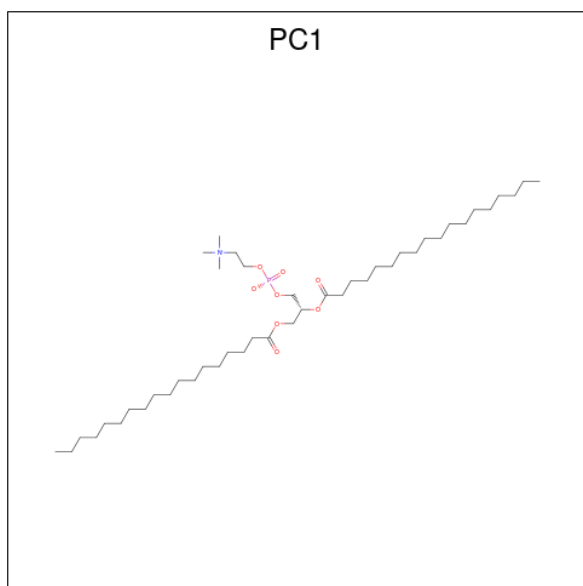
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 45  | M     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 30    | 20 | 1 | 8 | 1 |         |
| 45  | M     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 50    | 40 | 1 | 8 | 1 |         |
| 45  | M     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 34    | 24 | 1 | 8 | 1 |         |
| 45  | M     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 45  | N     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 45  | N     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 40    | 30 | 1 | 8 | 1 |         |
| 45  | N     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 49    | 39 | 1 | 8 | 1 |         |
| 45  | Y     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 27    | 17 | 1 | 8 | 1 |         |
| 45  | Y     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 45  | Y     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 45  | Y     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 45  | Y     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 46    | 36 | 1 | 8 | 1 |         |
| 45  | Y     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 34    | 24 | 1 | 8 | 1 |         |
| 45  | Y     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 45  | Z     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 37    | 27 | 1 | 8 | 1 |         |
| 45  | Z     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 45  | b     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 47    | 37 | 1 | 8 | 1 |         |
| 45  | b     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 45  | d     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 49    | 39 | 1 | 8 | 1 |         |
| 45  | f     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 45  | h     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 32    | 22 | 1 | 8 | 1 |         |

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| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 45  | m     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 41    | 31 | 1 | 8 | 1 |         |
| 45  | m     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 30    | 20 | 1 | 8 | 1 |         |
| 45  | q     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 45  | r     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 28    | 18 | 1 | 8 | 1 |         |

- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula:  $C_{44}H_{88}NO_8P$ ).



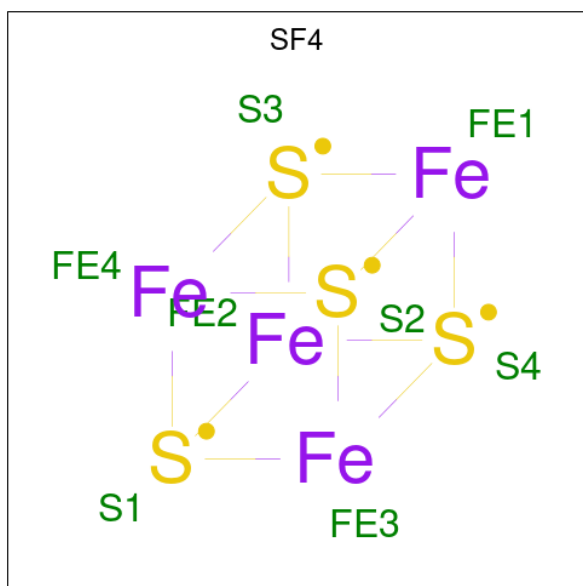
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 46  | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 35    | 25 | 1 | 8 | 1 |         |
| 46  | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 41    | 31 | 1 | 8 | 1 |         |
| 46  | B     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 48    | 38 | 1 | 8 | 1 |         |
| 46  | H     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 48    | 38 | 1 | 8 | 1 |         |
| 46  | H     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 39    | 29 | 1 | 8 | 1 |         |
| 46  | I     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 54    | 44 | 1 | 8 | 1 |         |
| 46  | L     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 54    | 44 | 1 | 8 | 1 |         |

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| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 46  | M     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 35    | 25 | 1 | 8 | 1 |         |
| 46  | Z     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 44    | 34 | 1 | 8 | 1 |         |
| 46  | d     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 39    | 29 | 1 | 8 | 1 |         |
| 46  | g     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 44    | 34 | 1 | 8 | 1 |         |
| 46  | h     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 40    | 30 | 1 | 8 | 1 |         |
| 46  | m     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 40    | 30 | 1 | 8 | 1 |         |
| 46  | q     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 23    | 13 | 1 | 8 | 1 |         |

- Molecule 47 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



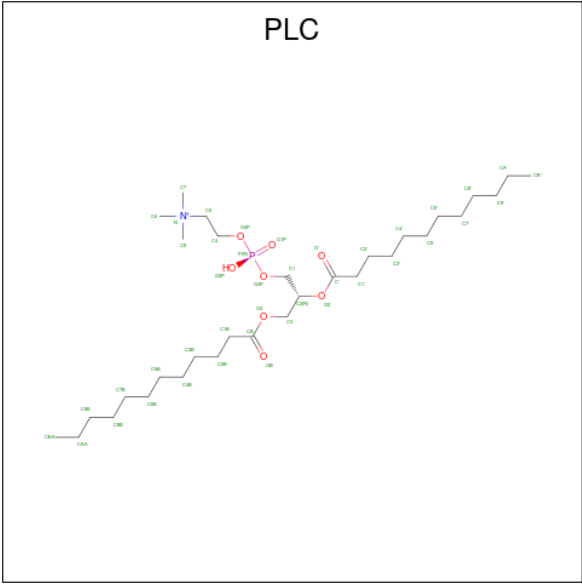
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 47  | B     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 47  | F     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 47  | G     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 47  | G     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 47  | I     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 47  | I     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

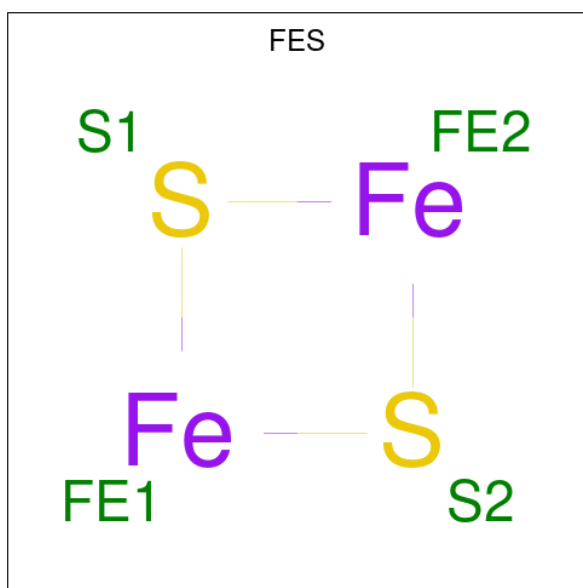
- Molecule 48 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula:  $C_{32}H_{65}NO_8P$ ).



| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 48  | B     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 28    | 18 | 1 | 8 | 1 |         |
| 48  | J     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 35    | 25 | 1 | 8 | 1 |         |
| 48  | L     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 42    | 32 | 1 | 8 | 1 |         |
| 48  | O     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 42    | 32 | 1 | 8 | 1 |         |
| 48  | Y     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 37    | 27 | 1 | 8 | 1 |         |
| 48  | Z     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 34    | 24 | 1 | 8 | 1 |         |
| 48  | b     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 38    | 28 | 1 | 8 | 1 |         |
| 48  | d     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 32    | 22 | 1 | 8 | 1 |         |
| 48  | g     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 28    | 18 | 1 | 8 | 1 |         |

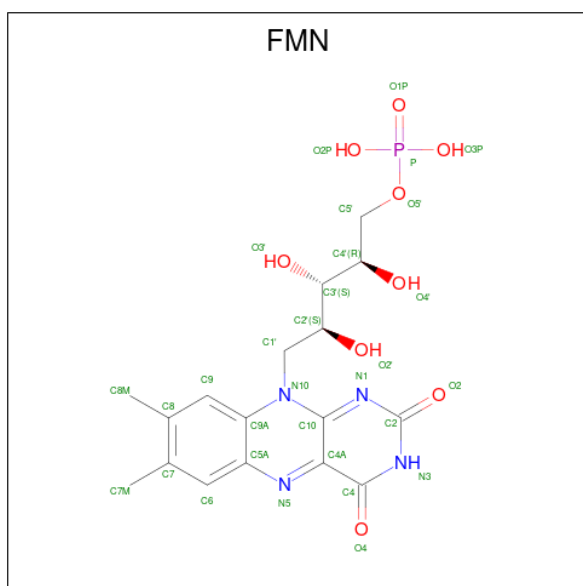


- Molecule 49 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 49  | E     | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |
| 49  | G     | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |

- Molecule 50 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$ ).



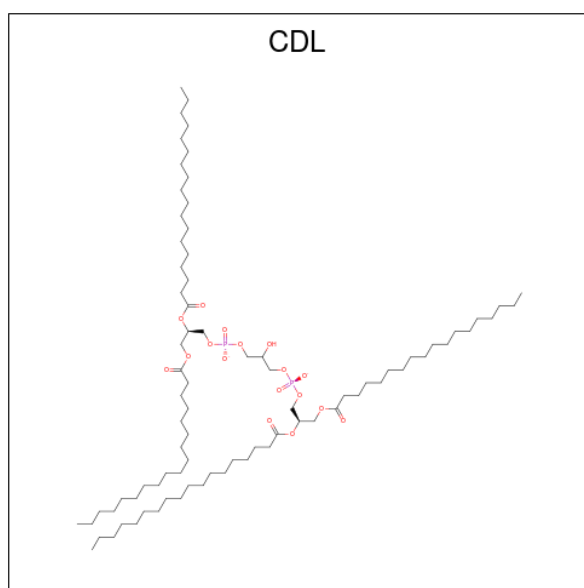
- Molecule 51 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms          | AltConf |
|-----|-------|----------|----------------|---------|
| 51  | G     | 1        | Total K<br>1 1 | 0       |

- Molecule 52 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms           | AltConf |
|-----|-------|----------|-----------------|---------|
| 52  | M     | 1        | Total Zn<br>1 1 | 0       |
| 52  | R     | 1        | Total Zn<br>1 1 | 0       |

- Molecule 53 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



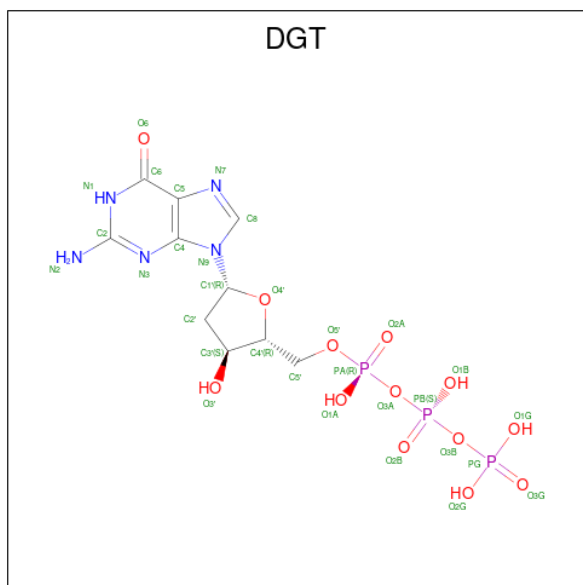
| Mol | Chain | Residues | Atoms                      | AltConf |
|-----|-------|----------|----------------------------|---------|
| 53  | M     | 1        | Total C O P<br>100 81 17 2 | 0       |
| 53  | N     | 1        | Total C O P<br>84 65 17 2  | 0       |
| 53  | X     | 1        | Total C O P<br>86 67 17 2  | 0       |
| 53  | d     | 1        | Total C O P<br>65 46 17 2  | 0       |
| 53  | h     | 1        | Total C O P<br>70 51 17 2  | 0       |
| 53  | i     | 1        | Total C O P<br>72 53 17 2  | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 53  | r     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 58    | 39 | 17 | 2 |         |

- Molecule 54 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 54  | O     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 55  | O     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).



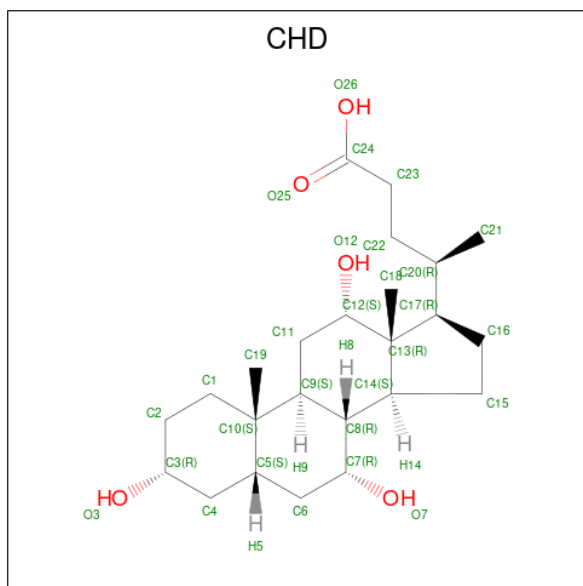
| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 56  | P     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 48    | 21 | 7 | 17 | 3 |         |

- Molecule 57 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: C<sub>25</sub>H<sub>49</sub>N<sub>2</sub>O<sub>9</sub>PS).



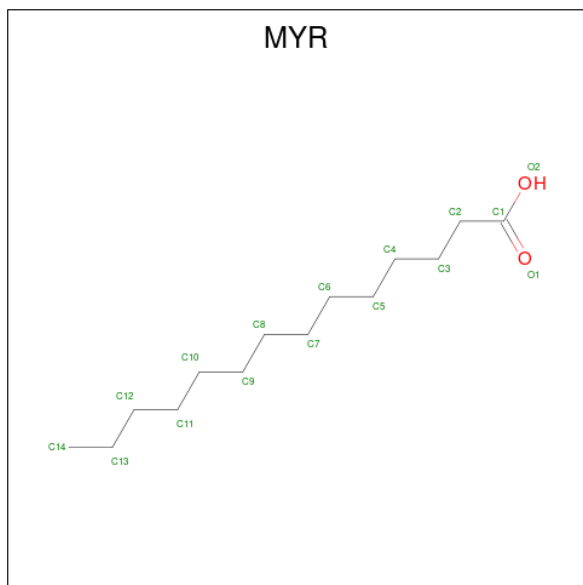
| Mol | Chain | Residues | Atoms       |         |        |        |        |        | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|--------|--------|---------|
| 57  | T     | 1        | Total<br>37 | C<br>25 | N<br>2 | O<br>8 | P<br>1 | S<br>1 | 0       |
| 57  | U     | 1        | Total<br>37 | C<br>25 | N<br>2 | O<br>8 | P<br>1 | S<br>1 | 0       |

- Molecule 58 is CHOLIC ACID (three-letter code: CHD) (formula:  $C_{24}H_{40}O_5$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 58  | i     | 1        | Total | C  | O | 0       |
|     |       |          | 29    | 24 | 5 |         |

- Molecule 59 is MYRISTIC ACID (three-letter code: MYR) (formula:  $C_{14}H_{28}O_2$ ).




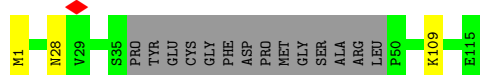
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 59  | o     | 1        | Total | C  | O | 0       |
|     |       |          | 15    | 14 | 1 |         |

### 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.

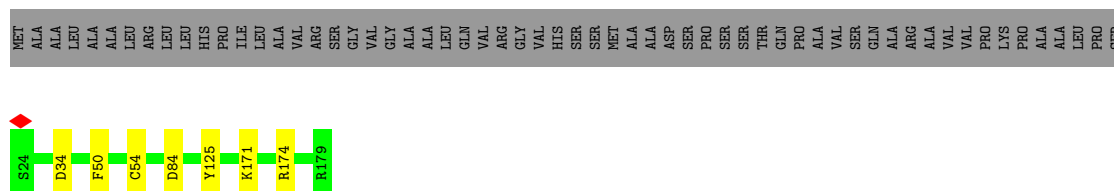
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A:  85% 12%




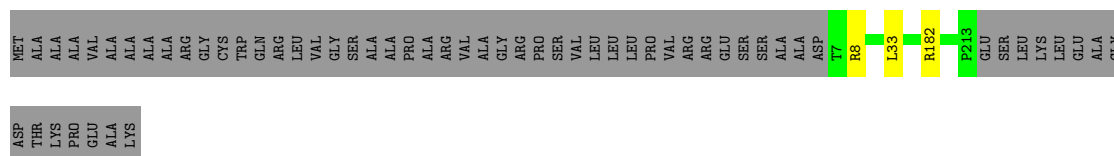
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B:  69% 28%




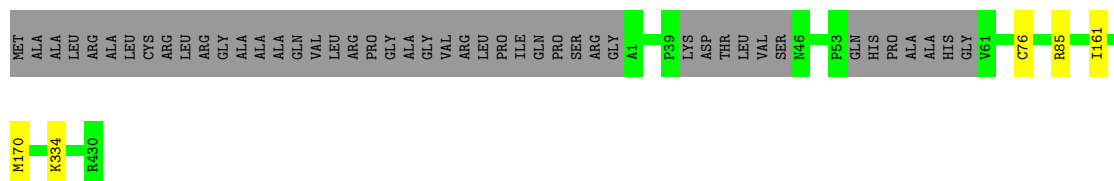
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C:  77% 22%




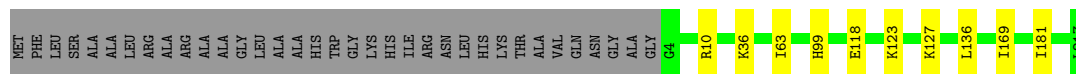
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D:  89% 10%




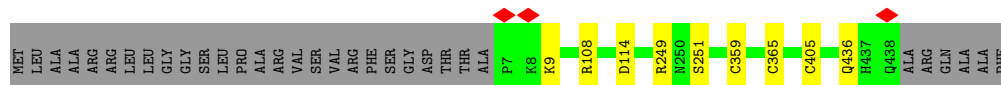
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:  82% 14%



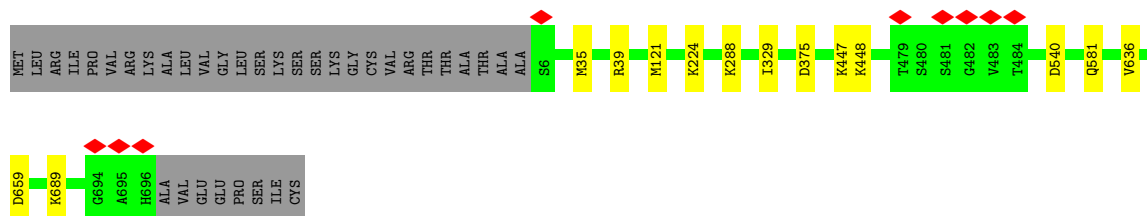
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F:  91% 7%



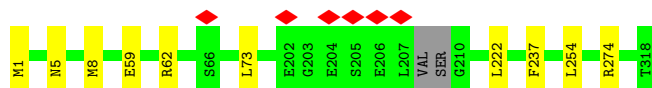
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G:  93% 5%




- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H:  96% 2%



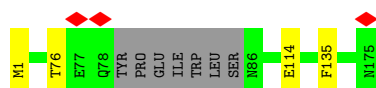
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:  82% 17%



- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:  94% 2%



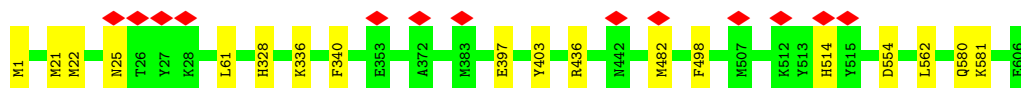
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:  96%



- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:  97%



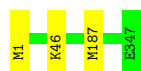
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:  98%



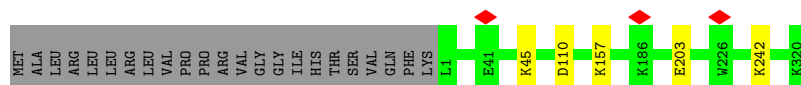
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:  99%




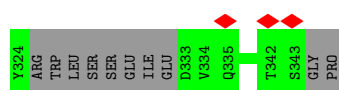
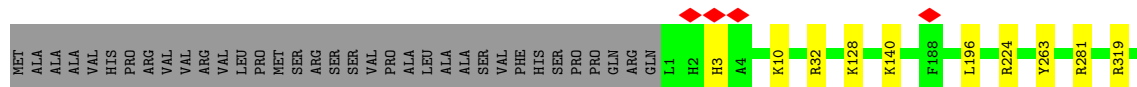
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:  92%



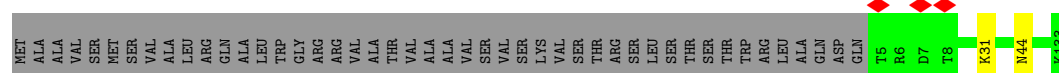
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:  86%

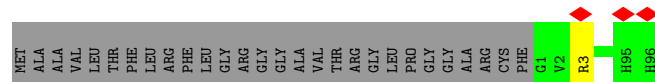
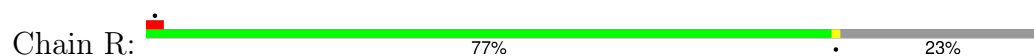


- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

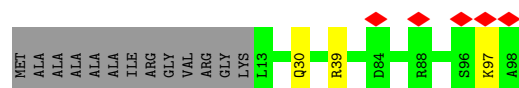
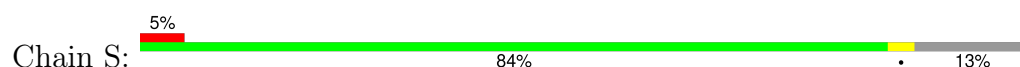




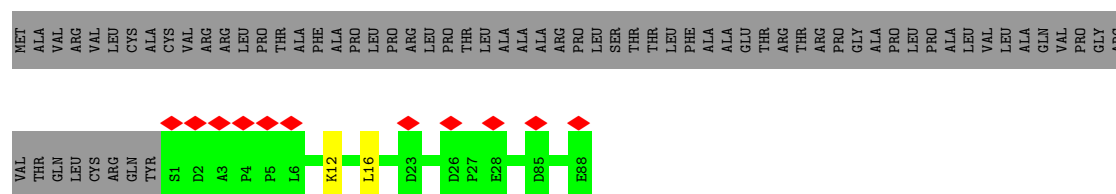
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



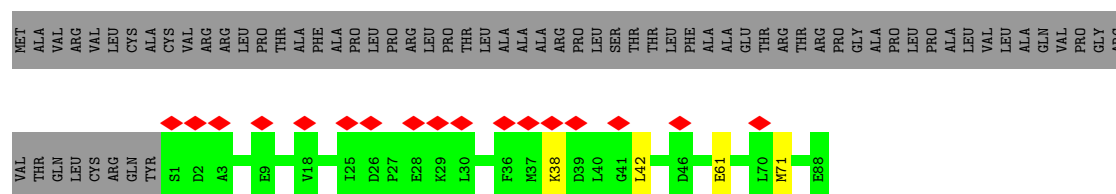
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



- Molecule 20: Acyl carrier protein, mitochondrial




- Molecule 20: Acyl carrier protein, mitochondrial

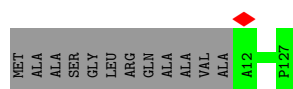


- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W:  91% 9%



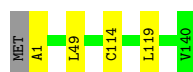
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X:  98% ..



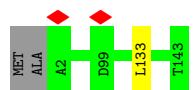
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y:  96% ..



- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z:  98% ..



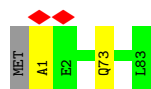
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a:  100%

There are no outlier residues recorded for this chain.

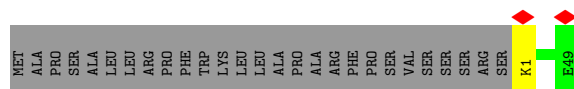
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b:  96% ..

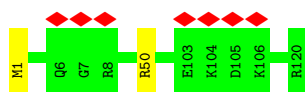


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

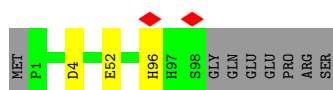
Chain c:  63% 36%



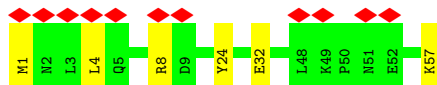
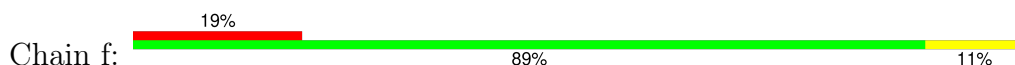
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



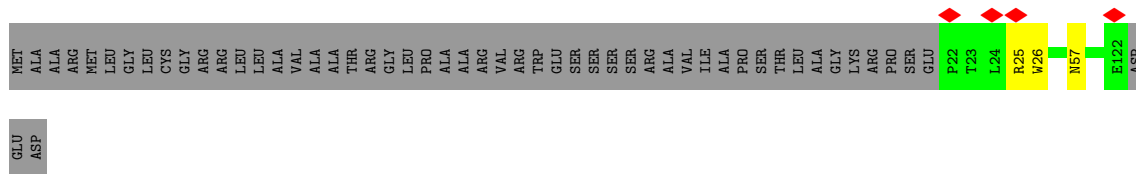
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



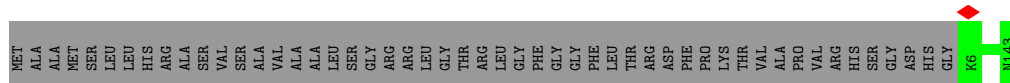
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



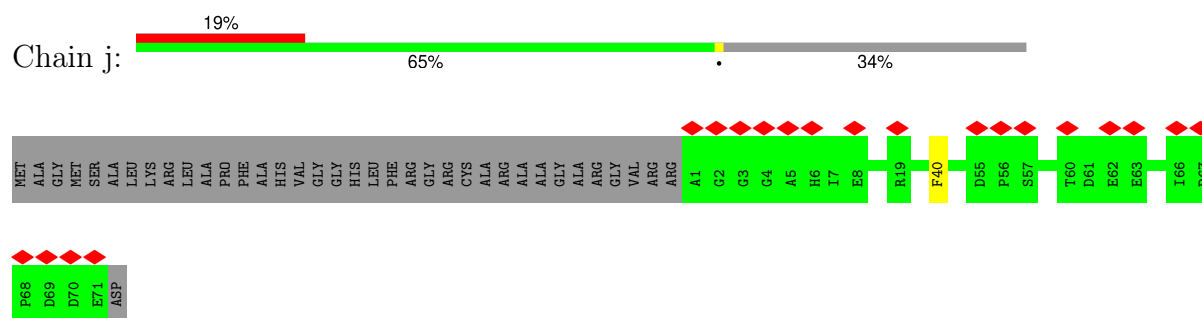
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



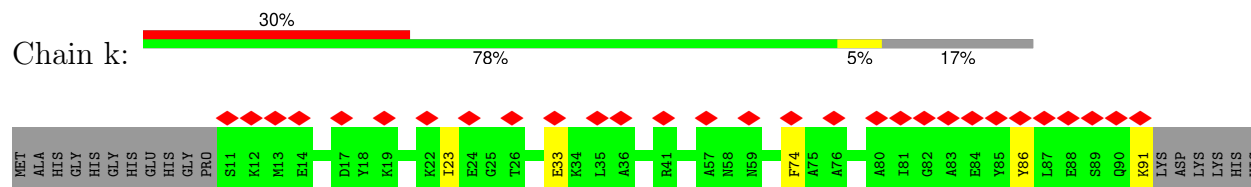
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



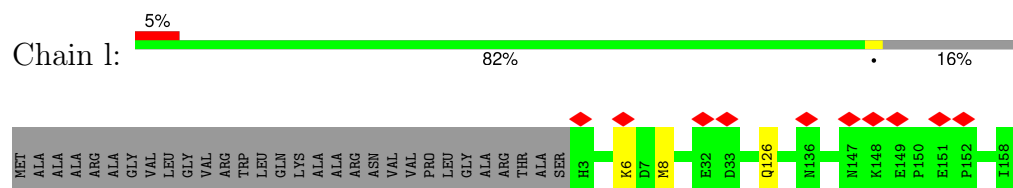
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



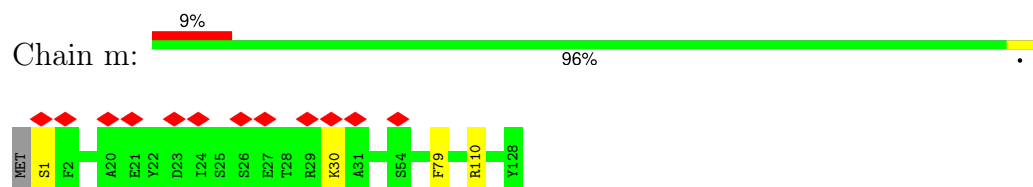
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



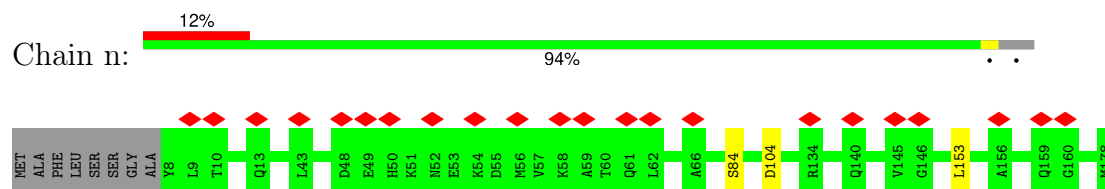
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



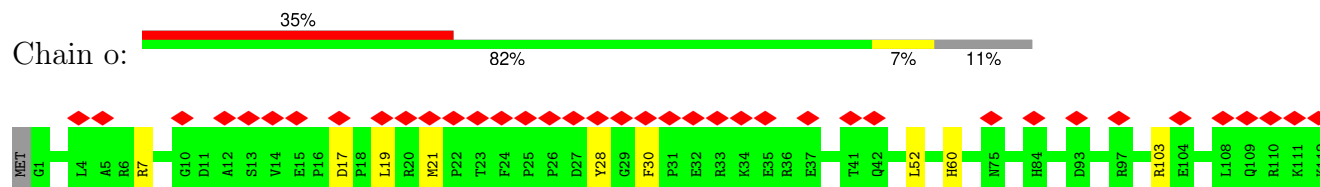
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

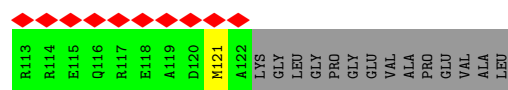


- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

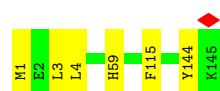




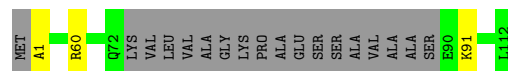
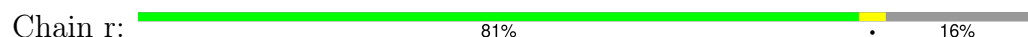
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



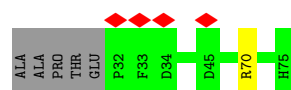
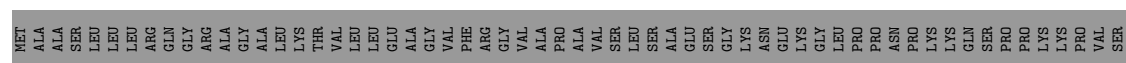
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



## 4 Experimental information

| Property                             | Value   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE   | Depositor |
| Imposed symmetry                     | POINT, C1   | Depositor |
| Number of particles used             | 93255   | 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 ( $e^-/\text{\AA}^2$ ) | 40, 40  | Depositor |
| Minimum defocus (nm)                 | 900   | Depositor |
| Maximum defocus (nm)                 | 2300  | Depositor |
| Magnification                        | 81000   | Depositor |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k),<br>GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value                    | 0.355   | Depositor |
| Minimum map value                    | -0.005  | Depositor |
| Average map value                    | -0.000  | Depositor |
| Map value standard deviation         | 0.004   | Depositor |
| Recommended contour level            | 0.022   | Depositor |
| Map size ( $\text{\AA}$ )            | 514.56, 514.56, 514.56  | wwPDB     |
| Map dimensions                       | 480, 480, 480   | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0  | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.072, 1.072, 1.072   | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MYR, NDP, CHD, PC1, AYA, CDL, SF4, MG, EHZ, DGT, K, FME, SAC, AME, ZN, PLC, FES, FMN, 3PE, 2MR

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     | 0.23         | 0/825   | 0.37        | 0/1128  |
| 2   | B     | 0.28         | 0/1278  | 0.52        | 0/1728  |
| 3   | C     | 0.27         | 0/1772  | 0.51        | 0/2413  |
| 4   | D     | 0.27         | 0/3437  | 0.49        | 0/4654  |
| 5   | E     | 0.26         | 0/1699  | 0.46        | 0/2312  |
| 6   | F     | 0.25         | 0/3401  | 0.50        | 0/4595  |
| 7   | G     | 0.25         | 0/5387  | 0.50        | 0/7301  |
| 8   | H     | 0.25         | 0/2557  | 0.44        | 0/3492  |
| 9   | I     | 0.28         | 0/1445  | 0.52        | 0/1956  |
| 10  | J     | 0.26         | 0/1301  | 0.40        | 0/1761  |
| 11  | K     | 0.24         | 0/745   | 0.42        | 0/1008  |
| 12  | L     | 0.24         | 0/4920  | 0.41        | 0/6694  |
| 13  | M     | 0.24         | 0/3738  | 0.42        | 0/5097  |
| 14  | N     | 0.24         | 0/2792  | 0.42        | 0/3800  |
| 15  | O     | 0.25         | 0/2651  | 0.42        | 0/3587  |
| 16  | P     | 0.25         | 0/2763  | 0.50        | 0/3747  |
| 17  | Q     | 0.24         | 0/1072  | 0.51        | 0/1449  |
| 18  | R     | 0.26         | 0/753   | 0.50        | 0/1014  |
| 19  | S     | 0.23         | 0/702   | 0.51        | 0/945   |
| 20  | T     | 0.24         | 0/719   | 0.39        | 0/971   |
| 20  | U     | 0.24         | 0/719   | 0.41        | 0/971   |
| 21  | V     | 0.23         | 0/943   | 0.40        | 0/1277  |
| 22  | W     | 0.24         | 0/1006  | 0.50        | 0/1352  |
| 23  | X     | 0.24         | 0/1439  | 0.47        | 0/1942  |
| 24  | Y     | 0.23         | 0/1042  | 0.45        | 0/1414  |
| 25  | Z     | 0.25         | 0/1186  | 0.50        | 0/1599  |
| 26  | a     | 0.26         | 0/584   | 0.51        | 0/786   |
| 27  | b     | 0.24         | 0/667   | 0.44        | 0/916   |
| 28  | c     | 0.25         | 0/427   | 0.39        | 0/579   |
| 29  | d     | 0.26         | 0/1018  | 0.48        | 0/1375  |
| 30  | e     | 0.24         | 0/846   | 0.49        | 0/1131  |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 31  | f     | 0.25         | 0/505   | 0.45        | 0/681   |
| 32  | g     | 0.24         | 0/873   | 0.46        | 0/1186  |
| 33  | h     | 0.24         | 0/1188  | 0.47        | 0/1607  |
| 34  | i     | 0.24         | 0/1127  | 0.46        | 0/1534  |
| 35  | j     | 0.24         | 0/624   | 0.43        | 0/855   |
| 36  | k     | 0.24         | 0/672   | 0.45        | 0/906   |
| 37  | l     | 0.24         | 0/1369  | 0.44        | 0/1873  |
| 38  | m     | 0.25         | 0/1088  | 0.51        | 0/1472  |
| 39  | n     | 0.24         | 0/1540  | 0.48        | 0/2085  |
| 40  | o     | 0.24         | 0/1073  | 0.52        | 0/1437  |
| 41  | p     | 0.24         | 0/1491  | 0.48        | 0/2011  |
| 42  | q     | 0.26         | 0/1242  | 0.49        | 0/1688  |
| 43  | r     | 0.26         | 0/789   | 0.50        | 0/1068  |
| 44  | s     | 0.24         | 0/383   | 0.48        | 0/518   |
| All | All   | 0.25         | 0/67798 | 0.47        | 0/91915 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [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     | 97/115 (84%)  | 94 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 2   | B     | 154/216 (71%) | 151 (98%) | 3 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 3   | C     | 205/266 (77%)  | 200 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 4   | D     | 410/463 (89%)  | 399 (97%) | 11 (3%) | 0        | 100         | 100 |
| 5   | E     | 212/249 (85%)  | 205 (97%) | 7 (3%)  | 0        | 100         | 100 |
| 6   | F     | 430/464 (93%)  | 419 (97%) | 11 (3%) | 0        | 100         | 100 |
| 7   | G     | 689/727 (95%)  | 664 (96%) | 25 (4%) | 0        | 100         | 100 |
| 8   | H     | 312/318 (98%)  | 300 (96%) | 12 (4%) | 0        | 100         | 100 |
| 9   | I     | 174/212 (82%)  | 170 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 10  | J     | 164/175 (94%)  | 156 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 11  | K     | 96/98 (98%)    | 93 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 12  | L     | 604/606 (100%) | 585 (97%) | 18 (3%) | 1 (0%)   | 44          | 66  |
| 13  | M     | 457/459 (100%) | 451 (99%) | 6 (1%)  | 0        | 100         | 100 |
| 14  | N     | 345/347 (99%)  | 336 (97%) | 9 (3%)  | 0        | 100         | 100 |
| 15  | O     | 318/343 (93%)  | 310 (98%) | 8 (2%)  | 0        | 100         | 100 |
| 16  | P     | 331/380 (87%)  | 322 (97%) | 9 (3%)  | 0        | 100         | 100 |
| 17  | Q     | 127/175 (73%)  | 124 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 18  | R     | 94/124 (76%)   | 93 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 19  | S     | 84/99 (85%)    | 81 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 20  | T     | 86/156 (55%)   | 83 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 20  | U     | 86/156 (55%)   | 82 (95%)  | 4 (5%)  | 0        | 100         | 100 |
| 21  | V     | 112/116 (97%)  | 111 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 22  | W     | 114/128 (89%)  | 111 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 23  | X     | 169/172 (98%)  | 167 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 24  | Y     | 138/141 (98%)  | 136 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 25  | Z     | 140/144 (97%)  | 137 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 26  | a     | 68/70 (97%)    | 67 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 27  | b     | 81/84 (96%)    | 78 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 28  | c     | 47/76 (62%)    | 47 (100%) | 0       | 0        | 100         | 100 |
| 29  | d     | 118/120 (98%)  | 117 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 30  | e     | 96/106 (91%)   | 94 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 31  | f     | 55/57 (96%)    | 53 (96%)  | 2 (4%)  | 0        | 100         | 100 |
| 32  | g     | 99/154 (64%)   | 91 (92%)  | 8 (8%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 33  | h     | 136/189 (72%)   | 135 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 34  | i     | 125/128 (98%)   | 120 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 35  | j     | 69/108 (64%)    | 64 (93%)   | 5 (7%)   | 0        | 100         | 100 |
| 36  | k     | 79/98 (81%)     | 75 (95%)   | 4 (5%)   | 0        | 100         | 100 |
| 37  | l     | 154/186 (83%)   | 141 (92%)  | 13 (8%)  | 0        | 100         | 100 |
| 38  | m     | 126/129 (98%)   | 123 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 39  | n     | 169/179 (94%)   | 160 (95%)  | 9 (5%)   | 0        | 100         | 100 |
| 40  | o     | 120/137 (88%)   | 108 (90%)  | 12 (10%) | 0        | 100         | 100 |
| 41  | p     | 172/176 (98%)   | 171 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 42  | q     | 143/145 (99%)   | 143 (100%) | 0        | 0        | 100         | 100 |
| 43  | r     | 91/113 (80%)    | 88 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 44  | s     | 42/109 (38%)    | 41 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| All | All   | 8138/9213 (88%) | 7896 (97%) | 241 (3%) | 1 (0%)   | 100         | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | L     | 562 | LEU  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 89/100 (89%)  | 87 (98%)  | 2 (2%)   | 47          | 72 |
| 2   | B     | 132/175 (75%) | 125 (95%) | 7 (5%)   | 19          | 40 |
| 3   | C     | 188/228 (82%) | 185 (98%) | 3 (2%)   | 58          | 79 |
| 4   | D     | 360/392 (92%) | 356 (99%) | 4 (1%)   | 70          | 86 |
| 5   | E     | 183/205 (89%) | 173 (94%) | 10 (6%)  | 18          | 38 |
| 6   | F     | 346/368 (94%) | 337 (97%) | 9 (3%)   | 41          | 67 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 7   | G     | 579/608 (95%)  | 565 (98%)  | 14 (2%)  | 44          | 70  |
| 8   | H     | 272/274 (99%)  | 263 (97%)  | 9 (3%)   | 33          | 59  |
| 9   | I     | 151/175 (86%)  | 149 (99%)  | 2 (1%)   | 65          | 84  |
| 10  | J     | 134/141 (95%)  | 131 (98%)  | 3 (2%)   | 47          | 72  |
| 11  | K     | 85/85 (100%)   | 82 (96%)   | 3 (4%)   | 31          | 57  |
| 12  | L     | 533/533 (100%) | 517 (97%)  | 16 (3%)  | 36          | 63  |
| 13  | M     | 412/412 (100%) | 404 (98%)  | 8 (2%)   | 52          | 75  |
| 14  | N     | 315/315 (100%) | 313 (99%)  | 2 (1%)   | 84          | 94  |
| 15  | O     | 283/303 (93%)  | 278 (98%)  | 5 (2%)   | 54          | 77  |
| 16  | P     | 289/327 (88%)  | 279 (96%)  | 10 (4%)  | 31          | 57  |
| 17  | Q     | 116/153 (76%)  | 114 (98%)  | 2 (2%)   | 56          | 78  |
| 18  | R     | 79/97 (81%)    | 78 (99%)   | 1 (1%)   | 65          | 84  |
| 19  | S     | 76/82 (93%)    | 73 (96%)   | 3 (4%)   | 27          | 53  |
| 20  | T     | 81/135 (60%)   | 79 (98%)   | 2 (2%)   | 42          | 68  |
| 20  | U     | 81/135 (60%)   | 77 (95%)   | 4 (5%)   | 21          | 43  |
| 21  | V     | 101/102 (99%)  | 100 (99%)  | 1 (1%)   | 73          | 88  |
| 22  | W     | 108/114 (95%)  | 108 (100%) | 0        | 100         | 100 |
| 23  | X     | 154/155 (99%)  | 151 (98%)  | 3 (2%)   | 52          | 75  |
| 24  | Y     | 101/102 (99%)  | 98 (97%)   | 3 (3%)   | 36          | 63  |
| 25  | Z     | 120/121 (99%)  | 119 (99%)  | 1 (1%)   | 79          | 91  |
| 26  | a     | 59/59 (100%)   | 59 (100%)  | 0        | 100         | 100 |
| 27  | b     | 71/72 (99%)    | 70 (99%)   | 1 (1%)   | 62          | 82  |
| 28  | c     | 45/68 (66%)    | 44 (98%)   | 1 (2%)   | 47          | 72  |
| 29  | d     | 105/105 (100%) | 104 (99%)  | 1 (1%)   | 73          | 88  |
| 30  | e     | 89/96 (93%)    | 86 (97%)   | 3 (3%)   | 32          | 58  |
| 31  | f     | 54/54 (100%)   | 48 (89%)   | 6 (11%)  | 5           | 10  |
| 32  | g     | 92/131 (70%)   | 89 (97%)   | 3 (3%)   | 33          | 59  |
| 33  | h     | 121/158 (77%)  | 121 (100%) | 0        | 100         | 100 |
| 34  | i     | 120/121 (99%)  | 116 (97%)  | 4 (3%)   | 33          | 59  |
| 35  | j     | 61/84 (73%)    | 60 (98%)   | 1 (2%)   | 58          | 79  |
| 36  | k     | 63/76 (83%)    | 58 (92%)   | 5 (8%)   | 10          | 21  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 37  | l     | 140/159 (88%)   | 137 (98%)  | 3 (2%)   | 48          | 73 |
| 38  | m     | 113/114 (99%)   | 110 (97%)  | 3 (3%)   | 40          | 66 |
| 39  | n     | 156/161 (97%)   | 153 (98%)  | 3 (2%)   | 52          | 75 |
| 40  | o     | 110/120 (92%)   | 100 (91%)  | 10 (9%)  | 7           | 16 |
| 41  | p     | 155/157 (99%)   | 152 (98%)  | 3 (2%)   | 52          | 75 |
| 42  | q     | 130/130 (100%)  | 125 (96%)  | 5 (4%)   | 28          | 54 |
| 43  | r     | 85/97 (88%)     | 83 (98%)   | 2 (2%)   | 44          | 70 |
| 44  | s     | 43/92 (47%)     | 42 (98%)   | 1 (2%)   | 45          | 71 |
| All | All   | 7180/7891 (91%) | 6998 (98%) | 182 (2%) | 43          | 68 |

All (182) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 28  | ASN  |
| 1   | A     | 109 | LYS  |
| 2   | B     | 34  | ASP  |
| 2   | B     | 50  | PHE  |
| 2   | B     | 54  | CYS  |
| 2   | B     | 84  | ASP  |
| 2   | B     | 125 | TYR  |
| 2   | B     | 171 | LYS  |
| 2   | B     | 174 | ARG  |
| 3   | C     | 8   | ARG  |
| 3   | C     | 33  | LEU  |
| 3   | C     | 182 | ARG  |
| 4   | D     | 76  | CYS  |
| 4   | D     | 161 | ILE  |
| 4   | D     | 170 | MET  |
| 4   | D     | 334 | LYS  |
| 5   | E     | 10  | ARG  |
| 5   | E     | 36  | LYS  |
| 5   | E     | 63  | ILE  |
| 5   | E     | 99  | HIS  |
| 5   | E     | 118 | GLU  |
| 5   | E     | 123 | LYS  |
| 5   | E     | 127 | LYS  |
| 5   | E     | 136 | LEU  |
| 5   | E     | 169 | ILE  |
| 5   | E     | 181 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | F     | 9   | LYS  |
| 6   | F     | 108 | ARG  |
| 6   | F     | 114 | ASP  |
| 6   | F     | 249 | ARG  |
| 6   | F     | 251 | SER  |
| 6   | F     | 359 | CYS  |
| 6   | F     | 365 | CYS  |
| 6   | F     | 405 | CYS  |
| 6   | F     | 436 | GLN  |
| 7   | G     | 35  | MET  |
| 7   | G     | 39  | ARG  |
| 7   | G     | 121 | MET  |
| 7   | G     | 224 | LYS  |
| 7   | G     | 288 | LYS  |
| 7   | G     | 329 | ILE  |
| 7   | G     | 375 | ASP  |
| 7   | G     | 447 | LYS  |
| 7   | G     | 448 | LYS  |
| 7   | G     | 540 | ASP  |
| 7   | G     | 581 | GLN  |
| 7   | G     | 636 | VAL  |
| 7   | G     | 659 | ASP  |
| 7   | G     | 689 | LYS  |
| 8   | H     | 5   | ASN  |
| 8   | H     | 8   | MET  |
| 8   | H     | 59  | GLU  |
| 8   | H     | 62  | ARG  |
| 8   | H     | 73  | LEU  |
| 8   | H     | 222 | LEU  |
| 8   | H     | 237 | PHE  |
| 8   | H     | 254 | LEU  |
| 8   | H     | 274 | ARG  |
| 9   | I     | 14  | MET  |
| 9   | I     | 144 | HIS  |
| 10  | J     | 76  | THR  |
| 10  | J     | 114 | GLU  |
| 10  | J     | 135 | PHE  |
| 11  | K     | 34  | GLU  |
| 11  | K     | 37  | MET  |
| 11  | K     | 53  | PHE  |
| 12  | L     | 21  | MET  |
| 12  | L     | 22  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | L     | 25  | ASN  |
| 12  | L     | 61  | LEU  |
| 12  | L     | 328 | HIS  |
| 12  | L     | 336 | LYS  |
| 12  | L     | 340 | PHE  |
| 12  | L     | 397 | GLU  |
| 12  | L     | 403 | TYR  |
| 12  | L     | 436 | ARG  |
| 12  | L     | 482 | MET  |
| 12  | L     | 498 | PHE  |
| 12  | L     | 514 | HIS  |
| 12  | L     | 554 | ASP  |
| 12  | L     | 580 | GLN  |
| 12  | L     | 581 | LYS  |
| 13  | M     | 3   | LYS  |
| 13  | M     | 57  | PHE  |
| 13  | M     | 72  | LEU  |
| 13  | M     | 207 | MET  |
| 13  | M     | 340 | ARG  |
| 13  | M     | 355 | MET  |
| 13  | M     | 413 | MET  |
| 13  | M     | 416 | ARG  |
| 14  | N     | 46  | LYS  |
| 14  | N     | 187 | MET  |
| 15  | O     | 45  | LYS  |
| 15  | O     | 110 | ASP  |
| 15  | O     | 157 | LYS  |
| 15  | O     | 203 | GLU  |
| 15  | O     | 242 | LYS  |
| 16  | P     | 3   | HIS  |
| 16  | P     | 10  | LYS  |
| 16  | P     | 32  | ARG  |
| 16  | P     | 128 | LYS  |
| 16  | P     | 140 | LYS  |
| 16  | P     | 196 | LEU  |
| 16  | P     | 224 | ARG  |
| 16  | P     | 263 | TYR  |
| 16  | P     | 281 | ARG  |
| 16  | P     | 319 | ARG  |
| 17  | Q     | 31  | LYS  |
| 17  | Q     | 44  | ASN  |
| 18  | R     | 3   | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | S     | 30  | GLN  |
| 19  | S     | 39  | ARG  |
| 19  | S     | 97  | LYS  |
| 20  | T     | 12  | LYS  |
| 20  | T     | 16  | LEU  |
| 20  | U     | 38  | LYS  |
| 20  | U     | 42  | LEU  |
| 20  | U     | 61  | GLU  |
| 20  | U     | 71  | MET  |
| 21  | V     | 65  | LYS  |
| 23  | X     | 25  | LYS  |
| 23  | X     | 47  | TRP  |
| 23  | X     | 76  | HIS  |
| 24  | Y     | 49  | LEU  |
| 24  | Y     | 114 | CYS  |
| 24  | Y     | 119 | LEU  |
| 25  | Z     | 133 | LEU  |
| 27  | b     | 73  | GLN  |
| 28  | c     | 1   | LYS  |
| 29  | d     | 50  | ARG  |
| 30  | e     | 4   | ASP  |
| 30  | e     | 52  | GLU  |
| 30  | e     | 96  | HIS  |
| 31  | f     | 1   | MET  |
| 31  | f     | 4   | LEU  |
| 31  | f     | 8   | ARG  |
| 31  | f     | 24  | TYR  |
| 31  | f     | 32  | GLU  |
| 31  | f     | 57  | LYS  |
| 32  | g     | 25  | ARG  |
| 32  | g     | 26  | TRP  |
| 32  | g     | 57  | ASN  |
| 34  | i     | 12  | GLN  |
| 34  | i     | 38  | ARG  |
| 34  | i     | 48  | LYS  |
| 34  | i     | 66  | HIS  |
| 35  | j     | 40  | PHE  |
| 36  | k     | 23  | ILE  |
| 36  | k     | 33  | GLU  |
| 36  | k     | 74  | PHE  |
| 36  | k     | 86  | TYR  |
| 36  | k     | 91  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | l     | 6   | LYS  |
| 37  | l     | 8   | MET  |
| 37  | l     | 126 | GLN  |
| 38  | m     | 30  | LYS  |
| 38  | m     | 79  | PHE  |
| 38  | m     | 110 | ARG  |
| 39  | n     | 84  | SER  |
| 39  | n     | 104 | ASP  |
| 39  | n     | 153 | LEU  |
| 40  | o     | 7   | ARG  |
| 40  | o     | 17  | ASP  |
| 40  | o     | 19  | LEU  |
| 40  | o     | 21  | MET  |
| 40  | o     | 28  | TYR  |
| 40  | o     | 30  | PHE  |
| 40  | o     | 52  | LEU  |
| 40  | o     | 60  | HIS  |
| 40  | o     | 103 | ARG  |
| 40  | o     | 121 | MET  |
| 41  | p     | 95  | TYR  |
| 41  | p     | 126 | LYS  |
| 41  | p     | 166 | ARG  |
| 42  | q     | 3   | LEU  |
| 42  | q     | 4   | LEU  |
| 42  | q     | 59  | HIS  |
| 42  | q     | 115 | PHE  |
| 42  | q     | 144 | TYR  |
| 43  | r     | 60  | ARG  |
| 43  | r     | 91  | LYS  |
| 44  | s     | 70  | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | M     | 338 | HIS  |
| 34  | i     | 82  | HIS  |
| 40  | o     | 60  | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 43  | AYA  | r     | 1   | 43   | 6,7,8        | 1.86 | 2 (33%)     | 6,8,10      | 1.39 | 1 (16%)     |
| 11  | FME  | K     | 1   | 11   | 8,9,10       | 1.52 | 1 (12%)     | 8,9,11      | 1.37 | 1 (12%)     |
| 29  | AME  | d     | 1   | 29   | 9,10,11      | 1.52 | 1 (11%)     | 9,11,13     | 1.30 | 1 (11%)     |
| 27  | AYA  | b     | 1   | 27   | 6,7,8        | 1.88 | 1 (16%)     | 6,8,10      | 1.26 | 1 (16%)     |
| 14  | FME  | N     | 1   | 14   | 8,9,10       | 1.51 | 1 (12%)     | 8,9,11      | 1.39 | 1 (12%)     |
| 1   | FME  | A     | 1   | 1    | 8,9,10       | 1.51 | 1 (12%)     | 8,9,11      | 1.37 | 1 (12%)     |
| 38  | SAC  | m     | 1   | 38   | 7,8,9        | 1.74 | 1 (14%)     | 7,9,11      | 1.23 | 1 (14%)     |
| 42  | AME  | q     | 1   | 42   | 9,10,11      | 1.53 | 1 (11%)     | 9,11,13     | 1.59 | 2 (22%)     |
| 12  | FME  | L     | 1   | 12   | 8,9,10       | 1.52 | 1 (12%)     | 8,9,11      | 1.47 | 2 (25%)     |
| 4   | 2MR  | D     | 85  | 4    | 10,12,13     | 2.46 | 2 (20%)     | 5,13,15     | 1.36 | 1 (20%)     |
| 24  | AYA  | Y     | 1   | 24   | 6,7,8        | 1.88 | 2 (33%)     | 6,8,10      | 1.50 | 1 (16%)     |
| 34  | SAC  | i     | 1   | 34   | 7,8,9        | 1.76 | 1 (14%)     | 7,9,11      | 1.63 | 1 (14%)     |
| 13  | FME  | M     | 1   | 13   | 8,9,10       | 1.49 | 1 (12%)     | 8,9,11      | 1.39 | 1 (12%)     |
| 10  | FME  | J     | 1   | 10   | 8,9,10       | 1.52 | 1 (12%)     | 8,9,11      | 1.41 | 1 (12%)     |
| 8   | FME  | H     | 1   | 8    | 8,9,10       | 1.51 | 1 (12%)     | 8,9,11      | 1.48 | 2 (25%)     |

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 |
|-----|------|-------|-----|------|---------|-----------|-------|
| 43  | AYA  | r     | 1   | 43   | -       | 0/5/6/8   | -     |
| 11  | FME  | K     | 1   | 11   | -       | 2/7/9/11  | -     |
| 29  | AME  | d     | 1   | 29   | -       | 0/9/10/12 | -     |
| 27  | AYA  | b     | 1   | 27   | -       | 1/5/6/8   | -     |
| 14  | FME  | N     | 1   | 14   | -       | 2/7/9/11  | -     |
| 1   | FME  | A     | 1   | 1    | -       | 1/7/9/11  | -     |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings |
|-----|------|-------|-----|------|---------|------------|-------|
| 38  | SAC  | m     | 1   | 38   | -       | 0/7/8/10   | -     |
| 42  | AME  | q     | 1   | 42   | -       | 5/9/10/12  | -     |
| 12  | FME  | L     | 1   | 12   | -       | 2/7/9/11   | -     |
| 4   | 2MR  | D     | 85  | 4    | -       | 0/10/13/15 | -     |
| 24  | AYA  | Y     | 1   | 24   | -       | 0/5/6/8    | -     |
| 34  | SAC  | i     | 1   | 34   | -       | 2/7/8/10   | -     |
| 13  | FME  | M     | 1   | 13   | -       | 2/7/9/11   | -     |
| 10  | FME  | J     | 1   | 10   | -       | 2/7/9/11   | -     |
| 8   | FME  | H     | 1   | 8    | -       | 1/7/9/11   | -     |

All (18) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4   | D     | 85  | 2MR  | CZ-NH2 | 5.51  | 1.45        | 1.33     |
| 4   | D     | 85  | 2MR  | CZ-NE  | 5.08  | 1.45        | 1.34     |
| 11  | K     | 1   | FME  | CN-N   | 3.77  | 1.45        | 1.33     |
| 12  | L     | 1   | FME  | CN-N   | 3.74  | 1.45        | 1.33     |
| 10  | J     | 1   | FME  | CN-N   | 3.74  | 1.45        | 1.33     |
| 1   | A     | 1   | FME  | CN-N   | 3.74  | 1.45        | 1.33     |
| 14  | N     | 1   | FME  | CN-N   | 3.73  | 1.45        | 1.33     |
| 8   | H     | 1   | FME  | CN-N   | 3.71  | 1.45        | 1.33     |
| 13  | M     | 1   | FME  | CN-N   | 3.70  | 1.45        | 1.33     |
| 34  | i     | 1   | SAC  | C1A-N  | 3.62  | 1.46        | 1.34     |
| 27  | b     | 1   | AYA  | CT-N   | 3.53  | 1.45        | 1.34     |
| 38  | m     | 1   | SAC  | C1A-N  | 3.52  | 1.45        | 1.34     |
| 42  | q     | 1   | AME  | CT1-N  | 3.48  | 1.45        | 1.34     |
| 29  | d     | 1   | AME  | CT1-N  | 3.48  | 1.45        | 1.34     |
| 43  | r     | 1   | AYA  | CT-N   | 3.42  | 1.45        | 1.34     |
| 24  | Y     | 1   | AYA  | CT-N   | 3.37  | 1.45        | 1.34     |
| 24  | Y     | 1   | AYA  | OT-CT  | -2.09 | 1.18        | 1.23     |
| 43  | r     | 1   | AYA  | OT-CT  | -2.06 | 1.18        | 1.23     |

All (18) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 34  | i     | 1   | SAC  | C2A-C1A-N | 3.21 | 121.45      | 116.12   |
| 42  | q     | 1   | AME  | CT2-CT1-N | 2.67 | 120.55      | 116.12   |
| 42  | q     | 1   | AME  | CE-SD-CG  | 2.66 | 114.08      | 100.32   |
| 24  | Y     | 1   | AYA  | CM-CT-N   | 2.53 | 120.31      | 116.12   |
| 43  | r     | 1   | AYA  | CM-CT-N   | 2.47 | 120.21      | 116.12   |
| 29  | d     | 1   | AME  | CT2-CT1-N | 2.40 | 120.10      | 116.12   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 38  | m     | 1   | SAC  | C2A-C1A-N | 2.24  | 119.83      | 116.12   |
| 27  | b     | 1   | AYA  | CM-CT-N   | 2.19  | 119.76      | 116.12   |
| 12  | L     | 1   | FME  | O1-CN-N   | -2.17 | 119.71      | 125.32   |
| 8   | H     | 1   | FME  | O1-CN-N   | -2.13 | 119.82      | 125.32   |
| 12  | L     | 1   | FME  | CA-N-CN   | -2.13 | 119.55      | 122.82   |
| 8   | H     | 1   | FME  | CA-N-CN   | -2.11 | 119.58      | 122.82   |
| 10  | J     | 1   | FME  | O1-CN-N   | -2.10 | 119.89      | 125.32   |
| 4   | D     | 85  | 2MR  | CD-NE-CZ  | -2.08 | 119.46      | 123.36   |
| 1   | A     | 1   | FME  | O1-CN-N   | -2.08 | 119.95      | 125.32   |
| 14  | N     | 1   | FME  | O1-CN-N   | -2.06 | 119.99      | 125.32   |
| 11  | K     | 1   | FME  | O1-CN-N   | -2.06 | 120.01      | 125.32   |
| 13  | M     | 1   | FME  | O1-CN-N   | -2.05 | 120.03      | 125.32   |

There are no chirality outliers.

All (20) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 1   | A     | 1   | FME  | C-CA-CB-CG   |
| 11  | K     | 1   | FME  | O1-CN-N-CA   |
| 13  | M     | 1   | FME  | C-CA-CB-CG   |
| 14  | N     | 1   | FME  | O1-CN-N-CA   |
| 27  | b     | 1   | AYA  | O-C-CA-CB    |
| 42  | q     | 1   | AME  | N-CA-CB-CG   |
| 34  | i     | 1   | SAC  | C2A-C1A-N-CA |
| 34  | i     | 1   | SAC  | OAC-C1A-N-CA |
| 42  | q     | 1   | AME  | CB-CG-SD-CE  |
| 12  | L     | 1   | FME  | CA-CB-CG-SD  |
| 42  | q     | 1   | AME  | CA-CB-CG-SD  |
| 13  | M     | 1   | FME  | N-CA-CB-CG   |
| 10  | J     | 1   | FME  | N-CA-CB-CG   |
| 14  | N     | 1   | FME  | N-CA-CB-CG   |
| 42  | q     | 1   | AME  | C-CA-CB-CG   |
| 12  | L     | 1   | FME  | CB-CA-N-CN   |
| 42  | q     | 1   | AME  | CB-CA-N-CT1  |
| 11  | K     | 1   | FME  | C-CA-CB-CG   |
| 8   | H     | 1   | FME  | CB-CA-N-CN   |
| 10  | J     | 1   | FME  | CB-CA-N-CN   |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 81 ligands modelled in this entry, 4 are monoatomic - leaving 77 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 |
| 46  | PC1  | m     | 203 | -    | 39,39,53     | 1.09 | 4 (10%)  | 45,47,61    | 1.08 | 2 (4%)   |
| 56  | NDP  | P     | 501 | -    | 47,52,52     | 4.33 | 25 (53%) | 61,80,80    | 1.99 | 4 (6%)   |
| 48  | PLC  | d     | 203 | -    | 31,31,41     | 0.58 | 0        | 37,39,49    | 0.60 | 0        |
| 45  | 3PE  | I     | 203 | -    | 36,36,50     | 1.02 | 4 (11%)  | 39,41,55    | 1.14 | 2 (5%)   |
| 45  | 3PE  | Y     | 204 | -    | 50,50,50     | 0.88 | 4 (8%)   | 53,55,55    | 1.05 | 2 (3%)   |
| 45  | 3PE  | m     | 202 | -    | 29,29,50     | 1.12 | 4 (13%)  | 32,34,55    | 1.19 | 2 (6%)   |
| 45  | 3PE  | Z     | 201 | -    | 36,36,50     | 1.02 | 4 (11%)  | 39,41,55    | 1.04 | 2 (5%)   |
| 54  | DGT  | O     | 401 | 55   | 29,33,33     | 2.94 | 11 (37%) | 37,52,52    | 1.49 | 8 (21%)  |
| 48  | PLC  | L     | 703 | -    | 41,41,41     | 0.51 | 0        | 47,49,49    | 0.51 | 0        |
| 48  | PLC  | Z     | 204 | -    | 33,33,41     | 0.57 | 0        | 39,41,49    | 0.59 | 0        |
| 45  | 3PE  | Y     | 207 | -    | 50,50,50     | 0.88 | 4 (8%)   | 53,55,55    | 1.05 | 2 (3%)   |
| 47  | SF4  | I     | 202 | 9    | 0,12,12      | -    | -        | -           | -    | -        |
| 45  | 3PE  | J     | 201 | -    | 30,30,50     | 1.10 | 4 (13%)  | 33,35,55    | 1.16 | 2 (6%)   |
| 45  | 3PE  | M     | 603 | -    | 49,49,50     | 0.88 | 4 (8%)   | 52,54,55    | 1.04 | 2 (3%)   |
| 47  | SF4  | B     | 201 | 2    | 0,12,12      | -    | -        | -           | -    | -        |
| 48  | PLC  | b     | 103 | -    | 37,37,41     | 0.53 | 0        | 43,45,49    | 0.54 | 0        |
| 45  | 3PE  | d     | 201 | -    | 48,48,50     | 0.89 | 4 (8%)   | 51,53,55    | 1.06 | 2 (3%)   |
| 46  | PC1  | H     | 403 | -    | 38,38,53     | 1.11 | 4 (10%)  | 44,46,61    | 0.98 | 2 (4%)   |
| 48  | PLC  | O     | 403 | -    | 41,41,41     | 0.51 | 0        | 47,49,49    | 0.56 | 0        |
| 45  | 3PE  | Y     | 203 | -    | 50,50,50     | 0.88 | 4 (8%)   | 53,55,55    | 1.08 | 2 (3%)   |
| 57  | EHZ  | U     | 101 | 20   | 31,36,37     | 1.58 | 5 (16%)  | 36,44,47    | 1.58 | 7 (19%)  |
| 53  | CDL  | h     | 203 | -    | 69,69,99     | 1.05 | 8 (11%)  | 75,81,111   | 1.09 | 4 (5%)   |
| 45  | 3PE  | N     | 403 | -    | 48,48,50     | 0.89 | 4 (8%)   | 51,53,55    | 1.07 | 2 (3%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 45  | 3PE  | N     | 402 | -    | 39,39,50     | 0.98 | 4 (10%)  | 42,44,55    | 1.13 | 2 (4%)   |
| 45  | 3PE  | J     | 202 | -    | 35,35,50     | 1.03 | 4 (11%)  | 38,40,55    | 1.14 | 2 (5%)   |
| 49  | FES  | G     | 803 | 7    | 0,4,4        | -    | -        | -           |      |          |
| 46  | PC1  | A     | 202 | -    | 34,34,53     | 1.18 | 4 (11%)  | 40,42,61    | 1.09 | 2 (5%)   |
| 45  | 3PE  | M     | 605 | -    | 44,44,50     | 0.92 | 4 (9%)   | 47,49,55    | 1.14 | 2 (4%)   |
| 48  | PLC  | J     | 203 | -    | 34,34,41     | 0.55 | 0        | 40,42,49    | 0.53 | 0        |
| 46  | PC1  | g     | 201 | -    | 43,43,53     | 1.05 | 4 (9%)   | 49,51,61    | 1.02 | 2 (4%)   |
| 45  | 3PE  | K     | 101 | -    | 43,43,50     | 0.95 | 4 (9%)   | 46,48,55    | 1.04 | 2 (4%)   |
| 46  | PC1  | L     | 701 | -    | 53,53,53     | 0.95 | 4 (7%)   | 59,61,61    | 0.96 | 2 (3%)   |
| 45  | 3PE  | H     | 401 | -    | 35,35,50     | 1.02 | 4 (11%)  | 38,40,55    | 1.00 | 2 (5%)   |
| 45  | 3PE  | M     | 602 | -    | 29,29,50     | 1.12 | 4 (13%)  | 32,34,55    | 1.00 | 2 (6%)   |
| 45  | 3PE  | f     | 101 | -    | 50,50,50     | 0.88 | 4 (8%)   | 53,55,55    | 1.07 | 2 (3%)   |
| 58  | CHD  | i     | 201 | -    | 32,32,32     | 3.27 | 10 (31%) | 51,51,51    | 2.42 | 17 (33%) |
| 45  | 3PE  | r     | 201 | -    | 27,27,50     | 1.17 | 4 (14%)  | 30,32,55    | 1.20 | 2 (6%)   |
| 46  | PC1  | M     | 606 | -    | 34,34,53     | 1.17 | 4 (11%)  | 40,42,61    | 1.10 | 2 (5%)   |
| 47  | SF4  | F     | 501 | 6    | 0,12,12      | -    | -        | -           |      |          |
| 53  | CDL  | X     | 201 | -    | 85,85,99     | 0.95 | 8 (9%)   | 91,97,111   | 1.10 | 4 (4%)   |
| 46  | PC1  | I     | 204 | -    | 53,53,53     | 0.94 | 4 (7%)   | 59,61,61    | 1.06 | 2 (3%)   |
| 45  | 3PE  | M     | 604 | -    | 33,33,50     | 1.06 | 4 (12%)  | 36,38,55    | 1.16 | 2 (5%)   |
| 45  | 3PE  | b     | 101 | -    | 46,46,50     | 0.90 | 4 (8%)   | 49,51,55    | 1.01 | 2 (4%)   |
| 59  | MYR  | o     | 201 | 40   | 13,14,15     | 0.41 | 0        | 12,13,15    | 0.90 | 0        |
| 45  | 3PE  | Y     | 205 | -    | 45,45,50     | 0.92 | 4 (8%)   | 48,50,55    | 1.10 | 2 (4%)   |
| 46  | PC1  | d     | 202 | -    | 38,38,53     | 1.12 | 4 (10%)  | 44,46,61    | 0.99 | 2 (4%)   |
| 50  | FMN  | F     | 502 | -    | 33,33,33     | 2.77 | 10 (30%) | 48,50,50    | 1.77 | 13 (27%) |
| 46  | PC1  | B     | 202 | -    | 47,47,53     | 1.02 | 4 (8%)   | 53,55,61    | 1.10 | 2 (3%)   |
| 45  | 3PE  | h     | 201 | -    | 31,31,50     | 1.10 | 4 (12%)  | 34,36,55    | 1.17 | 2 (5%)   |
| 45  | 3PE  | m     | 201 | -    | 40,40,50     | 0.98 | 4 (10%)  | 43,45,55    | 1.12 | 2 (4%)   |
| 45  | 3PE  | b     | 102 | -    | 50,50,50     | 0.88 | 4 (8%)   | 53,55,55    | 1.10 | 2 (3%)   |
| 47  | SF4  | I     | 201 | 9    | 0,12,12      | -    | -        | -           |      |          |
| 46  | PC1  | Z     | 203 | -    | 43,43,53     | 1.05 | 4 (9%)   | 49,51,61    | 1.03 | 2 (4%)   |
| 53  | CDL  | i     | 202 | -    | 71,71,99     | 1.04 | 8 (11%)  | 77,83,111   | 1.14 | 4 (5%)   |
| 45  | 3PE  | Z     | 202 | -    | 50,50,50     | 0.88 | 4 (8%)   | 53,55,55    | 1.03 | 2 (3%)   |
| 46  | PC1  | q     | 202 | -    | 22,22,53     | 1.36 | 3 (13%)  | 28,30,61    | 0.81 | 1 (3%)   |
| 45  | 3PE  | L     | 702 | -    | 44,44,50     | 0.92 | 4 (9%)   | 47,49,55    | 1.07 | 2 (4%)   |
| 45  | 3PE  | N     | 401 | -    | 44,44,50     | 0.93 | 4 (9%)   | 47,49,55    | 1.09 | 2 (4%)   |
| 45  | 3PE  | Y     | 202 | -    | 50,50,50     | 0.87 | 4 (8%)   | 53,55,55    | 1.09 | 2 (3%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 48  | PLC  | g     | 202 | -    | 27,27,41     | 0.61 | 0        | 33,35,49    | 0.66 | 1 (3%)   |
| 46  | PC1  | H     | 402 | -    | 47,47,53     | 1.02 | 4 (8%)   | 53,55,61    | 1.02 | 2 (3%)   |
| 45  | 3PE  | A     | 201 | -    | 42,42,50     | 0.95 | 4 (9%)   | 45,47,55    | 1.07 | 2 (4%)   |
| 53  | CDL  | N     | 404 | -    | 83,83,99     | 0.96 | 8 (9%)   | 89,95,111   | 1.06 | 4 (4%)   |
| 45  | 3PE  | Y     | 201 | -    | 26,26,50     | 1.19 | 4 (15%)  | 29,31,55    | 1.14 | 2 (6%)   |
| 47  | SF4  | G     | 802 | 7    | 0,12,12      | -    | -        | -           | -    | -        |
| 53  | CDL  | d     | 204 | -    | 64,64,99     | 1.08 | 8 (12%)  | 70,76,111   | 1.12 | 4 (5%)   |
| 45  | 3PE  | q     | 201 | -    | 50,50,50     | 0.87 | 4 (8%)   | 53,55,55    | 1.08 | 2 (3%)   |
| 53  | CDL  | M     | 607 | -    | 99,99,99     | 0.89 | 8 (8%)   | 105,111,111 | 1.10 | 4 (3%)   |
| 49  | FES  | E     | 301 | 5    | 0,4,4        | -    | -        | -           | -    | -        |
| 46  | PC1  | h     | 202 | -    | 39,39,53     | 1.09 | 4 (10%)  | 45,47,61    | 1.08 | 2 (4%)   |
| 47  | SF4  | G     | 801 | 7    | 0,12,12      | -    | -        | -           | -    | -        |
| 45  | 3PE  | Y     | 206 | -    | 33,33,50     | 1.06 | 4 (12%)  | 36,38,55    | 1.14 | 2 (5%)   |
| 53  | CDL  | r     | 202 | -    | 57,57,99     | 1.15 | 8 (14%)  | 63,69,111   | 1.12 | 4 (6%)   |
| 57  | EHZ  | T     | 101 | 20   | 31,36,37     | 1.61 | 5 (16%)  | 36,44,47    | 1.68 | 6 (16%)  |
| 48  | PLC  | B     | 203 | -    | 27,27,41     | 0.62 | 0        | 33,35,49    | 0.59 | 0        |
| 48  | PLC  | Y     | 208 | -    | 36,36,41     | 0.54 | 0        | 42,44,49    | 0.57 | 1 (2%)   |
| 46  | PC1  | A     | 203 | -    | 40,40,53     | 1.09 | 4 (10%)  | 46,48,61    | 1.05 | 2 (4%)   |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 46  | PC1  | m     | 203 | -    | -       | 16/43/43/57 | -       |
| 56  | NDP  | P     | 501 | -    | -       | 12/30/77/77 | 0/5/5/5 |
| 48  | PLC  | d     | 203 | -    | -       | 8/34/34/45  | -       |
| 45  | 3PE  | I     | 203 | -    | -       | 17/40/40/54 | -       |
| 45  | 3PE  | Y     | 204 | -    | -       | 25/54/54/54 | -       |
| 45  | 3PE  | m     | 202 | -    | -       | 16/33/33/54 | -       |
| 45  | 3PE  | Z     | 201 | -    | -       | 17/40/40/54 | -       |
| 54  | DGT  | O     | 401 | 55   | -       | 5/18/34/34  | 0/3/3/3 |
| 48  | PLC  | L     | 703 | -    | -       | 17/45/45/45 | -       |
| 48  | PLC  | Z     | 204 | -    | -       | 11/37/37/45 | -       |
| 45  | 3PE  | Y     | 207 | -    | -       | 25/54/54/54 | -       |
| 47  | SF4  | I     | 202 | 9    | -       | -           | 0/6/5/5 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions     | Rings   |
|-----|------|-------|-----|------|---------|--------------|---------|
| 45  | 3PE  | J     | 201 | -    | -       | 18/34/34/54  | -       |
| 45  | 3PE  | M     | 603 | -    | -       | 21/53/53/54  | -       |
| 47  | SF4  | B     | 201 | 2    | -       | -            | 0/6/5/5 |
| 48  | PLC  | b     | 103 | -    | -       | 16/41/41/45  | -       |
| 45  | 3PE  | d     | 201 | -    | -       | 22/52/52/54  | -       |
| 46  | PC1  | H     | 403 | -    | -       | 17/42/42/57  | -       |
| 48  | PLC  | O     | 403 | -    | -       | 15/45/45/45  | -       |
| 45  | 3PE  | Y     | 203 | -    | -       | 27/54/54/54  | -       |
| 57  | EHZ  | U     | 101 | 20   | -       | 20/42/44/45  | -       |
| 53  | CDL  | h     | 203 | -    | -       | 30/80/80/110 | -       |
| 45  | 3PE  | N     | 403 | -    | -       | 22/52/52/54  | -       |
| 45  | 3PE  | N     | 402 | -    | -       | 22/43/43/54  | -       |
| 45  | 3PE  | J     | 202 | -    | -       | 13/39/39/54  | -       |
| 49  | FES  | G     | 803 | 7    | -       | -            | 0/1/1/1 |
| 46  | PC1  | A     | 202 | -    | -       | 17/38/38/57  | -       |
| 45  | 3PE  | M     | 605 | -    | -       | 11/48/48/54  | -       |
| 48  | PLC  | J     | 203 | -    | -       | 12/38/38/45  | -       |
| 46  | PC1  | g     | 201 | -    | -       | 17/47/47/57  | -       |
| 45  | 3PE  | K     | 101 | -    | -       | 20/47/47/54  | -       |
| 46  | PC1  | L     | 701 | -    | -       | 23/57/57/57  | -       |
| 45  | 3PE  | H     | 401 | -    | -       | 15/39/39/54  | -       |
| 45  | 3PE  | M     | 602 | -    | -       | 12/33/33/54  | -       |
| 45  | 3PE  | f     | 101 | -    | -       | 23/54/54/54  | -       |
| 58  | CHD  | i     | 201 | -    | -       | 3/9/74/74    | 0/4/4/4 |
| 45  | 3PE  | r     | 201 | -    | -       | 14/31/31/54  | -       |
| 46  | PC1  | M     | 606 | -    | -       | 15/38/38/57  | -       |
| 47  | SF4  | F     | 501 | 6    | -       | -            | 0/6/5/5 |
| 53  | CDL  | X     | 201 | -    | -       | 46/96/96/110 | -       |
| 46  | PC1  | I     | 204 | -    | -       | 23/57/57/57  | -       |
| 45  | 3PE  | M     | 604 | -    | -       | 10/37/37/54  | -       |
| 45  | 3PE  | b     | 101 | -    | -       | 26/50/50/54  | -       |
| 59  | MYR  | o     | 201 | 40   | -       | 4/12/12/13   | -       |
| 45  | 3PE  | Y     | 205 | -    | -       | 25/49/49/54  | -       |
| 46  | PC1  | d     | 202 | -    | -       | 18/42/42/57  | -       |
| 50  | FMN  | F     | 502 | -    | -       | 2/18/18/18   | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions       | Rings   |
|-----|------|-------|-----|------|---------|----------------|---------|
| 46  | PC1  | B     | 202 | -    | -       | 22/51/51/57    | -       |
| 45  | 3PE  | h     | 201 | -    | -       | 17/35/35/54    | -       |
| 45  | 3PE  | m     | 201 | -    | -       | 20/44/44/54    | -       |
| 45  | 3PE  | b     | 102 | -    | -       | 21/54/54/54    | -       |
| 47  | SF4  | I     | 201 | 9    | -       | -              | 0/6/5/5 |
| 46  | PC1  | Z     | 203 | -    | -       | 17/47/47/57    | -       |
| 53  | CDL  | i     | 202 | -    | -       | 33/82/82/110   | -       |
| 45  | 3PE  | Z     | 202 | -    | -       | 22/54/54/54    | -       |
| 46  | PC1  | q     | 202 | -    | -       | 10/25/25/57    | -       |
| 45  | 3PE  | L     | 702 | -    | -       | 21/48/48/54    | -       |
| 45  | 3PE  | N     | 401 | -    | -       | 21/48/48/54    | -       |
| 45  | 3PE  | Y     | 202 | -    | -       | 19/54/54/54    | -       |
| 48  | PLC  | g     | 202 | -    | -       | 8/30/30/45     | -       |
| 46  | PC1  | H     | 402 | -    | -       | 23/51/51/57    | -       |
| 45  | 3PE  | A     | 201 | -    | -       | 21/46/46/54    | -       |
| 53  | CDL  | N     | 404 | -    | -       | 44/94/94/110   | -       |
| 45  | 3PE  | Y     | 201 | -    | -       | 12/30/30/54    | -       |
| 47  | SF4  | G     | 802 | 7    | -       | -              | 0/6/5/5 |
| 53  | CDL  | d     | 204 | -    | -       | 29/75/75/110   | -       |
| 45  | 3PE  | q     | 201 | -    | -       | 23/54/54/54    | -       |
| 53  | CDL  | M     | 607 | -    | -       | 51/110/110/110 | -       |
| 49  | FES  | E     | 301 | 5    | -       | -              | 0/1/1/1 |
| 46  | PC1  | h     | 202 | -    | -       | 15/43/43/57    | -       |
| 47  | SF4  | G     | 801 | 7    | -       | -              | 0/6/5/5 |
| 45  | 3PE  | Y     | 206 | -    | -       | 14/37/37/54    | -       |
| 53  | CDL  | r     | 202 | -    | -       | 23/68/68/110   | -       |
| 57  | EHZ  | T     | 101 | 20   | -       | 13/42/44/45    | -       |
| 48  | PLC  | B     | 203 | -    | -       | 10/31/31/45    | -       |
| 48  | PLC  | Y     | 208 | -    | -       | 13/40/40/45    | -       |
| 46  | PC1  | A     | 203 | -    | -       | 14/44/44/57    | -       |

All (305) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 56  | P     | 501 | NDP  | O4B-C1B | 16.04 | 1.61        | 1.40     |
| 56  | P     | 501 | NDP  | PA-O3   | 10.41 | 1.70        | 1.59     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 58  | i     | 201 | CHD  | C11-C12 | 9.11  | 1.68        | 1.53     |
| 56  | P     | 501 | NDP  | O4D-C1D | 8.27  | 1.61        | 1.42     |
| 56  | P     | 501 | NDP  | C7N-N7N | 7.66  | 1.55        | 1.33     |
| 54  | O     | 401 | DGT  | O6-C6   | 7.30  | 1.40        | 1.23     |
| 56  | P     | 501 | NDP  | C2D-C1D | -7.25 | 1.30        | 1.53     |
| 58  | i     | 201 | CHD  | C16-C15 | 7.22  | 1.73        | 1.54     |
| 56  | P     | 501 | NDP  | C6N-C5N | 7.18  | 1.55        | 1.33     |
| 50  | F     | 502 | FMN  | C10-N1  | 6.60  | 1.46        | 1.33     |
| 50  | F     | 502 | FMN  | C4A-N5  | 6.52  | 1.44        | 1.30     |
| 56  | P     | 501 | NDP  | O4D-C4D | -6.49 | 1.30        | 1.45     |
| 58  | i     | 201 | CHD  | C20-C17 | -6.19 | 1.43        | 1.54     |
| 56  | P     | 501 | NDP  | P2B-O2B | 5.72  | 1.69        | 1.59     |
| 50  | F     | 502 | FMN  | C5A-N5  | 5.45  | 1.49        | 1.39     |
| 58  | i     | 201 | CHD  | C13-C17 | 5.35  | 1.64        | 1.55     |
| 58  | i     | 201 | CHD  | C8-C9   | 5.31  | 1.64        | 1.53     |
| 57  | T     | 101 | EHZ  | C12-N1  | 5.20  | 1.45        | 1.33     |
| 58  | i     | 201 | CHD  | O12-C12 | -5.19 | 1.35        | 1.43     |
| 54  | O     | 401 | DGT  | PA-O3A  | 5.18  | 1.65        | 1.59     |
| 54  | O     | 401 | DGT  | PB-O3A  | 5.15  | 1.65        | 1.59     |
| 57  | U     | 101 | EHZ  | C12-N1  | 5.14  | 1.45        | 1.33     |
| 50  | F     | 502 | FMN  | C9A-N10 | 5.08  | 1.50        | 1.41     |
| 57  | U     | 101 | EHZ  | C15-N2  | 5.07  | 1.45        | 1.33     |
| 54  | O     | 401 | DGT  | PB-O3B  | 5.05  | 1.65        | 1.59     |
| 50  | F     | 502 | FMN  | C2-N1   | 5.04  | 1.48        | 1.36     |
| 56  | P     | 501 | NDP  | O4B-C4B | -5.04 | 1.33        | 1.45     |
| 57  | T     | 101 | EHZ  | C15-N2  | 4.99  | 1.45        | 1.33     |
| 56  | P     | 501 | NDP  | PN-O3   | 4.93  | 1.64        | 1.59     |
| 54  | O     | 401 | DGT  | C2-N2   | 4.85  | 1.45        | 1.34     |
| 54  | O     | 401 | DGT  | C2-N1   | 4.79  | 1.49        | 1.37     |
| 58  | i     | 201 | CHD  | C6-C5   | 4.58  | 1.61        | 1.53     |
| 56  | P     | 501 | NDP  | C2N-C3N | 4.57  | 1.47        | 1.35     |
| 50  | F     | 502 | FMN  | C2-N3   | 4.56  | 1.49        | 1.39     |
| 54  | O     | 401 | DGT  | C2-N3   | 4.30  | 1.43        | 1.33     |
| 58  | i     | 201 | CHD  | C15-C14 | 4.21  | 1.63        | 1.54     |
| 56  | P     | 501 | NDP  | O7N-C7N | -4.10 | 1.14        | 1.24     |
| 56  | P     | 501 | NDP  | C6A-N6A | 3.86  | 1.47        | 1.34     |
| 50  | F     | 502 | FMN  | C10-N10 | 3.83  | 1.45        | 1.37     |
| 56  | P     | 501 | NDP  | O2D-C2D | 3.80  | 1.52        | 1.43     |
| 50  | F     | 502 | FMN  | C4-N3   | 3.76  | 1.45        | 1.38     |
| 58  | i     | 201 | CHD  | C6-C7   | 3.54  | 1.59        | 1.52     |
| 56  | P     | 501 | NDP  | C4N-C3N | 3.24  | 1.56        | 1.50     |
| 56  | P     | 501 | NDP  | C2A-N3A | 2.87  | 1.36        | 1.32     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 50  | F     | 502 | FMN  | O2-C2   | -2.87 | 1.18        | 1.24     |
| 54  | O     | 401 | DGT  | C5-C6   | -2.85 | 1.41        | 1.47     |
| 54  | O     | 401 | DGT  | C1'-N9  | -2.83 | 1.41        | 1.49     |
| 53  | r     | 202 | CDL  | OB6-CB4 | -2.79 | 1.40        | 1.46     |
| 53  | M     | 607 | CDL  | OB6-CB4 | -2.78 | 1.40        | 1.46     |
| 56  | P     | 501 | NDP  | C4N-C5N | 2.78  | 1.56        | 1.49     |
| 53  | r     | 202 | CDL  | OA6-CA4 | -2.77 | 1.40        | 1.46     |
| 45  | Z     | 201 | 3PE  | O21-C2  | -2.76 | 1.40        | 1.46     |
| 53  | X     | 201 | CDL  | OB6-CB4 | -2.76 | 1.40        | 1.46     |
| 45  | J     | 202 | 3PE  | O21-C2  | -2.75 | 1.40        | 1.46     |
| 53  | d     | 204 | CDL  | OA6-CA4 | -2.75 | 1.40        | 1.46     |
| 53  | N     | 404 | CDL  | OB6-CB4 | -2.74 | 1.40        | 1.46     |
| 53  | d     | 204 | CDL  | OB6-CB4 | -2.73 | 1.40        | 1.46     |
| 46  | H     | 402 | PC1  | O21-C2  | -2.73 | 1.40        | 1.46     |
| 45  | q     | 201 | 3PE  | O21-C2  | -2.72 | 1.40        | 1.46     |
| 46  | A     | 203 | PC1  | O21-C2  | -2.72 | 1.40        | 1.46     |
| 45  | N     | 403 | 3PE  | O21-C2  | -2.72 | 1.40        | 1.46     |
| 46  | L     | 701 | PC1  | O21-C2  | -2.71 | 1.40        | 1.46     |
| 45  | h     | 201 | 3PE  | O21-C2  | -2.71 | 1.40        | 1.46     |
| 45  | K     | 101 | 3PE  | O21-C2  | -2.70 | 1.40        | 1.46     |
| 45  | r     | 201 | 3PE  | O21-C2  | -2.70 | 1.40        | 1.46     |
| 53  | i     | 202 | CDL  | OA6-CA4 | -2.69 | 1.40        | 1.46     |
| 46  | M     | 606 | PC1  | O21-C2  | -2.68 | 1.40        | 1.46     |
| 45  | d     | 201 | 3PE  | O21-C2  | -2.68 | 1.40        | 1.46     |
| 53  | h     | 203 | CDL  | OA6-CA4 | -2.68 | 1.40        | 1.46     |
| 45  | Z     | 202 | 3PE  | O21-C2  | -2.68 | 1.40        | 1.46     |
| 46  | I     | 204 | PC1  | O21-C2  | -2.67 | 1.40        | 1.46     |
| 53  | i     | 202 | CDL  | OB6-CB4 | -2.67 | 1.40        | 1.46     |
| 45  | m     | 201 | 3PE  | O21-C2  | -2.67 | 1.40        | 1.46     |
| 46  | Z     | 203 | PC1  | O21-C2  | -2.67 | 1.40        | 1.46     |
| 46  | q     | 202 | PC1  | O21-C2  | -2.67 | 1.40        | 1.46     |
| 46  | A     | 202 | PC1  | O21-C2  | -2.66 | 1.40        | 1.46     |
| 45  | N     | 402 | 3PE  | O21-C2  | -2.66 | 1.40        | 1.46     |
| 46  | d     | 202 | PC1  | O21-C2  | -2.65 | 1.40        | 1.46     |
| 45  | M     | 604 | 3PE  | O21-C2  | -2.65 | 1.40        | 1.46     |
| 45  | Y     | 203 | 3PE  | O21-C2  | -2.65 | 1.40        | 1.46     |
| 53  | M     | 607 | CDL  | OA6-CA4 | -2.65 | 1.40        | 1.46     |
| 45  | b     | 101 | 3PE  | O21-C2  | -2.64 | 1.40        | 1.46     |
| 45  | I     | 203 | 3PE  | O21-C2  | -2.64 | 1.40        | 1.46     |
| 45  | H     | 401 | 3PE  | O21-C2  | -2.63 | 1.40        | 1.46     |
| 53  | h     | 203 | CDL  | OB6-CB4 | -2.63 | 1.40        | 1.46     |
| 45  | Y     | 207 | 3PE  | O21-C2  | -2.63 | 1.40        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 45  | Y     | 201 | 3PE  | O21-C2  | -2.63 | 1.40        | 1.46     |
| 45  | Y     | 205 | 3PE  | O21-C2  | -2.62 | 1.40        | 1.46     |
| 45  | m     | 202 | 3PE  | O21-C2  | -2.62 | 1.40        | 1.46     |
| 56  | P     | 501 | NDP  | C6N-N1N | 2.61  | 1.43        | 1.37     |
| 45  | Y     | 204 | 3PE  | O21-C2  | -2.61 | 1.40        | 1.46     |
| 45  | Y     | 206 | 3PE  | O21-C2  | -2.61 | 1.40        | 1.46     |
| 46  | H     | 403 | PC1  | O21-C2  | -2.61 | 1.40        | 1.46     |
| 45  | A     | 201 | 3PE  | O21-C2  | -2.61 | 1.40        | 1.46     |
| 46  | B     | 202 | PC1  | O21-C2  | -2.61 | 1.40        | 1.46     |
| 46  | m     | 203 | PC1  | O21-C2  | -2.60 | 1.40        | 1.46     |
| 45  | M     | 602 | 3PE  | O21-C2  | -2.59 | 1.40        | 1.46     |
| 46  | g     | 201 | PC1  | O21-C2  | -2.59 | 1.40        | 1.46     |
| 45  | M     | 603 | 3PE  | O21-C2  | -2.59 | 1.40        | 1.46     |
| 45  | b     | 102 | 3PE  | O21-C2  | -2.59 | 1.40        | 1.46     |
| 46  | h     | 202 | PC1  | O21-C2  | -2.59 | 1.40        | 1.46     |
| 45  | J     | 201 | 3PE  | O21-C2  | -2.58 | 1.40        | 1.46     |
| 50  | F     | 502 | FMN  | O4-C4   | -2.58 | 1.18        | 1.23     |
| 45  | f     | 101 | 3PE  | O21-C2  | -2.57 | 1.40        | 1.46     |
| 45  | M     | 605 | 3PE  | O21-C2  | -2.57 | 1.40        | 1.46     |
| 53  | N     | 404 | CDL  | OA6-CA4 | -2.56 | 1.40        | 1.46     |
| 45  | Y     | 202 | 3PE  | O21-C2  | -2.50 | 1.40        | 1.46     |
| 57  | T     | 101 | EHZ  | C9-S1   | 2.49  | 1.82        | 1.76     |
| 53  | h     | 203 | CDL  | OB8-CB7 | 2.48  | 1.40        | 1.33     |
| 53  | i     | 202 | CDL  | OB8-CB7 | 2.48  | 1.40        | 1.33     |
| 46  | g     | 201 | PC1  | O31-C31 | 2.47  | 1.40        | 1.33     |
| 53  | X     | 201 | CDL  | OA6-CA4 | -2.46 | 1.40        | 1.46     |
| 45  | N     | 401 | 3PE  | O31-C31 | 2.46  | 1.40        | 1.33     |
| 53  | r     | 202 | CDL  | OA8-CA7 | 2.46  | 1.40        | 1.33     |
| 45  | N     | 401 | 3PE  | O21-C2  | -2.44 | 1.40        | 1.46     |
| 53  | r     | 202 | CDL  | OB8-CB7 | 2.43  | 1.40        | 1.33     |
| 57  | T     | 101 | EHZ  | O3-C12  | -2.43 | 1.18        | 1.23     |
| 45  | L     | 702 | 3PE  | O21-C2  | -2.42 | 1.40        | 1.46     |
| 53  | M     | 607 | CDL  | OA8-CA7 | 2.42  | 1.40        | 1.33     |
| 53  | N     | 404 | CDL  | OB8-CB7 | 2.41  | 1.40        | 1.33     |
| 53  | X     | 201 | CDL  | OA8-CA7 | 2.41  | 1.40        | 1.33     |
| 46  | H     | 402 | PC1  | O31-C31 | 2.41  | 1.40        | 1.33     |
| 46  | A     | 203 | PC1  | O31-C31 | 2.41  | 1.40        | 1.33     |
| 53  | d     | 204 | CDL  | OB8-CB7 | 2.41  | 1.40        | 1.33     |
| 45  | J     | 202 | 3PE  | O31-C31 | 2.40  | 1.40        | 1.33     |
| 45  | N     | 402 | 3PE  | O31-C31 | 2.40  | 1.40        | 1.33     |
| 45  | I     | 203 | 3PE  | O31-C31 | 2.40  | 1.40        | 1.33     |
| 45  | m     | 201 | 3PE  | O31-C31 | 2.40  | 1.40        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 53  | d     | 204 | CDL  | OA8-CA6 | -2.40 | 1.39        | 1.45     |
| 46  | h     | 202 | PC1  | O31-C31 | 2.40  | 1.40        | 1.33     |
| 56  | P     | 501 | NDP  | O3D-C3D | -2.40 | 1.37        | 1.43     |
| 46  | M     | 606 | PC1  | O31-C31 | 2.40  | 1.40        | 1.33     |
| 53  | N     | 404 | CDL  | OA8-CA7 | 2.39  | 1.40        | 1.33     |
| 53  | X     | 201 | CDL  | OB8-CB7 | 2.39  | 1.40        | 1.33     |
| 45  | Y     | 207 | 3PE  | O31-C31 | 2.39  | 1.40        | 1.33     |
| 58  | i     | 201 | CHD  | C13-C12 | -2.39 | 1.50        | 1.54     |
| 56  | P     | 501 | NDP  | O3B-C3B | -2.39 | 1.37        | 1.43     |
| 45  | d     | 201 | 3PE  | O31-C31 | 2.39  | 1.40        | 1.33     |
| 56  | P     | 501 | NDP  | PA-O5B  | 2.38  | 1.68        | 1.59     |
| 46  | B     | 202 | PC1  | O31-C3  | -2.38 | 1.39        | 1.45     |
| 45  | M     | 604 | 3PE  | O31-C31 | 2.38  | 1.40        | 1.33     |
| 46  | d     | 202 | PC1  | O31-C31 | 2.38  | 1.40        | 1.33     |
| 57  | T     | 101 | EHZ  | O4-C15  | -2.38 | 1.18        | 1.23     |
| 45  | K     | 101 | 3PE  | O31-C31 | 2.38  | 1.40        | 1.33     |
| 45  | Y     | 202 | 3PE  | O31-C31 | 2.38  | 1.40        | 1.33     |
| 45  | Y     | 201 | 3PE  | O31-C31 | 2.38  | 1.40        | 1.33     |
| 53  | M     | 607 | CDL  | OB8-CB7 | 2.38  | 1.40        | 1.33     |
| 57  | U     | 101 | EHZ  | C9-S1   | 2.38  | 1.81        | 1.76     |
| 46  | H     | 403 | PC1  | O31-C31 | 2.37  | 1.40        | 1.33     |
| 45  | r     | 201 | 3PE  | O31-C31 | 2.37  | 1.40        | 1.33     |
| 46  | A     | 202 | PC1  | O31-C31 | 2.36  | 1.40        | 1.33     |
| 45  | Y     | 204 | 3PE  | O31-C31 | 2.36  | 1.40        | 1.33     |
| 45  | Z     | 201 | 3PE  | O31-C31 | 2.36  | 1.40        | 1.33     |
| 45  | H     | 401 | 3PE  | O31-C31 | 2.36  | 1.40        | 1.33     |
| 45  | f     | 101 | 3PE  | O31-C31 | 2.36  | 1.40        | 1.33     |
| 45  | h     | 201 | 3PE  | O31-C31 | 2.36  | 1.40        | 1.33     |
| 45  | J     | 201 | 3PE  | O31-C31 | 2.36  | 1.40        | 1.33     |
| 45  | A     | 201 | 3PE  | O31-C31 | 2.35  | 1.40        | 1.33     |
| 46  | m     | 203 | PC1  | O31-C31 | 2.35  | 1.40        | 1.33     |
| 45  | Y     | 205 | 3PE  | O31-C31 | 2.34  | 1.40        | 1.33     |
| 45  | m     | 202 | 3PE  | O31-C31 | 2.34  | 1.40        | 1.33     |
| 45  | Y     | 206 | 3PE  | O31-C31 | 2.34  | 1.40        | 1.33     |
| 45  | M     | 602 | 3PE  | O31-C31 | 2.34  | 1.40        | 1.33     |
| 46  | I     | 204 | PC1  | O31-C31 | 2.34  | 1.40        | 1.33     |
| 57  | U     | 101 | EHZ  | O4-C15  | -2.34 | 1.18        | 1.23     |
| 45  | M     | 603 | 3PE  | O31-C31 | 2.33  | 1.40        | 1.33     |
| 46  | L     | 701 | PC1  | O31-C31 | 2.33  | 1.40        | 1.33     |
| 45  | L     | 702 | 3PE  | O31-C31 | 2.33  | 1.40        | 1.33     |
| 56  | P     | 501 | NDP  | P2B-O1X | 2.33  | 1.57        | 1.50     |
| 53  | i     | 202 | CDL  | OA8-CA7 | 2.33  | 1.40        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 45  | N     | 403 | 3PE  | O31-C31 | 2.32  | 1.40        | 1.33     |
| 45  | b     | 101 | 3PE  | O31-C31 | 2.32  | 1.40        | 1.33     |
| 46  | Z     | 203 | PC1  | O31-C31 | 2.32  | 1.40        | 1.33     |
| 45  | b     | 102 | 3PE  | O31-C31 | 2.32  | 1.40        | 1.33     |
| 45  | Z     | 202 | 3PE  | O31-C31 | 2.32  | 1.40        | 1.33     |
| 57  | U     | 101 | EHZ  | O3-C12  | -2.31 | 1.18        | 1.23     |
| 53  | h     | 203 | CDL  | OA8-CA7 | 2.31  | 1.40        | 1.33     |
| 56  | P     | 501 | NDP  | C7N-C3N | 2.30  | 1.53        | 1.48     |
| 45  | Y     | 203 | 3PE  | O31-C31 | 2.30  | 1.40        | 1.33     |
| 45  | M     | 605 | 3PE  | O31-C31 | 2.29  | 1.40        | 1.33     |
| 45  | K     | 101 | 3PE  | O31-C3  | -2.29 | 1.40        | 1.45     |
| 46  | B     | 202 | PC1  | O31-C31 | 2.29  | 1.40        | 1.33     |
| 45  | m     | 201 | 3PE  | O31-C3  | -2.28 | 1.40        | 1.45     |
| 45  | q     | 201 | 3PE  | O31-C31 | 2.27  | 1.40        | 1.33     |
| 45  | b     | 102 | 3PE  | O31-C3  | -2.27 | 1.40        | 1.45     |
| 45  | M     | 603 | 3PE  | O31-C3  | -2.26 | 1.40        | 1.45     |
| 45  | b     | 101 | 3PE  | O31-C3  | -2.26 | 1.40        | 1.45     |
| 45  | N     | 401 | 3PE  | O21-C21 | 2.26  | 1.40        | 1.34     |
| 53  | d     | 204 | CDL  | OA8-CA7 | 2.26  | 1.39        | 1.33     |
| 45  | m     | 202 | 3PE  | O31-C3  | -2.25 | 1.40        | 1.45     |
| 46  | Z     | 203 | PC1  | O31-C3  | -2.25 | 1.40        | 1.45     |
| 45  | h     | 201 | 3PE  | O31-C3  | -2.25 | 1.40        | 1.45     |
| 46  | L     | 701 | PC1  | O31-C3  | -2.25 | 1.40        | 1.45     |
| 45  | Y     | 204 | 3PE  | O31-C3  | -2.24 | 1.40        | 1.45     |
| 45  | f     | 101 | 3PE  | O31-C3  | -2.24 | 1.40        | 1.45     |
| 46  | A     | 203 | PC1  | O31-C3  | -2.24 | 1.40        | 1.45     |
| 45  | q     | 201 | 3PE  | O31-C3  | -2.24 | 1.40        | 1.45     |
| 53  | X     | 201 | CDL  | OB8-CB6 | -2.24 | 1.40        | 1.45     |
| 45  | H     | 401 | 3PE  | O31-C3  | -2.24 | 1.40        | 1.45     |
| 45  | Y     | 203 | 3PE  | O31-C3  | -2.24 | 1.40        | 1.45     |
| 46  | B     | 202 | PC1  | O21-C21 | 2.24  | 1.40        | 1.34     |
| 56  | P     | 501 | NDP  | C5B-C4B | 2.23  | 1.58        | 1.51     |
| 54  | O     | 401 | DGT  | PG-O2G  | -2.23 | 1.46        | 1.54     |
| 45  | I     | 203 | 3PE  | O31-C3  | -2.23 | 1.40        | 1.45     |
| 45  | M     | 602 | 3PE  | O31-C3  | -2.23 | 1.40        | 1.45     |
| 45  | A     | 201 | 3PE  | O31-C3  | -2.22 | 1.40        | 1.45     |
| 46  | H     | 403 | PC1  | O31-C3  | -2.22 | 1.40        | 1.45     |
| 45  | L     | 702 | 3PE  | O31-C3  | -2.22 | 1.40        | 1.45     |
| 45  | N     | 403 | 3PE  | O31-C3  | -2.22 | 1.40        | 1.45     |
| 54  | O     | 401 | DGT  | PG-O1G  | -2.22 | 1.46        | 1.54     |
| 45  | Y     | 205 | 3PE  | O31-C3  | -2.22 | 1.40        | 1.45     |
| 46  | d     | 202 | PC1  | O21-C21 | 2.22  | 1.40        | 1.34     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 45  | Y     | 206 | 3PE  | O31-C3  | -2.22 | 1.40        | 1.45     |
| 53  | i     | 202 | CDL  | OA8-CA6 | -2.21 | 1.40        | 1.45     |
| 53  | h     | 203 | CDL  | OA8-CA6 | -2.20 | 1.40        | 1.45     |
| 46  | d     | 202 | PC1  | O31-C3  | -2.20 | 1.40        | 1.45     |
| 45  | M     | 604 | 3PE  | O31-C3  | -2.20 | 1.40        | 1.45     |
| 45  | Y     | 203 | 3PE  | O21-C21 | 2.20  | 1.40        | 1.34     |
| 45  | Z     | 202 | 3PE  | O31-C3  | -2.19 | 1.40        | 1.45     |
| 45  | r     | 201 | 3PE  | O31-C3  | -2.19 | 1.40        | 1.45     |
| 45  | f     | 101 | 3PE  | O21-C21 | 2.19  | 1.40        | 1.34     |
| 46  | h     | 202 | PC1  | O21-C21 | 2.19  | 1.40        | 1.34     |
| 45  | b     | 102 | 3PE  | O21-C21 | 2.19  | 1.40        | 1.34     |
| 46  | A     | 202 | PC1  | O21-C21 | 2.19  | 1.40        | 1.34     |
| 45  | N     | 401 | 3PE  | O31-C3  | -2.19 | 1.40        | 1.45     |
| 45  | M     | 602 | 3PE  | O21-C21 | 2.19  | 1.40        | 1.34     |
| 53  | N     | 404 | CDL  | OA6-CA5 | 2.19  | 1.40        | 1.34     |
| 45  | Z     | 201 | 3PE  | O31-C3  | -2.18 | 1.40        | 1.45     |
| 53  | M     | 607 | CDL  | OB8-CB6 | -2.18 | 1.40        | 1.45     |
| 45  | b     | 101 | 3PE  | O21-C21 | 2.18  | 1.40        | 1.34     |
| 46  | m     | 203 | PC1  | O21-C21 | 2.18  | 1.40        | 1.34     |
| 46  | M     | 606 | PC1  | O31-C3  | -2.18 | 1.40        | 1.45     |
| 46  | L     | 701 | PC1  | O21-C21 | 2.18  | 1.40        | 1.34     |
| 53  | r     | 202 | CDL  | OB8-CB6 | -2.18 | 1.40        | 1.45     |
| 46  | H     | 402 | PC1  | O21-C21 | 2.17  | 1.40        | 1.34     |
| 45  | A     | 201 | 3PE  | O21-C21 | 2.17  | 1.40        | 1.34     |
| 46  | A     | 202 | PC1  | O31-C3  | -2.17 | 1.40        | 1.45     |
| 45  | Y     | 205 | 3PE  | O21-C21 | 2.17  | 1.40        | 1.34     |
| 45  | Z     | 202 | 3PE  | O21-C21 | 2.17  | 1.40        | 1.34     |
| 53  | h     | 203 | CDL  | OB6-CB5 | 2.17  | 1.40        | 1.34     |
| 53  | i     | 202 | CDL  | OB8-CB6 | -2.17 | 1.40        | 1.45     |
| 45  | Y     | 207 | 3PE  | O31-C3  | -2.17 | 1.40        | 1.45     |
| 45  | J     | 201 | 3PE  | O21-C21 | 2.17  | 1.40        | 1.34     |
| 45  | M     | 605 | 3PE  | O31-C3  | -2.16 | 1.40        | 1.45     |
| 53  | M     | 607 | CDL  | OA8-CA6 | -2.16 | 1.40        | 1.45     |
| 46  | H     | 403 | PC1  | O21-C21 | 2.16  | 1.40        | 1.34     |
| 46  | h     | 202 | PC1  | O31-C3  | -2.16 | 1.40        | 1.45     |
| 53  | h     | 203 | CDL  | OA6-CA5 | 2.16  | 1.40        | 1.34     |
| 45  | m     | 202 | 3PE  | O21-C21 | 2.16  | 1.40        | 1.34     |
| 53  | N     | 404 | CDL  | OB8-CB6 | -2.16 | 1.40        | 1.45     |
| 46  | Z     | 203 | PC1  | O21-C21 | 2.16  | 1.40        | 1.34     |
| 53  | d     | 204 | CDL  | OB8-CB6 | -2.16 | 1.40        | 1.45     |
| 53  | X     | 201 | CDL  | OA6-CA5 | 2.16  | 1.40        | 1.34     |
| 45  | L     | 702 | 3PE  | O21-C21 | 2.16  | 1.40        | 1.34     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 53  | i     | 202 | CDL  | OB6-CB5 | 2.15  | 1.40        | 1.34     |
| 45  | d     | 201 | 3PE  | O31-C3  | -2.15 | 1.40        | 1.45     |
| 53  | M     | 607 | CDL  | OA6-CA5 | 2.15  | 1.40        | 1.34     |
| 46  | g     | 201 | PC1  | O21-C21 | 2.15  | 1.40        | 1.34     |
| 45  | Y     | 207 | 3PE  | O21-C21 | 2.15  | 1.40        | 1.34     |
| 45  | M     | 603 | 3PE  | O21-C21 | 2.15  | 1.40        | 1.34     |
| 45  | Y     | 202 | 3PE  | O21-C21 | 2.15  | 1.40        | 1.34     |
| 45  | I     | 203 | 3PE  | O21-C21 | 2.14  | 1.40        | 1.34     |
| 53  | h     | 203 | CDL  | OB8-CB6 | -2.14 | 1.40        | 1.45     |
| 45  | M     | 604 | 3PE  | O21-C21 | 2.14  | 1.40        | 1.34     |
| 45  | J     | 202 | 3PE  | O31-C3  | -2.14 | 1.40        | 1.45     |
| 46  | m     | 203 | PC1  | O31-C3  | -2.14 | 1.40        | 1.45     |
| 46  | q     | 202 | PC1  | O31-C3  | -2.13 | 1.40        | 1.45     |
| 53  | d     | 204 | CDL  | OB6-CB5 | 2.13  | 1.40        | 1.34     |
| 45  | Y     | 201 | 3PE  | O21-C21 | 2.13  | 1.40        | 1.34     |
| 46  | I     | 204 | PC1  | O31-C3  | -2.13 | 1.40        | 1.45     |
| 56  | P     | 501 | NDP  | C5D-C4D | 2.13  | 1.58        | 1.51     |
| 46  | M     | 606 | PC1  | O21-C21 | 2.13  | 1.40        | 1.34     |
| 53  | r     | 202 | CDL  | OA8-CA6 | -2.13 | 1.40        | 1.45     |
| 53  | N     | 404 | CDL  | OA8-CA6 | -2.12 | 1.40        | 1.45     |
| 53  | i     | 202 | CDL  | OA6-CA5 | 2.12  | 1.40        | 1.34     |
| 45  | K     | 101 | 3PE  | O21-C21 | 2.12  | 1.40        | 1.34     |
| 45  | Y     | 202 | 3PE  | O31-C3  | -2.12 | 1.40        | 1.45     |
| 45  | H     | 401 | 3PE  | O21-C21 | 2.12  | 1.40        | 1.34     |
| 45  | Y     | 204 | 3PE  | O21-C21 | 2.12  | 1.40        | 1.34     |
| 46  | H     | 402 | PC1  | O31-C3  | -2.11 | 1.40        | 1.45     |
| 46  | q     | 202 | PC1  | O21-C21 | 2.11  | 1.40        | 1.34     |
| 53  | X     | 201 | CDL  | OB6-CB5 | 2.11  | 1.40        | 1.34     |
| 46  | g     | 201 | PC1  | O31-C3  | -2.11 | 1.40        | 1.45     |
| 45  | Y     | 201 | 3PE  | O31-C3  | -2.11 | 1.40        | 1.45     |
| 45  | J     | 201 | 3PE  | O31-C3  | -2.11 | 1.40        | 1.45     |
| 45  | r     | 201 | 3PE  | O21-C21 | 2.10  | 1.40        | 1.34     |
| 45  | Y     | 206 | 3PE  | O21-C21 | 2.10  | 1.40        | 1.34     |
| 45  | J     | 202 | 3PE  | O21-C21 | 2.10  | 1.40        | 1.34     |
| 45  | N     | 402 | 3PE  | O21-C21 | 2.10  | 1.40        | 1.34     |
| 45  | m     | 201 | 3PE  | O21-C21 | 2.09  | 1.40        | 1.34     |
| 45  | M     | 605 | 3PE  | O21-C21 | 2.09  | 1.40        | 1.34     |
| 53  | M     | 607 | CDL  | OB6-CB5 | 2.09  | 1.40        | 1.34     |
| 46  | A     | 203 | PC1  | O21-C21 | 2.08  | 1.40        | 1.34     |
| 45  | h     | 201 | 3PE  | O21-C21 | 2.08  | 1.40        | 1.34     |
| 45  | Z     | 201 | 3PE  | O21-C21 | 2.08  | 1.40        | 1.34     |
| 53  | N     | 404 | CDL  | OB6-CB5 | 2.07  | 1.40        | 1.34     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 45  | N     | 402 | 3PE  | O31-C3  | -2.07 | 1.40        | 1.45     |
| 53  | d     | 204 | CDL  | OA6-CA5 | 2.07  | 1.40        | 1.34     |
| 45  | d     | 201 | 3PE  | O21-C21 | 2.07  | 1.40        | 1.34     |
| 53  | X     | 201 | CDL  | OA8-CA6 | -2.07 | 1.40        | 1.45     |
| 46  | I     | 204 | PC1  | O21-C21 | 2.06  | 1.40        | 1.34     |
| 45  | N     | 403 | 3PE  | O21-C21 | 2.06  | 1.40        | 1.34     |
| 45  | q     | 201 | 3PE  | O21-C21 | 2.05  | 1.40        | 1.34     |
| 53  | r     | 202 | CDL  | OA6-CA5 | 2.04  | 1.40        | 1.34     |
| 53  | r     | 202 | CDL  | OB6-CB5 | 2.04  | 1.40        | 1.34     |

All (176) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 56  | P     | 501 | NDP  | C5A-C6A-N6A | 8.87  | 133.82      | 120.31   |
| 58  | i     | 201 | CHD  | C13-C17-C20 | -7.39 | 110.53      | 119.48   |
| 56  | P     | 501 | NDP  | C1B-N9A-C4A | -7.14 | 114.09      | 126.64   |
| 56  | P     | 501 | NDP  | N3A-C2A-N1A | -6.30 | 120.12      | 128.67   |
| 58  | i     | 201 | CHD  | C14-C13-C12 | 6.17  | 113.06      | 107.42   |
| 56  | P     | 501 | NDP  | N6A-C6A-N1A | -5.93 | 105.66      | 118.33   |
| 57  | T     | 101 | EHZ  | C8-C9-S1    | 5.84  | 120.92      | 113.56   |
| 58  | i     | 201 | CHD  | C17-C13-C14 | 5.41  | 105.54      | 100.11   |
| 57  | U     | 101 | EHZ  | C8-C9-S1    | 4.92  | 119.77      | 113.56   |
| 50  | F     | 502 | FMN  | C9-C8-C7    | 4.72  | 126.62      | 119.69   |
| 50  | F     | 502 | FMN  | C7M-C7-C6   | 4.72  | 127.89      | 119.57   |
| 45  | M     | 605 | 3PE  | O21-C21-C22 | 4.54  | 121.31      | 111.48   |
| 46  | B     | 202 | PC1  | O21-C21-C22 | 4.40  | 120.99      | 111.48   |
| 45  | m     | 201 | 3PE  | O21-C21-C22 | 4.29  | 120.77      | 111.48   |
| 58  | i     | 201 | CHD  | C18-C13-C12 | -4.29 | 104.77      | 109.06   |
| 53  | M     | 607 | CDL  | OA6-CA5-C11 | 4.28  | 120.75      | 111.48   |
| 46  | h     | 202 | PC1  | O21-C21-C22 | 4.26  | 120.70      | 111.48   |
| 45  | b     | 102 | 3PE  | O21-C21-C22 | 4.22  | 120.61      | 111.48   |
| 46  | H     | 402 | PC1  | O21-C21-C22 | 4.22  | 120.61      | 111.48   |
| 45  | f     | 101 | 3PE  | O21-C21-C22 | 4.22  | 120.60      | 111.48   |
| 58  | i     | 201 | CHD  | C17-C13-C12 | 4.21  | 121.46      | 117.67   |
| 45  | N     | 402 | 3PE  | O21-C21-C22 | 4.17  | 120.50      | 111.48   |
| 45  | J     | 201 | 3PE  | O21-C21-C22 | 4.16  | 120.49      | 111.48   |
| 46  | I     | 204 | PC1  | O21-C21-C22 | 4.14  | 120.43      | 111.48   |
| 46  | m     | 203 | PC1  | O21-C21-C22 | 4.10  | 120.36      | 111.48   |
| 45  | M     | 604 | 3PE  | O21-C21-C22 | 4.10  | 120.35      | 111.48   |
| 45  | m     | 202 | 3PE  | O21-C21-C22 | 4.09  | 120.33      | 111.48   |
| 53  | M     | 607 | CDL  | OB6-CB5-C51 | 4.09  | 120.32      | 111.48   |
| 45  | N     | 403 | 3PE  | O21-C21-C22 | 4.08  | 120.31      | 111.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 53  | X     | 201 | CDL  | OB6-CB5-C51 | 4.08  | 120.31      | 111.48   |
| 53  | i     | 202 | CDL  | OA6-CA5-C11 | 4.07  | 120.29      | 111.48   |
| 45  | Y     | 205 | 3PE  | O21-C21-C22 | 4.06  | 120.27      | 111.48   |
| 45  | q     | 201 | 3PE  | O21-C21-C22 | 4.05  | 120.25      | 111.48   |
| 45  | Y     | 206 | 3PE  | O21-C21-C22 | 4.04  | 120.21      | 111.48   |
| 45  | I     | 203 | 3PE  | O21-C21-C22 | 4.01  | 120.16      | 111.48   |
| 45  | h     | 201 | 3PE  | O21-C21-C22 | 3.99  | 120.12      | 111.48   |
| 45  | Y     | 207 | 3PE  | O21-C21-C22 | 3.99  | 120.11      | 111.48   |
| 45  | Y     | 204 | 3PE  | O21-C21-C22 | 3.96  | 120.05      | 111.48   |
| 45  | N     | 401 | 3PE  | O21-C21-C22 | 3.95  | 120.03      | 111.48   |
| 46  | Z     | 203 | PC1  | O21-C21-C22 | 3.95  | 120.02      | 111.48   |
| 45  | Y     | 203 | 3PE  | O21-C21-C22 | 3.94  | 120.01      | 111.48   |
| 53  | h     | 203 | CDL  | OB6-CB5-C51 | 3.94  | 120.01      | 111.48   |
| 46  | g     | 201 | PC1  | O21-C21-C22 | 3.94  | 120.00      | 111.48   |
| 46  | A     | 202 | PC1  | O21-C21-C22 | 3.94  | 120.00      | 111.48   |
| 46  | M     | 606 | PC1  | O21-C21-C22 | 3.93  | 119.98      | 111.48   |
| 53  | d     | 204 | CDL  | OA6-CA5-C11 | 3.92  | 119.95      | 111.48   |
| 53  | r     | 202 | CDL  | OA6-CA5-C11 | 3.91  | 119.94      | 111.48   |
| 45  | r     | 201 | 3PE  | O21-C21-C22 | 3.91  | 119.94      | 111.48   |
| 46  | A     | 203 | PC1  | O21-C21-C22 | 3.90  | 119.91      | 111.48   |
| 53  | N     | 404 | CDL  | OB6-CB5-C51 | 3.89  | 119.89      | 111.48   |
| 45  | J     | 202 | 3PE  | O21-C21-C22 | 3.89  | 119.89      | 111.48   |
| 53  | i     | 202 | CDL  | OB6-CB5-C51 | 3.88  | 119.88      | 111.48   |
| 45  | M     | 603 | 3PE  | O21-C21-C22 | 3.86  | 119.84      | 111.48   |
| 45  | A     | 201 | 3PE  | O21-C21-C22 | 3.85  | 119.82      | 111.48   |
| 58  | i     | 201 | CHD  | C18-C13-C17 | -3.84 | 105.19      | 111.20   |
| 45  | Z     | 202 | 3PE  | O21-C21-C22 | 3.83  | 119.77      | 111.48   |
| 45  | Y     | 201 | 3PE  | O21-C21-C22 | 3.80  | 119.71      | 111.48   |
| 45  | L     | 702 | 3PE  | O21-C21-C22 | 3.80  | 119.70      | 111.48   |
| 45  | Y     | 202 | 3PE  | O21-C21-C22 | 3.80  | 119.70      | 111.48   |
| 45  | d     | 201 | 3PE  | O21-C21-C22 | 3.79  | 119.68      | 111.48   |
| 45  | K     | 101 | 3PE  | O21-C21-C22 | 3.77  | 119.63      | 111.48   |
| 53  | X     | 201 | CDL  | OA6-CA5-C11 | 3.72  | 119.52      | 111.48   |
| 46  | d     | 202 | PC1  | O21-C21-C22 | 3.71  | 119.51      | 111.48   |
| 53  | N     | 404 | CDL  | OA6-CA5-C11 | 3.67  | 119.42      | 111.48   |
| 53  | h     | 203 | CDL  | OA6-CA5-C11 | 3.67  | 119.41      | 111.48   |
| 58  | i     | 201 | CHD  | C18-C13-C14 | -3.63 | 105.52      | 111.20   |
| 53  | r     | 202 | CDL  | OB6-CB5-C51 | 3.60  | 119.27      | 111.48   |
| 45  | b     | 101 | 3PE  | O21-C21-C22 | 3.58  | 119.23      | 111.48   |
| 46  | L     | 701 | PC1  | O21-C21-C22 | 3.45  | 118.95      | 111.48   |
| 45  | Z     | 201 | 3PE  | O21-C21-C22 | 3.43  | 118.91      | 111.48   |
| 50  | F     | 502 | FMN  | C4-N3-C2    | -3.38 | 119.64      | 125.64   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 50  | F     | 502 | FMN  | C8M-C8-C7   | -3.34 | 113.93      | 120.76   |
| 57  | T     | 101 | EHZ  | C13-C12-N1  | 3.24  | 122.25      | 116.34   |
| 54  | O     | 401 | DGT  | C2-N1-C6    | -3.16 | 119.32      | 125.11   |
| 53  | X     | 201 | CDL  | OB8-CB7-C71 | 3.14  | 121.41      | 111.83   |
| 58  | i     | 201 | CHD  | C1-C10-C5   | 3.13  | 112.25      | 107.75   |
| 58  | i     | 201 | CHD  | C15-C14-C8  | 3.06  | 122.56      | 118.36   |
| 45  | Y     | 202 | 3PE  | O31-C31-C32 | 3.04  | 121.11      | 111.83   |
| 45  | N     | 401 | 3PE  | O31-C31-C32 | 3.00  | 120.97      | 111.83   |
| 54  | O     | 401 | DGT  | O2G-PG-O3B  | 2.97  | 114.60      | 104.64   |
| 46  | I     | 204 | PC1  | O31-C31-C32 | 2.95  | 120.84      | 111.83   |
| 45  | J     | 202 | 3PE  | O31-C31-C32 | 2.91  | 119.98      | 111.15   |
| 54  | O     | 401 | DGT  | C5-C6-N1    | 2.88  | 119.57      | 114.07   |
| 46  | A     | 203 | PC1  | O31-C31-C32 | 2.88  | 120.61      | 111.83   |
| 46  | B     | 202 | PC1  | O31-C31-C32 | 2.85  | 120.52      | 111.83   |
| 57  | U     | 101 | EHZ  | C10-S1-C9   | 2.85  | 110.26      | 101.84   |
| 57  | T     | 101 | EHZ  | C10-S1-C9   | 2.84  | 110.25      | 101.84   |
| 46  | H     | 403 | PC1  | O31-C31-C32 | 2.82  | 120.44      | 111.83   |
| 46  | A     | 202 | PC1  | O31-C31-C32 | 2.82  | 120.44      | 111.83   |
| 45  | r     | 201 | 3PE  | O31-C31-C32 | 2.82  | 120.44      | 111.83   |
| 53  | M     | 607 | CDL  | OB8-CB7-C71 | 2.82  | 120.43      | 111.83   |
| 45  | m     | 201 | 3PE  | O31-C31-C32 | 2.82  | 120.43      | 111.83   |
| 58  | i     | 201 | CHD  | C6-C5-C4    | -2.81 | 108.02      | 111.23   |
| 46  | m     | 203 | PC1  | O31-C31-C32 | 2.80  | 120.37      | 111.83   |
| 45  | I     | 203 | 3PE  | O31-C31-C32 | 2.79  | 120.33      | 111.83   |
| 53  | M     | 607 | CDL  | OA8-CA7-C31 | 2.78  | 120.31      | 111.83   |
| 45  | Y     | 203 | 3PE  | O31-C31-C32 | 2.77  | 120.30      | 111.83   |
| 45  | N     | 402 | 3PE  | O31-C31-C32 | 2.77  | 120.28      | 111.83   |
| 53  | i     | 202 | CDL  | OA8-CA7-C31 | 2.77  | 120.27      | 111.83   |
| 50  | F     | 502 | FMN  | C6-C7-C8    | -2.76 | 115.63      | 119.69   |
| 45  | M     | 602 | 3PE  | O31-C31-C32 | 2.76  | 120.24      | 111.83   |
| 46  | M     | 606 | PC1  | O31-C31-C32 | 2.76  | 120.24      | 111.83   |
| 46  | H     | 402 | PC1  | O31-C31-C32 | 2.76  | 120.24      | 111.83   |
| 45  | Y     | 204 | 3PE  | O31-C31-C32 | 2.75  | 120.21      | 111.83   |
| 46  | h     | 202 | PC1  | O31-C31-C32 | 2.75  | 120.21      | 111.83   |
| 53  | d     | 204 | CDL  | OB8-CB7-C71 | 2.74  | 120.20      | 111.83   |
| 58  | i     | 201 | CHD  | C9-C10-C5   | 2.74  | 112.33      | 108.51   |
| 45  | H     | 401 | 3PE  | O31-C31-C32 | 2.73  | 120.16      | 111.83   |
| 53  | h     | 203 | CDL  | OA8-CA7-C31 | 2.73  | 120.16      | 111.83   |
| 53  | N     | 404 | CDL  | OA8-CA7-C31 | 2.73  | 120.15      | 111.83   |
| 54  | O     | 401 | DGT  | O1G-PG-O3B  | 2.73  | 113.78      | 104.64   |
| 45  | h     | 201 | 3PE  | O31-C31-C32 | 2.73  | 120.14      | 111.83   |
| 45  | f     | 101 | 3PE  | O31-C31-C32 | 2.72  | 120.12      | 111.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 53  | i     | 202 | CDL  | OB8-CB7-C71 | 2.71  | 120.09      | 111.83   |
| 45  | Y     | 205 | 3PE  | O31-C31-C32 | 2.71  | 120.09      | 111.83   |
| 45  | b     | 102 | 3PE  | O31-C31-C32 | 2.71  | 120.08      | 111.83   |
| 46  | g     | 201 | PC1  | O31-C31-C32 | 2.70  | 120.07      | 111.83   |
| 45  | Y     | 206 | 3PE  | O31-C31-C32 | 2.69  | 120.03      | 111.83   |
| 50  | F     | 502 | FMN  | C4A-C10-N10 | 2.69  | 120.33      | 116.48   |
| 45  | q     | 201 | 3PE  | O31-C31-C32 | 2.69  | 120.03      | 111.83   |
| 45  | A     | 201 | 3PE  | O31-C31-C32 | 2.69  | 120.02      | 111.83   |
| 45  | N     | 403 | 3PE  | O31-C31-C32 | 2.68  | 120.02      | 111.83   |
| 45  | M     | 605 | 3PE  | O31-C31-C32 | 2.68  | 119.99      | 111.83   |
| 45  | Y     | 207 | 3PE  | O31-C31-C32 | 2.68  | 119.99      | 111.83   |
| 53  | d     | 204 | CDL  | OA8-CA7-C31 | 2.67  | 119.98      | 111.83   |
| 50  | F     | 502 | FMN  | C5A-C9A-N10 | 2.67  | 120.38      | 117.97   |
| 46  | L     | 701 | PC1  | O31-C31-C32 | 2.67  | 119.97      | 111.83   |
| 45  | L     | 702 | 3PE  | O31-C31-C32 | 2.67  | 119.96      | 111.83   |
| 45  | Y     | 201 | 3PE  | O31-C31-C32 | 2.66  | 119.95      | 111.83   |
| 45  | Z     | 201 | 3PE  | O31-C31-C32 | 2.65  | 119.93      | 111.83   |
| 45  | M     | 604 | 3PE  | O31-C31-C32 | 2.65  | 119.90      | 111.83   |
| 45  | m     | 202 | 3PE  | O31-C31-C32 | 2.64  | 119.89      | 111.83   |
| 53  | d     | 204 | CDL  | OB6-CB5-C51 | 2.64  | 120.62      | 110.93   |
| 57  | T     | 101 | EHZ  | O2-C9-C8    | -2.63 | 119.60      | 123.74   |
| 53  | X     | 201 | CDL  | OA8-CA7-C31 | 2.63  | 119.86      | 111.83   |
| 45  | d     | 201 | 3PE  | O31-C31-C32 | 2.60  | 119.76      | 111.83   |
| 46  | d     | 202 | PC1  | O31-C31-C32 | 2.60  | 119.75      | 111.83   |
| 53  | N     | 404 | CDL  | OB8-CB7-C71 | 2.59  | 119.74      | 111.83   |
| 53  | r     | 202 | CDL  | OB8-CB7-C71 | 2.59  | 119.73      | 111.83   |
| 45  | J     | 201 | 3PE  | O31-C31-C32 | 2.59  | 119.73      | 111.83   |
| 45  | K     | 101 | 3PE  | O31-C31-C32 | 2.59  | 119.72      | 111.83   |
| 45  | Z     | 202 | 3PE  | O31-C31-C32 | 2.58  | 119.69      | 111.83   |
| 53  | h     | 203 | CDL  | OB8-CB7-C71 | 2.58  | 119.69      | 111.83   |
| 46  | Z     | 203 | PC1  | O31-C31-C32 | 2.55  | 119.61      | 111.83   |
| 57  | T     | 101 | EHZ  | O2-C9-S1    | -2.52 | 119.48      | 122.68   |
| 45  | b     | 101 | 3PE  | O31-C31-C32 | 2.52  | 119.51      | 111.83   |
| 45  | H     | 401 | 3PE  | O21-C21-C22 | 2.50  | 120.12      | 110.93   |
| 45  | M     | 603 | 3PE  | O31-C31-C32 | 2.49  | 119.44      | 111.83   |
| 50  | F     | 502 | FMN  | C9A-C5A-N5  | -2.49 | 119.81      | 122.45   |
| 50  | F     | 502 | FMN  | C4A-C4-N3   | 2.48  | 119.58      | 113.25   |
| 53  | r     | 202 | CDL  | OA8-CA7-C31 | 2.47  | 119.37      | 111.83   |
| 50  | F     | 502 | FMN  | O4-C4-C4A   | -2.45 | 120.08      | 126.53   |
| 45  | M     | 602 | 3PE  | O21-C21-C22 | 2.42  | 119.81      | 110.93   |
| 58  | i     | 201 | CHD  | C19-C10-C9  | -2.40 | 107.95      | 111.18   |
| 54  | O     | 401 | DGT  | O1A-PA-O2A  | -2.39 | 101.35      | 112.44   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 46  | H     | 403 | PC1  | O21-C21-C22 | 2.38  | 119.68      | 110.93   |
| 50  | F     | 502 | FMN  | C6-C5A-C9A  | 2.35  | 122.28      | 119.05   |
| 54  | O     | 401 | DGT  | O1B-PB-O2B  | -2.33 | 101.59      | 112.44   |
| 54  | O     | 401 | DGT  | C2'-C3'-C4' | 2.32  | 107.51      | 102.80   |
| 58  | i     | 201 | CHD  | C1-C2-C3    | 2.31  | 113.54      | 110.48   |
| 46  | q     | 202 | PC1  | O21-C21-C22 | 2.29  | 119.35      | 110.93   |
| 57  | U     | 101 | EHZ  | C13-C12-N1  | 2.28  | 120.50      | 116.34   |
| 57  | U     | 101 | EHZ  | C16-C15-N2  | 2.25  | 120.76      | 116.48   |
| 57  | U     | 101 | EHZ  | O2-C9-C8    | -2.23 | 120.23      | 123.74   |
| 58  | i     | 201 | CHD  | C1-C10-C9   | -2.21 | 107.91      | 111.34   |
| 50  | F     | 502 | FMN  | C10-C4A-N5  | -2.20 | 120.31      | 124.81   |
| 58  | i     | 201 | CHD  | C13-C14-C8  | -2.15 | 112.00      | 114.72   |
| 58  | i     | 201 | CHD  | C11-C9-C10  | -2.12 | 111.55      | 113.70   |
| 57  | U     | 101 | EHZ  | O2-C9-S1    | -2.12 | 119.99      | 122.68   |
| 48  | g     | 202 | PLC  | C3-C2-C1    | 2.10  | 116.69      | 111.78   |
| 50  | F     | 502 | FMN  | C7M-C7-C8   | -2.10 | 116.48      | 120.76   |
| 57  | T     | 101 | EHZ  | O3-C12-N1   | -2.08 | 118.94      | 123.03   |
| 57  | U     | 101 | EHZ  | C14-N2-C15  | -2.05 | 118.87      | 122.55   |
| 54  | O     | 401 | DGT  | O6-C6-C5    | -2.04 | 120.28      | 124.32   |
| 48  | Y     | 208 | PLC  | C3-C2-C1    | 2.03  | 116.52      | 111.78   |
| 58  | i     | 201 | CHD  | C16-C17-C13 | 2.01  | 105.50      | 103.54   |

There are no chirality outliers.

All (1284) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 45  | A     | 201 | 3PE  | C11-O13-P-O11  |
| 45  | A     | 201 | 3PE  | C11-O13-P-O12  |
| 45  | A     | 201 | 3PE  | C11-O13-P-O14  |
| 45  | H     | 401 | 3PE  | C11-O13-P-O11  |
| 45  | H     | 401 | 3PE  | C11-O13-P-O12  |
| 45  | H     | 401 | 3PE  | C22-C21-O21-C2 |
| 45  | I     | 203 | 3PE  | C11-O13-P-O11  |
| 45  | I     | 203 | 3PE  | C11-O13-P-O14  |
| 45  | I     | 203 | 3PE  | O13-C11-C12-N  |
| 45  | I     | 203 | 3PE  | O22-C21-O21-C2 |
| 45  | I     | 203 | 3PE  | C22-C21-O21-C2 |
| 45  | J     | 201 | 3PE  | C11-O13-P-O11  |
| 45  | J     | 201 | 3PE  | C11-O13-P-O14  |
| 45  | J     | 201 | 3PE  | C12-C11-O13-P  |
| 45  | J     | 201 | 3PE  | O22-C21-O21-C2 |
| 45  | J     | 202 | 3PE  | C11-O13-P-O11  |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 45  | J     | 202 | 3PE  | C11-O13-P-O12  |
| 45  | K     | 101 | 3PE  | C1-O11-P-O12   |
| 45  | K     | 101 | 3PE  | C1-O11-P-O13   |
| 45  | K     | 101 | 3PE  | C11-O13-P-O12  |
| 45  | K     | 101 | 3PE  | O11-C1-C2-O21  |
| 45  | L     | 702 | 3PE  | C1-O11-P-O12   |
| 45  | L     | 702 | 3PE  | C1-O11-P-O13   |
| 45  | L     | 702 | 3PE  | C11-O13-P-O11  |
| 45  | L     | 702 | 3PE  | C11-O13-P-O12  |
| 45  | L     | 702 | 3PE  | C11-O13-P-O14  |
| 45  | L     | 702 | 3PE  | C22-C21-O21-C2 |
| 45  | M     | 602 | 3PE  | C11-O13-P-O14  |
| 45  | M     | 602 | 3PE  | C12-C11-O13-P  |
| 45  | M     | 603 | 3PE  | C1-O11-P-O13   |
| 45  | M     | 603 | 3PE  | C1-O11-P-O14   |
| 45  | M     | 603 | 3PE  | C12-C11-O13-P  |
| 45  | M     | 604 | 3PE  | O22-C21-O21-C2 |
| 45  | M     | 604 | 3PE  | C22-C21-O21-C2 |
| 45  | M     | 605 | 3PE  | C1-O11-P-O14   |
| 45  | N     | 401 | 3PE  | C11-O13-P-O11  |
| 45  | N     | 401 | 3PE  | C11-O13-P-O14  |
| 45  | N     | 401 | 3PE  | C12-C11-O13-P  |
| 45  | N     | 402 | 3PE  | C11-O13-P-O11  |
| 45  | N     | 402 | 3PE  | C11-O13-P-O12  |
| 45  | N     | 402 | 3PE  | C11-O13-P-O14  |
| 45  | N     | 402 | 3PE  | O22-C21-O21-C2 |
| 45  | Y     | 201 | 3PE  | C1-O11-P-O13   |
| 45  | Y     | 201 | 3PE  | C1-O11-P-O14   |
| 45  | Y     | 201 | 3PE  | O13-C11-C12-N  |
| 45  | Y     | 202 | 3PE  | C1-O11-P-O14   |
| 45  | Y     | 202 | 3PE  | C11-O13-P-O11  |
| 45  | Y     | 202 | 3PE  | C11-O13-P-O14  |
| 45  | Y     | 202 | 3PE  | C22-C21-O21-C2 |
| 45  | Y     | 203 | 3PE  | C1-O11-P-O12   |
| 45  | Y     | 203 | 3PE  | C1-O11-P-O13   |
| 45  | Y     | 203 | 3PE  | C1-O11-P-O14   |
| 45  | Y     | 203 | 3PE  | C11-O13-P-O11  |
| 45  | Y     | 203 | 3PE  | C11-O13-P-O12  |
| 45  | Y     | 203 | 3PE  | C11-O13-P-O14  |
| 45  | Y     | 203 | 3PE  | C22-C21-O21-C2 |
| 45  | Y     | 204 | 3PE  | C1-O11-P-O13   |
| 45  | Y     | 204 | 3PE  | C1-O11-P-O14   |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 45  | Y     | 204 | 3PE  | C11-O13-P-O11  |
| 45  | Y     | 204 | 3PE  | C11-O13-P-O14  |
| 45  | Y     | 204 | 3PE  | C22-C21-O21-C2 |
| 45  | Y     | 205 | 3PE  | C11-O13-P-O11  |
| 45  | Y     | 205 | 3PE  | C11-O13-P-O12  |
| 45  | Y     | 205 | 3PE  | C11-O13-P-O14  |
| 45  | Y     | 206 | 3PE  | C11-O13-P-O11  |
| 45  | Y     | 206 | 3PE  | C11-O13-P-O12  |
| 45  | Y     | 206 | 3PE  | C11-O13-P-O14  |
| 45  | Y     | 206 | 3PE  | O22-C21-O21-C2 |
| 45  | Y     | 207 | 3PE  | C1-O11-P-O12   |
| 45  | Y     | 207 | 3PE  | C11-O13-P-O11  |
| 45  | Y     | 207 | 3PE  | C11-O13-P-O12  |
| 45  | Y     | 207 | 3PE  | O22-C21-O21-C2 |
| 45  | Y     | 207 | 3PE  | C22-C21-O21-C2 |
| 45  | Z     | 201 | 3PE  | C1-O11-P-O12   |
| 45  | Z     | 201 | 3PE  | C1-O11-P-O13   |
| 45  | Z     | 201 | 3PE  | C1-O11-P-O14   |
| 45  | Z     | 201 | 3PE  | C11-O13-P-O14  |
| 45  | Z     | 201 | 3PE  | O13-C11-C12-N  |
| 45  | Z     | 202 | 3PE  | C1-O11-P-O12   |
| 45  | Z     | 202 | 3PE  | C1-O11-P-O13   |
| 45  | Z     | 202 | 3PE  | C1-O11-P-O14   |
| 45  | b     | 101 | 3PE  | C1-O11-P-O13   |
| 45  | b     | 101 | 3PE  | C1-O11-P-O14   |
| 45  | b     | 102 | 3PE  | C1-O11-P-O12   |
| 45  | b     | 102 | 3PE  | C1-O11-P-O13   |
| 45  | b     | 102 | 3PE  | C12-C11-O13-P  |
| 45  | b     | 102 | 3PE  | O22-C21-O21-C2 |
| 45  | d     | 201 | 3PE  | C11-O13-P-O11  |
| 45  | d     | 201 | 3PE  | C11-O13-P-O12  |
| 45  | d     | 201 | 3PE  | C11-O13-P-O14  |
| 45  | d     | 201 | 3PE  | C22-C21-O21-C2 |
| 45  | f     | 101 | 3PE  | C1-O11-P-O13   |
| 45  | f     | 101 | 3PE  | C11-O13-P-O11  |
| 45  | f     | 101 | 3PE  | C11-O13-P-O12  |
| 45  | f     | 101 | 3PE  | C22-C21-O21-C2 |
| 45  | h     | 201 | 3PE  | C1-O11-P-O14   |
| 45  | h     | 201 | 3PE  | C11-O13-P-O11  |
| 45  | h     | 201 | 3PE  | C11-O13-P-O12  |
| 45  | h     | 201 | 3PE  | C11-O13-P-O14  |
| 45  | h     | 201 | 3PE  | O11-C1-C2-O21  |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 45  | h     | 201 | 3PE  | C22-C21-O21-C2 |
| 45  | m     | 201 | 3PE  | C11-O13-P-O12  |
| 45  | m     | 201 | 3PE  | O13-C11-C12-N  |
| 45  | m     | 201 | 3PE  | O32-C31-O31-C3 |
| 45  | m     | 201 | 3PE  | C32-C31-O31-C3 |
| 45  | m     | 201 | 3PE  | O22-C21-O21-C2 |
| 45  | m     | 202 | 3PE  | C1-O11-P-O13   |
| 45  | m     | 202 | 3PE  | C11-O13-P-O11  |
| 45  | m     | 202 | 3PE  | C11-O13-P-O12  |
| 45  | m     | 202 | 3PE  | C11-O13-P-O14  |
| 45  | m     | 202 | 3PE  | O13-C11-C12-N  |
| 45  | m     | 202 | 3PE  | O22-C21-O21-C2 |
| 45  | q     | 201 | 3PE  | C11-O13-P-O11  |
| 45  | q     | 201 | 3PE  | C11-O13-P-O12  |
| 45  | q     | 201 | 3PE  | C11-O13-P-O14  |
| 45  | q     | 201 | 3PE  | O22-C21-O21-C2 |
| 45  | r     | 201 | 3PE  | C1-O11-P-O12   |
| 45  | r     | 201 | 3PE  | C1-O11-P-O13   |
| 45  | r     | 201 | 3PE  | C1-O11-P-O14   |
| 45  | r     | 201 | 3PE  | C11-O13-P-O11  |
| 45  | r     | 201 | 3PE  | C11-O13-P-O12  |
| 45  | r     | 201 | 3PE  | C11-O13-P-O14  |
| 45  | r     | 201 | 3PE  | O32-C31-O31-C3 |
| 45  | r     | 201 | 3PE  | C22-C21-O21-C2 |
| 46  | A     | 202 | PC1  | C11-O13-P-O12  |
| 46  | A     | 202 | PC1  | C11-O13-P-O11  |
| 46  | A     | 202 | PC1  | O13-C11-C12-N  |
| 46  | A     | 203 | PC1  | C11-O13-P-O14  |
| 46  | A     | 203 | PC1  | C11-O13-P-O11  |
| 46  | A     | 203 | PC1  | C22-C21-O21-C2 |
| 46  | B     | 202 | PC1  | C11-O13-P-O14  |
| 46  | B     | 202 | PC1  | C11-O13-P-O11  |
| 46  | B     | 202 | PC1  | C1-O11-P-O12   |
| 46  | B     | 202 | PC1  | C1-O11-P-O14   |
| 46  | B     | 202 | PC1  | C1-O11-P-O13   |
| 46  | B     | 202 | PC1  | C2-C1-O11-P    |
| 46  | B     | 202 | PC1  | O22-C21-O21-C2 |
| 46  | H     | 402 | PC1  | C1-O11-P-O12   |
| 46  | H     | 402 | PC1  | C1-O11-P-O14   |
| 46  | H     | 402 | PC1  | C1-O11-P-O13   |
| 46  | H     | 402 | PC1  | O13-C11-C12-N  |
| 46  | H     | 403 | PC1  | C1-O11-P-O12   |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 46  | H     | 403 | PC1  | C1-O11-P-O13   |
| 46  | H     | 403 | PC1  | O13-C11-C12-N  |
| 46  | I     | 204 | PC1  | C1-O11-P-O12   |
| 46  | I     | 204 | PC1  | C1-O11-P-O14   |
| 46  | I     | 204 | PC1  | C1-O11-P-O13   |
| 46  | I     | 204 | PC1  | O13-C11-C12-N  |
| 46  | L     | 701 | PC1  | C11-O13-P-O12  |
| 46  | L     | 701 | PC1  | C11-O13-P-O14  |
| 46  | L     | 701 | PC1  | C11-O13-P-O11  |
| 46  | L     | 701 | PC1  | O21-C2-C3-O31  |
| 46  | L     | 701 | PC1  | O32-C31-O31-C3 |
| 46  | M     | 606 | PC1  | C1-O11-P-O14   |
| 46  | Z     | 203 | PC1  | C11-O13-P-O14  |
| 46  | Z     | 203 | PC1  | C11-O13-P-O11  |
| 46  | Z     | 203 | PC1  | C1-O11-P-O12   |
| 46  | d     | 202 | PC1  | C11-O13-P-O12  |
| 46  | d     | 202 | PC1  | C1-O11-P-O12   |
| 46  | d     | 202 | PC1  | C1-O11-P-O14   |
| 46  | d     | 202 | PC1  | C1-O11-P-O13   |
| 46  | d     | 202 | PC1  | O32-C31-O31-C3 |
| 46  | g     | 201 | PC1  | C11-O13-P-O12  |
| 46  | g     | 201 | PC1  | C1-O11-P-O12   |
| 46  | g     | 201 | PC1  | C1-O11-P-O14   |
| 46  | g     | 201 | PC1  | C1-O11-P-O13   |
| 46  | g     | 201 | PC1  | O13-C11-C12-N  |
| 46  | h     | 202 | PC1  | C11-O13-P-O12  |
| 46  | h     | 202 | PC1  | C11-O13-P-O14  |
| 46  | h     | 202 | PC1  | C11-O13-P-O11  |
| 46  | m     | 203 | PC1  | C11-O13-P-O12  |
| 46  | m     | 203 | PC1  | C11-O13-P-O14  |
| 46  | m     | 203 | PC1  | C11-O13-P-O11  |
| 46  | m     | 203 | PC1  | C1-O11-P-O14   |
| 46  | m     | 203 | PC1  | C1-O11-P-O13   |
| 46  | m     | 203 | PC1  | C22-C21-O21-C2 |
| 46  | q     | 202 | PC1  | C11-O13-P-O14  |
| 46  | q     | 202 | PC1  | C11-O13-P-O11  |
| 46  | q     | 202 | PC1  | O11-C1-C2-O21  |
| 48  | B     | 203 | PLC  | C4-O4P-P-O1P   |
| 48  | B     | 203 | PLC  | C4-O4P-P-O3P   |
| 48  | J     | 203 | PLC  | C4-O4P-P-O1P   |
| 48  | J     | 203 | PLC  | C4-O4P-P-O2P   |
| 48  | J     | 203 | PLC  | C4-O4P-P-O3P   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 48  | L     | 703 | PLC  | C2-C1-O3P-P     |
| 48  | L     | 703 | PLC  | C1-O3P-P-O1P    |
| 48  | L     | 703 | PLC  | C1-O3P-P-O2P    |
| 48  | L     | 703 | PLC  | C1-O3P-P-O4P    |
| 48  | Y     | 208 | PLC  | C1-O3P-P-O2P    |
| 48  | Y     | 208 | PLC  | C1-O3P-P-O4P    |
| 48  | Y     | 208 | PLC  | C4-O4P-P-O1P    |
| 48  | Z     | 204 | PLC  | C1'-C'-O2-C2    |
| 48  | Z     | 204 | PLC  | C1-O3P-P-O1P    |
| 48  | b     | 103 | PLC  | C1-O3P-P-O2P    |
| 48  | b     | 103 | PLC  | C1-O3P-P-O4P    |
| 48  | b     | 103 | PLC  | C4-O4P-P-O1P    |
| 48  | d     | 203 | PLC  | C1-O3P-P-O2P    |
| 48  | d     | 203 | PLC  | C4-O4P-P-O3P    |
| 48  | g     | 202 | PLC  | C1-O3P-P-O2P    |
| 48  | g     | 202 | PLC  | C1-O3P-P-O4P    |
| 50  | F     | 502 | FMN  | N10-C1'-C2'-O2' |
| 53  | M     | 607 | CDL  | CA2-OA2-PA1-OA3 |
| 53  | M     | 607 | CDL  | CA2-OA2-PA1-OA4 |
| 53  | M     | 607 | CDL  | CA2-OA2-PA1-OA5 |
| 53  | M     | 607 | CDL  | CA3-OA5-PA1-OA2 |
| 53  | M     | 607 | CDL  | CA3-OA5-PA1-OA3 |
| 53  | M     | 607 | CDL  | CA3-OA5-PA1-OA4 |
| 53  | M     | 607 | CDL  | CB2-OB2-PB2-OB4 |
| 53  | M     | 607 | CDL  | CB2-OB2-PB2-OB5 |
| 53  | M     | 607 | CDL  | CB3-OB5-PB2-OB2 |
| 53  | M     | 607 | CDL  | OB7-CB5-OB6-CB4 |
| 53  | N     | 404 | CDL  | CB2-OB2-PB2-OB3 |
| 53  | N     | 404 | CDL  | C51-CB5-OB6-CB4 |
| 53  | X     | 201 | CDL  | C1-CA2-OA2-PA1  |
| 53  | X     | 201 | CDL  | CA2-OA2-PA1-OA5 |
| 53  | X     | 201 | CDL  | CB3-OB5-PB2-OB2 |
| 53  | X     | 201 | CDL  | CB3-OB5-PB2-OB3 |
| 53  | X     | 201 | CDL  | CB3-OB5-PB2-OB4 |
| 53  | X     | 201 | CDL  | C51-CB5-OB6-CB4 |
| 53  | d     | 204 | CDL  | CB2-OB2-PB2-OB3 |
| 53  | d     | 204 | CDL  | CB2-OB2-PB2-OB5 |
| 53  | d     | 204 | CDL  | CB3-OB5-PB2-OB3 |
| 53  | d     | 204 | CDL  | OB7-CB5-OB6-CB4 |
| 53  | i     | 202 | CDL  | CB2-OB2-PB2-OB3 |
| 53  | i     | 202 | CDL  | CB2-OB2-PB2-OB4 |
| 53  | i     | 202 | CDL  | CB2-OB2-PB2-OB5 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 53  | r     | 202 | CDL  | CA3-OA5-PA1-OA2 |
| 53  | r     | 202 | CDL  | CA3-OA5-PA1-OA3 |
| 53  | r     | 202 | CDL  | C11-CA5-OA6-CA4 |
| 53  | r     | 202 | CDL  | OB5-CB3-CB4-OB6 |
| 54  | O     | 401 | DGT  | C5'-O5'-PA-O2A  |
| 56  | P     | 501 | NDP  | C5B-O5B-PA-O1A  |
| 56  | P     | 501 | NDP  | C5B-O5B-PA-O2A  |
| 56  | P     | 501 | NDP  | C5B-O5B-PA-O3   |
| 56  | P     | 501 | NDP  | C5D-O5D-PN-O3   |
| 56  | P     | 501 | NDP  | C5D-O5D-PN-O2N  |
| 57  | T     | 101 | EHZ  | C6-C7-C8-C9     |
| 57  | T     | 101 | EHZ  | C11-C10-S1-C9   |
| 57  | T     | 101 | EHZ  | C16-C17-C20-O6  |
| 57  | U     | 101 | EHZ  | O1-C7-C8-C9     |
| 57  | U     | 101 | EHZ  | S1-C10-C11-N1   |
| 57  | U     | 101 | EHZ  | C15-C16-C17-C19 |
| 57  | U     | 101 | EHZ  | C15-C16-C17-C20 |
| 57  | U     | 101 | EHZ  | C16-C17-C20-O6  |
| 57  | U     | 101 | EHZ  | C18-C17-C20-O6  |
| 57  | U     | 101 | EHZ  | C19-C17-C20-O6  |
| 57  | U     | 101 | EHZ  | O2-C9-S1-C10    |
| 57  | U     | 101 | EHZ  | C8-C9-S1-C10    |
| 45  | A     | 201 | 3PE  | O32-C31-O31-C3  |
| 45  | N     | 403 | 3PE  | O32-C31-O31-C3  |
| 45  | Y     | 204 | 3PE  | O32-C31-O31-C3  |
| 53  | X     | 201 | CDL  | OA9-CA7-OA8-CA6 |
| 53  | X     | 201 | CDL  | OB9-CB7-OB8-CB6 |
| 53  | d     | 204 | CDL  | OB9-CB7-OB8-CB6 |
| 45  | N     | 403 | 3PE  | C32-C31-O31-C3  |
| 45  | Y     | 204 | 3PE  | C32-C31-O31-C3  |
| 46  | L     | 701 | PC1  | C32-C31-O31-C3  |
| 53  | X     | 201 | CDL  | C31-CA7-OA8-CA6 |
| 53  | X     | 201 | CDL  | C71-CB7-OB8-CB6 |
| 53  | d     | 204 | CDL  | C71-CB7-OB8-CB6 |
| 45  | H     | 401 | 3PE  | O32-C31-O31-C3  |
| 45  | I     | 203 | 3PE  | O32-C31-O31-C3  |
| 45  | J     | 201 | 3PE  | O32-C31-O31-C3  |
| 45  | M     | 604 | 3PE  | O32-C31-O31-C3  |
| 45  | N     | 401 | 3PE  | O32-C31-O31-C3  |
| 45  | Y     | 203 | 3PE  | O32-C31-O31-C3  |
| 45  | Y     | 205 | 3PE  | O32-C31-O31-C3  |
| 45  | Y     | 206 | 3PE  | O32-C31-O31-C3  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 45  | h     | 201 | 3PE  | O32-C31-O31-C3  |
| 46  | A     | 203 | PC1  | O32-C31-O31-C3  |
| 46  | B     | 202 | PC1  | O32-C31-O31-C3  |
| 46  | H     | 403 | PC1  | O32-C31-O31-C3  |
| 46  | h     | 202 | PC1  | O32-C31-O31-C3  |
| 53  | M     | 607 | CDL  | OA9-CA7-OA8-CA6 |
| 53  | M     | 607 | CDL  | OB9-CB7-OB8-CB6 |
| 53  | h     | 203 | CDL  | OA9-CA7-OA8-CA6 |
| 53  | h     | 203 | CDL  | OB9-CB7-OB8-CB6 |
| 45  | H     | 401 | 3PE  | O22-C21-O21-C2  |
| 45  | L     | 702 | 3PE  | O22-C21-O21-C2  |
| 45  | Y     | 204 | 3PE  | O22-C21-O21-C2  |
| 45  | d     | 201 | 3PE  | O22-C21-O21-C2  |
| 45  | f     | 101 | 3PE  | O22-C21-O21-C2  |
| 45  | h     | 201 | 3PE  | O22-C21-O21-C2  |
| 45  | r     | 201 | 3PE  | O22-C21-O21-C2  |
| 46  | A     | 203 | PC1  | O22-C21-O21-C2  |
| 46  | I     | 204 | PC1  | O22-C21-O21-C2  |
| 46  | m     | 203 | PC1  | O22-C21-O21-C2  |
| 53  | N     | 404 | CDL  | OB7-CB5-OB6-CB4 |
| 53  | X     | 201 | CDL  | OB7-CB5-OB6-CB4 |
| 45  | A     | 201 | 3PE  | C32-C31-O31-C3  |
| 45  | H     | 401 | 3PE  | C32-C31-O31-C3  |
| 45  | J     | 201 | 3PE  | C32-C31-O31-C3  |
| 45  | M     | 604 | 3PE  | C32-C31-O31-C3  |
| 45  | N     | 401 | 3PE  | C32-C31-O31-C3  |
| 45  | Y     | 203 | 3PE  | C32-C31-O31-C3  |
| 45  | Y     | 205 | 3PE  | C32-C31-O31-C3  |
| 45  | Y     | 206 | 3PE  | C32-C31-O31-C3  |
| 45  | b     | 102 | 3PE  | C32-C31-O31-C3  |
| 45  | h     | 201 | 3PE  | C32-C31-O31-C3  |
| 45  | r     | 201 | 3PE  | C32-C31-O31-C3  |
| 46  | A     | 203 | PC1  | C32-C31-O31-C3  |
| 46  | B     | 202 | PC1  | C32-C31-O31-C3  |
| 46  | H     | 403 | PC1  | C32-C31-O31-C3  |
| 46  | M     | 606 | PC1  | C32-C31-O31-C3  |
| 46  | d     | 202 | PC1  | C32-C31-O31-C3  |
| 46  | h     | 202 | PC1  | C32-C31-O31-C3  |
| 53  | M     | 607 | CDL  | C31-CA7-OA8-CA6 |
| 53  | M     | 607 | CDL  | C71-CB7-OB8-CB6 |
| 53  | h     | 203 | CDL  | C31-CA7-OA8-CA6 |
| 45  | J     | 201 | 3PE  | C22-C21-O21-C2  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 45  | N     | 402 | 3PE  | C22-C21-O21-C2  |
| 45  | Y     | 206 | 3PE  | C22-C21-O21-C2  |
| 45  | b     | 102 | 3PE  | C22-C21-O21-C2  |
| 45  | m     | 201 | 3PE  | C22-C21-O21-C2  |
| 45  | m     | 202 | 3PE  | C22-C21-O21-C2  |
| 45  | q     | 201 | 3PE  | C22-C21-O21-C2  |
| 46  | B     | 202 | PC1  | C22-C21-O21-C2  |
| 46  | I     | 204 | PC1  | C22-C21-O21-C2  |
| 53  | M     | 607 | CDL  | C51-CB5-OB6-CB4 |
| 53  | d     | 204 | CDL  | C51-CB5-OB6-CB4 |
| 46  | m     | 203 | PC1  | O32-C31-O31-C3  |
| 53  | d     | 204 | CDL  | OA9-CA7-OA8-CA6 |
| 46  | q     | 202 | PC1  | O32-C31-O31-C3  |
| 45  | d     | 201 | 3PE  | O32-C31-O31-C3  |
| 45  | I     | 203 | 3PE  | C32-C31-O31-C3  |
| 45  | d     | 201 | 3PE  | C32-C31-O31-C3  |
| 46  | m     | 203 | PC1  | C32-C31-O31-C3  |
| 53  | N     | 404 | CDL  | C71-CB7-OB8-CB6 |
| 53  | h     | 203 | CDL  | C71-CB7-OB8-CB6 |
| 46  | M     | 606 | PC1  | O32-C31-O31-C3  |
| 53  | i     | 202 | CDL  | OA9-CA7-OA8-CA6 |
| 45  | Y     | 202 | 3PE  | O22-C21-O21-C2  |
| 45  | Y     | 203 | 3PE  | O22-C21-O21-C2  |
| 48  | Z     | 204 | PLC  | O'-C'-O2-C2     |
| 53  | r     | 202 | CDL  | OA7-CA5-OA6-CA4 |
| 46  | q     | 202 | PC1  | C32-C31-O31-C3  |
| 53  | M     | 607 | CDL  | O1-C1-CA2-OA2   |
| 53  | N     | 404 | CDL  | O1-C1-CA2-OA2   |
| 53  | d     | 204 | CDL  | O1-C1-CA2-OA2   |
| 46  | A     | 202 | PC1  | C32-C31-O31-C3  |
| 53  | d     | 204 | CDL  | C31-CA7-OA8-CA6 |
| 45  | b     | 102 | 3PE  | O32-C31-O31-C3  |
| 46  | A     | 202 | PC1  | O32-C31-O31-C3  |
| 53  | N     | 404 | CDL  | OB9-CB7-OB8-CB6 |
| 46  | M     | 606 | PC1  | C22-C21-O21-C2  |
| 46  | h     | 202 | PC1  | C22-C21-O21-C2  |
| 53  | X     | 201 | CDL  | C11-CA5-OA6-CA4 |
| 53  | i     | 202 | CDL  | C31-CA7-OA8-CA6 |
| 53  | X     | 201 | CDL  | OA7-CA5-OA6-CA4 |
| 45  | Y     | 207 | 3PE  | C32-C31-O31-C3  |
| 53  | i     | 202 | CDL  | C71-CB7-OB8-CB6 |
| 45  | Y     | 207 | 3PE  | O32-C31-O31-C3  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 53  | i     | 202 | CDL  | OB9-CB7-OB8-CB6 |
| 46  | H     | 403 | PC1  | C22-C21-O21-C2  |
| 46  | h     | 202 | PC1  | O22-C21-O21-C2  |
| 45  | Z     | 201 | 3PE  | C32-C31-O31-C3  |
| 45  | f     | 101 | 3PE  | C32-C31-O31-C3  |
| 45  | m     | 202 | 3PE  | C32-C31-O31-C3  |
| 46  | Z     | 203 | PC1  | C32-C31-O31-C3  |
| 53  | N     | 404 | CDL  | C31-CA7-OA8-CA6 |
| 48  | O     | 403 | PLC  | C4-C5-N-C8      |
| 45  | m     | 202 | 3PE  | O32-C31-O31-C3  |
| 53  | N     | 404 | CDL  | OA9-CA7-OA8-CA6 |
| 53  | d     | 204 | CDL  | CB7-C71-C72-C73 |
| 45  | f     | 101 | 3PE  | O32-C31-O31-C3  |
| 53  | M     | 607 | CDL  | OB5-CB3-CB4-OB6 |
| 46  | M     | 606 | PC1  | O21-C2-C3-O31   |
| 48  | O     | 403 | PLC  | O2-C2-C3-O3     |
| 53  | M     | 607 | CDL  | CB7-C71-C72-C73 |
| 45  | Y     | 204 | 3PE  | C21-C22-C23-C24 |
| 53  | r     | 202 | CDL  | CB5-C51-C52-C53 |
| 46  | B     | 202 | PC1  | C21-C22-C23-C24 |
| 48  | O     | 403 | PLC  | CB-C1B-C2B-C3B  |
| 46  | M     | 606 | PC1  | O22-C21-O21-C2  |
| 45  | N     | 401 | 3PE  | C31-C32-C33-C34 |
| 45  | Z     | 201 | 3PE  | C21-C22-C23-C24 |
| 46  | H     | 402 | PC1  | C21-C22-C23-C24 |
| 46  | Z     | 203 | PC1  | C31-C32-C33-C34 |
| 46  | d     | 202 | PC1  | C31-C32-C33-C34 |
| 45  | Z     | 201 | 3PE  | O32-C31-O31-C3  |
| 45  | A     | 201 | 3PE  | C31-C32-C33-C34 |
| 45  | b     | 102 | 3PE  | C21-C22-C23-C24 |
| 45  | f     | 101 | 3PE  | C21-C22-C23-C24 |
| 46  | A     | 202 | PC1  | C21-C22-C23-C24 |
| 46  | Z     | 203 | PC1  | O32-C31-O31-C3  |
| 45  | Y     | 201 | 3PE  | C32-C31-O31-C3  |
| 48  | b     | 103 | PLC  | C1B-CB-O3-C3    |
| 53  | M     | 607 | CDL  | CB5-C51-C52-C53 |
| 46  | H     | 403 | PC1  | O22-C21-O21-C2  |
| 45  | J     | 202 | 3PE  | C21-C22-C23-C24 |
| 45  | d     | 201 | 3PE  | C31-C32-C33-C34 |
| 45  | Z     | 202 | 3PE  | C32-C31-O31-C3  |
| 45  | Y     | 203 | 3PE  | C21-C22-C23-C24 |
| 53  | r     | 202 | CDL  | CA5-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 53  | N     | 404 | CDL  | CB2-C1-CA2-OA2  |
| 48  | O     | 403 | PLC  | C4-C5-N-C7      |
| 46  | g     | 201 | PC1  | C32-C31-O31-C3  |
| 46  | d     | 202 | PC1  | C21-C22-C23-C24 |
| 53  | M     | 607 | CDL  | C11-CA5-OA6-CA4 |
| 53  | d     | 204 | CDL  | C11-CA5-OA6-CA4 |
| 53  | M     | 607 | CDL  | OA7-CA5-OA6-CA4 |
| 53  | d     | 204 | CDL  | OA7-CA5-OA6-CA4 |
| 46  | I     | 204 | PC1  | C21-C22-C23-C24 |
| 45  | M     | 603 | 3PE  | C2-C1-O11-P     |
| 45  | Z     | 202 | 3PE  | C31-C32-C33-C34 |
| 45  | Y     | 201 | 3PE  | O32-C31-O31-C3  |
| 45  | K     | 101 | 3PE  | C22-C21-O21-C2  |
| 45  | M     | 603 | 3PE  | C22-C21-O21-C2  |
| 45  | M     | 605 | 3PE  | C22-C21-O21-C2  |
| 45  | N     | 401 | 3PE  | C22-C21-O21-C2  |
| 53  | i     | 202 | CDL  | C11-CA5-OA6-CA4 |
| 48  | O     | 403 | PLC  | C4-C5-N-C6      |
| 45  | K     | 101 | 3PE  | C35-C36-C37-C38 |
| 45  | Y     | 204 | 3PE  | C39-C3A-C3B-C3C |
| 45  | Y     | 206 | 3PE  | C36-C37-C38-C39 |
| 45  | Z     | 202 | 3PE  | C38-C39-C3A-C3B |
| 46  | L     | 701 | PC1  | C3B-C3C-C3D-C3E |
| 53  | X     | 201 | CDL  | C35-C36-C37-C38 |
| 45  | M     | 605 | 3PE  | C35-C36-C37-C38 |
| 45  | Y     | 203 | 3PE  | C26-C27-C28-C29 |
| 45  | Y     | 205 | 3PE  | C2A-C2B-C2C-C2D |
| 45  | b     | 102 | 3PE  | C28-C29-C2A-C2B |
| 46  | L     | 701 | PC1  | C29-C2A-C2B-C2C |
| 53  | M     | 607 | CDL  | C37-C38-C39-C40 |
| 53  | d     | 204 | CDL  | C72-C73-C74-C75 |
| 45  | Y     | 204 | 3PE  | C25-C26-C27-C28 |
| 45  | Y     | 207 | 3PE  | C2C-C2D-C2E-C2F |
| 46  | L     | 701 | PC1  | C32-C33-C34-C35 |
| 53  | M     | 607 | CDL  | C13-C14-C15-C16 |
| 59  | o     | 201 | MYR  | C2-C3-C4-C5     |
| 45  | Z     | 202 | 3PE  | O32-C31-O31-C3  |
| 48  | b     | 103 | PLC  | OB-CB-O3-C3     |
| 45  | A     | 201 | 3PE  | C24-C25-C26-C27 |
| 45  | M     | 605 | 3PE  | C33-C34-C35-C36 |
| 45  | N     | 403 | 3PE  | C24-C25-C26-C27 |
| 45  | Y     | 202 | 3PE  | C2C-C2D-C2E-C2F |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 45  | Y     | 207 | 3PE  | C3B-C3C-C3D-C3E |
| 45  | Z     | 202 | 3PE  | C29-C2A-C2B-C2C |
| 45  | h     | 201 | 3PE  | C33-C34-C35-C36 |
| 46  | H     | 403 | PC1  | C36-C37-C38-C39 |
| 53  | M     | 607 | CDL  | C18-C19-C20-C21 |
| 53  | X     | 201 | CDL  | C82-C83-C84-C85 |
| 57  | T     | 101 | EHZ  | C2-C3-C4-C5     |
| 45  | M     | 603 | 3PE  | C2D-C2E-C2F-C2G |
| 45  | Y     | 206 | 3PE  | C33-C34-C35-C36 |
| 45  | Z     | 202 | 3PE  | C2B-C2C-C2D-C2E |
| 53  | X     | 201 | CDL  | C37-C38-C39-C40 |
| 45  | q     | 201 | 3PE  | C21-C22-C23-C24 |
| 46  | M     | 606 | PC1  | C31-C32-C33-C34 |
| 45  | N     | 402 | 3PE  | C2C-C2D-C2E-C2F |
| 53  | h     | 203 | CDL  | C60-C61-C62-C63 |
| 45  | K     | 101 | 3PE  | C22-C23-C24-C25 |
| 45  | Z     | 202 | 3PE  | C35-C36-C37-C38 |
| 45  | f     | 101 | 3PE  | C24-C25-C26-C27 |
| 45  | J     | 202 | 3PE  | C22-C21-O21-C2  |
| 53  | r     | 202 | CDL  | C51-CB5-OB6-CB4 |
| 45  | H     | 401 | 3PE  | C3E-C3F-C3G-C3H |
| 45  | J     | 202 | 3PE  | C27-C28-C29-C2A |
| 45  | Y     | 202 | 3PE  | C2B-C2C-C2D-C2E |
| 57  | U     | 101 | EHZ  | C5-C6-C7-C8     |
| 45  | N     | 403 | 3PE  | C2A-C2B-C2C-C2D |
| 45  | Y     | 204 | 3PE  | C33-C34-C35-C36 |
| 53  | N     | 404 | CDL  | C17-C18-C19-C20 |
| 48  | b     | 103 | PLC  | C'-C1'-C2'-C3'  |
| 45  | L     | 702 | 3PE  | C3A-C3B-C3C-C3D |
| 46  | d     | 202 | PC1  | C36-C37-C38-C39 |
| 53  | N     | 404 | CDL  | C78-C79-C80-C81 |
| 53  | X     | 201 | CDL  | C58-C59-C60-C61 |
| 53  | i     | 202 | CDL  | C16-C17-C18-C19 |
| 45  | b     | 101 | 3PE  | C26-C27-C28-C29 |
| 45  | q     | 201 | 3PE  | C27-C28-C29-C2A |
| 48  | L     | 703 | PLC  | C3'-C4'-C5'-C6' |
| 53  | X     | 201 | CDL  | C61-C62-C63-C64 |
| 46  | I     | 204 | PC1  | C36-C37-C38-C39 |
| 53  | M     | 607 | CDL  | C32-C33-C34-C35 |
| 45  | M     | 603 | 3PE  | C3A-C3B-C3C-C3D |
| 45  | Y     | 205 | 3PE  | C33-C34-C35-C36 |
| 45  | Y     | 207 | 3PE  | C39-C3A-C3B-C3C |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 46  | L     | 701 | PC1  | C39-C3A-C3B-C3C |
| 57  | T     | 101 | EHZ  | C1-C2-C3-C4     |
| 45  | K     | 101 | 3PE  | O22-C21-O21-C2  |
| 45  | M     | 605 | 3PE  | O22-C21-O21-C2  |
| 45  | q     | 201 | 3PE  | C25-C26-C27-C28 |
| 45  | A     | 201 | 3PE  | C3C-C3D-C3E-C3F |
| 45  | N     | 401 | 3PE  | C24-C25-C26-C27 |
| 46  | H     | 403 | PC1  | C3A-C3B-C3C-C3D |
| 46  | I     | 204 | PC1  | C35-C36-C37-C38 |
| 53  | h     | 203 | CDL  | C34-C35-C36-C37 |
| 45  | N     | 403 | 3PE  | C31-C32-C33-C34 |
| 45  | Y     | 207 | 3PE  | C21-C22-C23-C24 |
| 45  | A     | 201 | 3PE  | C36-C37-C38-C39 |
| 45  | A     | 201 | 3PE  | C3E-C3F-C3G-C3H |
| 45  | M     | 604 | 3PE  | C35-C36-C37-C38 |
| 45  | M     | 605 | 3PE  | C2A-C2B-C2C-C2D |
| 45  | N     | 403 | 3PE  | C2D-C2E-C2F-C2G |
| 45  | Y     | 201 | 3PE  | C22-C23-C24-C25 |
| 45  | m     | 202 | 3PE  | C35-C36-C37-C38 |
| 46  | B     | 202 | PC1  | C38-C39-C3A-C3B |
| 48  | b     | 103 | PLC  | C4'-C5'-C6'-C7' |
| 53  | M     | 607 | CDL  | C57-C58-C59-C60 |
| 53  | N     | 404 | CDL  | C22-C23-C24-C25 |
| 53  | X     | 201 | CDL  | C51-C52-C53-C54 |
| 45  | N     | 403 | 3PE  | C28-C29-C2A-C2B |
| 45  | Y     | 207 | 3PE  | C33-C34-C35-C36 |
| 48  | O     | 403 | PLC  | C2'-C3'-C4'-C5' |
| 45  | f     | 101 | 3PE  | C34-C35-C36-C37 |
| 45  | m     | 202 | 3PE  | C33-C34-C35-C36 |
| 45  | A     | 201 | 3PE  | C34-C35-C36-C37 |
| 45  | Y     | 205 | 3PE  | C38-C39-C3A-C3B |
| 45  | q     | 201 | 3PE  | C3B-C3C-C3D-C3E |
| 46  | H     | 402 | PC1  | C24-C25-C26-C27 |
| 46  | H     | 402 | PC1  | C33-C34-C35-C36 |
| 53  | N     | 404 | CDL  | CA5-C11-C12-C13 |
| 53  | N     | 404 | CDL  | CB7-C71-C72-C73 |
| 46  | g     | 201 | PC1  | O32-C31-O31-C3  |
| 46  | d     | 202 | PC1  | C33-C34-C35-C36 |
| 46  | L     | 701 | PC1  | C35-C36-C37-C38 |
| 45  | K     | 101 | 3PE  | C32-C33-C34-C35 |
| 45  | N     | 401 | 3PE  | C2B-C2C-C2D-C2E |
| 46  | H     | 402 | PC1  | C34-C35-C36-C37 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 46  | M     | 606 | PC1  | C25-C26-C27-C28 |
| 53  | N     | 404 | CDL  | C12-C13-C14-C15 |
| 45  | Z     | 202 | 3PE  | C21-C22-C23-C24 |
| 53  | i     | 202 | CDL  | C12-C13-C14-C15 |
| 53  | M     | 607 | CDL  | C83-C84-C85-C86 |
| 53  | X     | 201 | CDL  | C77-C78-C79-C80 |
| 53  | i     | 202 | CDL  | C32-C33-C34-C35 |
| 45  | J     | 202 | 3PE  | O22-C21-O21-C2  |
| 45  | M     | 603 | 3PE  | O22-C21-O21-C2  |
| 45  | N     | 401 | 3PE  | O22-C21-O21-C2  |
| 53  | i     | 202 | CDL  | OA7-CA5-OA6-CA4 |
| 53  | r     | 202 | CDL  | OB7-CB5-OB6-CB4 |
| 45  | b     | 101 | 3PE  | C34-C35-C36-C37 |
| 46  | A     | 202 | PC1  | C23-C24-C25-C26 |
| 45  | N     | 401 | 3PE  | C32-C33-C34-C35 |
| 45  | Y     | 203 | 3PE  | C29-C2A-C2B-C2C |
| 45  | Y     | 205 | 3PE  | C25-C26-C27-C28 |
| 46  | H     | 402 | PC1  | C29-C2A-C2B-C2C |
| 45  | M     | 602 | 3PE  | C32-C31-O31-C3  |
| 46  | g     | 201 | PC1  | C26-C27-C28-C29 |
| 53  | N     | 404 | CDL  | C51-C52-C53-C54 |
| 45  | Y     | 203 | 3PE  | C2D-C2E-C2F-C2G |
| 45  | b     | 102 | 3PE  | C23-C24-C25-C26 |
| 45  | M     | 602 | 3PE  | C33-C34-C35-C36 |
| 45  | Y     | 207 | 3PE  | C35-C36-C37-C38 |
| 53  | M     | 607 | CDL  | C23-C24-C25-C26 |
| 45  | r     | 201 | 3PE  | C31-C32-C33-C34 |
| 53  | M     | 607 | CDL  | CA5-C11-C12-C13 |
| 45  | M     | 603 | 3PE  | C35-C36-C37-C38 |
| 45  | N     | 402 | 3PE  | C26-C27-C28-C29 |
| 53  | d     | 204 | CDL  | C35-C36-C37-C38 |
| 45  | J     | 202 | 3PE  | C29-C2A-C2B-C2C |
| 45  | N     | 401 | 3PE  | C27-C28-C29-C2A |
| 46  | m     | 203 | PC1  | C24-C25-C26-C27 |
| 45  | N     | 402 | 3PE  | C32-C31-O31-C3  |
| 45  | M     | 602 | 3PE  | C22-C21-O21-C2  |
| 45  | Z     | 201 | 3PE  | C22-C21-O21-C2  |
| 57  | T     | 101 | EHZ  | C12-C13-C14-N2  |
| 46  | h     | 202 | PC1  | C29-C2A-C2B-C2C |
| 48  | L     | 703 | PLC  | C5B-C6B-C7B-C8B |
| 45  | Z     | 201 | 3PE  | O22-C21-O21-C2  |
| 45  | Y     | 206 | 3PE  | C38-C39-C3A-C3B |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 48  | L     | 703 | PLC  | C7'-C8'-C9'-CA' |
| 45  | N     | 402 | 3PE  | C33-C34-C35-C36 |
| 46  | H     | 402 | PC1  | C32-C33-C34-C35 |
| 45  | Y     | 203 | 3PE  | C31-C32-C33-C34 |
| 45  | q     | 201 | 3PE  | C32-C33-C34-C35 |
| 45  | q     | 201 | 3PE  | C35-C36-C37-C38 |
| 53  | M     | 607 | CDL  | C14-C15-C16-C17 |
| 53  | h     | 203 | CDL  | C72-C73-C74-C75 |
| 53  | r     | 202 | CDL  | C71-C72-C73-C74 |
| 57  | U     | 101 | EHZ  | C5-C6-C7-O1     |
| 45  | b     | 102 | 3PE  | C33-C34-C35-C36 |
| 45  | M     | 602 | 3PE  | C31-C32-C33-C34 |
| 45  | b     | 102 | 3PE  | C2D-C2E-C2F-C2G |
| 46  | H     | 402 | PC1  | C28-C29-C2A-C2B |
| 45  | H     | 401 | 3PE  | O11-C1-C2-O21   |
| 45  | N     | 403 | 3PE  | O11-C1-C2-O21   |
| 53  | N     | 404 | CDL  | OA5-CA3-CA4-OA6 |
| 46  | Z     | 203 | PC1  | C22-C21-O21-C2  |
| 45  | A     | 201 | 3PE  | C3A-C3B-C3C-C3D |
| 45  | Y     | 203 | 3PE  | C3B-C3C-C3D-C3E |
| 53  | N     | 404 | CDL  | C55-C56-C57-C58 |
| 45  | f     | 101 | 3PE  | C32-C33-C34-C35 |
| 45  | M     | 603 | 3PE  | C31-C32-C33-C34 |
| 45  | L     | 702 | 3PE  | C35-C36-C37-C38 |
| 46  | A     | 203 | PC1  | C3C-C3D-C3E-C3F |
| 46  | H     | 402 | PC1  | O21-C2-C3-O31   |
| 46  | m     | 203 | PC1  | O21-C2-C3-O31   |
| 45  | N     | 401 | 3PE  | C2E-C2F-C2G-C2H |
| 48  | g     | 202 | PLC  | C1'-C2'-C3'-C4' |
| 45  | K     | 101 | 3PE  | C3A-C3B-C3C-C3D |
| 56  | P     | 501 | NDP  | O4D-C1D-N1N-C6N |
| 45  | Y     | 207 | 3PE  | C38-C39-C3A-C3B |
| 46  | A     | 203 | PC1  | C34-C35-C36-C37 |
| 45  | Z     | 202 | 3PE  | C2-C1-O11-P     |
| 45  | M     | 605 | 3PE  | C27-C28-C29-C2A |
| 46  | H     | 403 | PC1  | C3E-C3F-C3G-C3H |
| 45  | N     | 401 | 3PE  | C22-C23-C24-C25 |
| 45  | Y     | 204 | 3PE  | C34-C35-C36-C37 |
| 48  | J     | 203 | PLC  | C2B-C3B-C4B-C5B |
| 53  | d     | 204 | CDL  | C74-C75-C76-C77 |
| 45  | d     | 201 | 3PE  | C28-C29-C2A-C2B |
| 57  | U     | 101 | EHZ  | C22-C23-C24-C25 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 57  | T     | 101 | EHZ  | C22-C23-C24-C25 |
| 53  | N     | 404 | CDL  | C71-C72-C73-C74 |
| 45  | K     | 101 | 3PE  | O11-C1-C2-C3    |
| 45  | N     | 403 | 3PE  | O11-C1-C2-C3    |
| 45  | Y     | 202 | 3PE  | O11-C1-C2-C3    |
| 45  | Y     | 204 | 3PE  | O11-C1-C2-C3    |
| 45  | h     | 201 | 3PE  | O11-C1-C2-C3    |
| 45  | r     | 201 | 3PE  | O11-C1-C2-C3    |
| 53  | M     | 607 | CDL  | OB5-CB3-CB4-CB6 |
| 53  | N     | 404 | CDL  | OA5-CA3-CA4-CA6 |
| 53  | X     | 201 | CDL  | OA5-CA3-CA4-CA6 |
| 53  | i     | 202 | CDL  | OB5-CB3-CB4-CB6 |
| 53  | N     | 404 | CDL  | C72-C73-C74-C75 |
| 53  | i     | 202 | CDL  | CA5-C11-C12-C13 |
| 53  | M     | 607 | CDL  | C73-C74-C75-C76 |
| 45  | M     | 602 | 3PE  | O32-C31-O31-C3  |
| 45  | Y     | 204 | 3PE  | C29-C2A-C2B-C2C |
| 46  | d     | 202 | PC1  | C34-C35-C36-C37 |
| 45  | Y     | 203 | 3PE  | C34-C35-C36-C37 |
| 48  | B     | 203 | PLC  | C'-C1'-C2'-C3'  |
| 48  | B     | 203 | PLC  | C1'-C'-O2-C2    |
| 46  | L     | 701 | PC1  | C27-C28-C29-C2A |
| 45  | N     | 401 | 3PE  | C28-C29-C2A-C2B |
| 45  | q     | 201 | 3PE  | C1-C2-C3-O31    |
| 46  | H     | 402 | PC1  | C1-C2-C3-O31    |
| 46  | M     | 606 | PC1  | C1-C2-C3-O31    |
| 46  | h     | 202 | PC1  | C1-C2-C3-O31    |
| 48  | O     | 403 | PLC  | C1-C2-C3-O3     |
| 48  | Z     | 204 | PLC  | C1-C2-C3-O3     |
| 53  | h     | 203 | CDL  | CB3-CB4-CB6-OB8 |
| 45  | Y     | 202 | 3PE  | C35-C36-C37-C38 |
| 46  | Z     | 203 | PC1  | C37-C38-C39-C3A |
| 45  | M     | 605 | 3PE  | C23-C24-C25-C26 |
| 46  | H     | 403 | PC1  | C3B-C3C-C3D-C3E |
| 45  | N     | 403 | 3PE  | C23-C24-C25-C26 |
| 53  | h     | 203 | CDL  | C35-C36-C37-C38 |
| 45  | Y     | 203 | 3PE  | C38-C39-C3A-C3B |
| 45  | b     | 101 | 3PE  | C38-C39-C3A-C3B |
| 53  | h     | 203 | CDL  | C33-C34-C35-C36 |
| 53  | h     | 203 | CDL  | CA5-C11-C12-C13 |
| 45  | N     | 402 | 3PE  | O32-C31-O31-C3  |
| 46  | I     | 204 | PC1  | C25-C26-C27-C28 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 48  | J     | 203 | PLC  | C6B-C7B-C8B-C9B |
| 45  | N     | 403 | 3PE  | C34-C35-C36-C37 |
| 45  | Y     | 207 | 3PE  | C28-C29-C2A-C2B |
| 45  | f     | 101 | 3PE  | C2E-C2F-C2G-C2H |
| 48  | Z     | 204 | PLC  | CB-C1B-C2B-C3B  |
| 45  | Y     | 204 | 3PE  | C3-C2-O21-C21   |
| 45  | A     | 201 | 3PE  | C38-C39-C3A-C3B |
| 45  | M     | 603 | 3PE  | C2A-C2B-C2C-C2D |
| 45  | m     | 201 | 3PE  | C22-C23-C24-C25 |
| 45  | I     | 203 | 3PE  | C24-C25-C26-C27 |
| 45  | Z     | 202 | 3PE  | C3B-C3C-C3D-C3E |
| 53  | M     | 607 | CDL  | CB2-C1-CA2-OA2  |
| 48  | L     | 703 | PLC  | O3P-C1-C2-O2    |
| 48  | d     | 203 | PLC  | O3P-C1-C2-O2    |
| 45  | N     | 401 | 3PE  | C34-C35-C36-C37 |
| 48  | Z     | 204 | PLC  | C1B-CB-O3-C3    |
| 53  | X     | 201 | CDL  | C44-C45-C46-C47 |
| 53  | i     | 202 | CDL  | C72-C73-C74-C75 |
| 45  | I     | 203 | 3PE  | C22-C23-C24-C25 |
| 45  | M     | 602 | 3PE  | C35-C36-C37-C38 |
| 45  | M     | 603 | 3PE  | C23-C24-C25-C26 |
| 46  | L     | 701 | PC1  | C3E-C3F-C3G-C3H |
| 46  | g     | 201 | PC1  | C2F-C2G-C2H-C2I |
| 48  | g     | 202 | PLC  | C'-C1'-C2'-C3'  |
| 45  | M     | 603 | 3PE  | C3C-C3D-C3E-C3F |
| 53  | X     | 201 | CDL  | C71-C72-C73-C74 |
| 45  | A     | 201 | 3PE  | O21-C2-C3-O31   |
| 45  | q     | 201 | 3PE  | O21-C2-C3-O31   |
| 46  | d     | 202 | PC1  | O21-C2-C3-O31   |
| 53  | r     | 202 | CDL  | OA6-CA4-CA6-OA8 |
| 45  | Z     | 201 | 3PE  | C24-C25-C26-C27 |
| 53  | i     | 202 | CDL  | C39-C40-C41-C42 |
| 46  | H     | 402 | PC1  | C2F-C2G-C2H-C2I |
| 45  | b     | 102 | 3PE  | C35-C36-C37-C38 |
| 46  | Z     | 203 | PC1  | C26-C27-C28-C29 |
| 53  | M     | 607 | CDL  | C42-C43-C44-C45 |
| 45  | q     | 201 | 3PE  | C2F-C2G-C2H-C2I |
| 58  | i     | 201 | CHD  | C20-C22-C23-C24 |
| 45  | Y     | 207 | 3PE  | C3E-C3F-C3G-C3H |
| 53  | N     | 404 | CDL  | C35-C36-C37-C38 |
| 45  | Y     | 205 | 3PE  | C3A-C3B-C3C-C3D |
| 57  | U     | 101 | EHZ  | O5-C16-C17-C18  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 57  | U     | 101 | EHZ  | O5-C16-C17-C19  |
| 45  | Z     | 201 | 3PE  | C25-C26-C27-C28 |
| 46  | M     | 606 | PC1  | C23-C24-C25-C26 |
| 45  | Y     | 205 | 3PE  | C26-C27-C28-C29 |
| 56  | P     | 501 | NDP  | PN-O3-PA-O1A    |
| 46  | B     | 202 | PC1  | C33-C34-C35-C36 |
| 53  | N     | 404 | CDL  | C11-CA5-OA6-CA4 |
| 53  | h     | 203 | CDL  | C38-C39-C40-C41 |
| 45  | J     | 202 | 3PE  | C2F-C2G-C2H-C2I |
| 48  | b     | 103 | PLC  | C4B-C5B-C6B-C7B |
| 53  | N     | 404 | CDL  | C60-C61-C62-C63 |
| 46  | m     | 203 | PC1  | C21-C22-C23-C24 |
| 45  | b     | 101 | 3PE  | C29-C2A-C2B-C2C |
| 53  | i     | 202 | CDL  | C41-C42-C43-C44 |
| 45  | M     | 602 | 3PE  | O22-C21-O21-C2  |
| 53  | r     | 202 | CDL  | C1-CB2-OB2-PB2  |
| 57  | T     | 101 | EHZ  | S1-C10-C11-N1   |
| 45  | K     | 101 | 3PE  | C25-C26-C27-C28 |
| 45  | L     | 702 | 3PE  | C32-C33-C34-C35 |
| 45  | N     | 402 | 3PE  | C21-C22-C23-C24 |
| 45  | H     | 401 | 3PE  | O11-C1-C2-C3    |
| 45  | b     | 101 | 3PE  | O11-C1-C2-C3    |
| 46  | L     | 701 | PC1  | O11-C1-C2-C3    |
| 48  | O     | 403 | PLC  | O3P-C1-C2-C3    |
| 53  | d     | 204 | CDL  | OA5-CA3-CA4-CA6 |
| 53  | r     | 202 | CDL  | OB5-CB3-CB4-CB6 |
| 53  | i     | 202 | CDL  | C51-CB5-OB6-CB4 |
| 46  | B     | 202 | PC1  | C39-C3A-C3B-C3C |
| 45  | N     | 403 | 3PE  | O21-C21-C22-C23 |
| 45  | b     | 102 | 3PE  | C37-C38-C39-C3A |
| 45  | M     | 603 | 3PE  | C39-C3A-C3B-C3C |
| 45  | Y     | 203 | 3PE  | C24-C25-C26-C27 |
| 53  | r     | 202 | CDL  | C16-C17-C18-C19 |
| 45  | q     | 201 | 3PE  | C3F-C3G-C3H-C3I |
| 48  | J     | 203 | PLC  | C5B-C6B-C7B-C8B |
| 45  | K     | 101 | 3PE  | C23-C24-C25-C26 |
| 45  | Y     | 207 | 3PE  | C2E-C2F-C2G-C2H |
| 45  | Z     | 201 | 3PE  | C27-C28-C29-C2A |
| 45  | q     | 201 | 3PE  | C3D-C3E-C3F-C3G |
| 53  | N     | 404 | CDL  | C31-C32-C33-C34 |
| 45  | H     | 401 | 3PE  | C33-C34-C35-C36 |
| 45  | m     | 201 | 3PE  | C29-C2A-C2B-C2C |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 45  | J     | 202 | 3PE  | C1-C2-C3-O31    |
| 45  | L     | 702 | 3PE  | C1-C2-C3-O31    |
| 45  | M     | 603 | 3PE  | C1-C2-C3-O31    |
| 45  | Z     | 202 | 3PE  | C1-C2-C3-O31    |
| 46  | A     | 202 | PC1  | C1-C2-C3-O31    |
| 46  | m     | 203 | PC1  | C1-C2-C3-O31    |
| 48  | L     | 703 | PLC  | C1-C2-C3-O3     |
| 53  | M     | 607 | CDL  | CA3-CA4-CA6-OA8 |
| 53  | i     | 202 | CDL  | CA3-CA4-CA6-OA8 |
| 53  | i     | 202 | CDL  | C36-C37-C38-C39 |
| 45  | Y     | 203 | 3PE  | C2C-C2D-C2E-C2F |
| 45  | Y     | 202 | 3PE  | C33-C34-C35-C36 |
| 53  | h     | 203 | CDL  | C31-C32-C33-C34 |
| 45  | Y     | 205 | 3PE  | C28-C29-C2A-C2B |
| 45  | b     | 101 | 3PE  | C36-C37-C38-C39 |
| 53  | N     | 404 | CDL  | C20-C21-C22-C23 |
| 46  | h     | 202 | PC1  | C31-C32-C33-C34 |
| 45  | I     | 203 | 3PE  | O11-C1-C2-O21   |
| 45  | Y     | 202 | 3PE  | O11-C1-C2-O21   |
| 45  | Y     | 204 | 3PE  | O11-C1-C2-O21   |
| 45  | d     | 201 | 3PE  | O11-C1-C2-O21   |
| 48  | O     | 403 | PLC  | O3P-C1-C2-O2    |
| 53  | i     | 202 | CDL  | OB5-CB3-CB4-OB6 |
| 45  | L     | 702 | 3PE  | C38-C39-C3A-C3B |
| 46  | A     | 203 | PC1  | C32-C33-C34-C35 |
| 48  | O     | 403 | PLC  | C6B-C7B-C8B-C9B |
| 53  | X     | 201 | CDL  | C41-C42-C43-C44 |
| 45  | J     | 201 | 3PE  | C2-C1-O11-P     |
| 57  | T     | 101 | EHZ  | O1-C7-C8-C9     |
| 45  | d     | 201 | 3PE  | C39-C3A-C3B-C3C |
| 45  | J     | 201 | 3PE  | C32-C33-C34-C35 |
| 45  | K     | 101 | 3PE  | C37-C38-C39-C3A |
| 46  | H     | 403 | PC1  | C32-C33-C34-C35 |
| 46  | L     | 701 | PC1  | C26-C27-C28-C29 |
| 45  | Y     | 203 | 3PE  | C28-C29-C2A-C2B |
| 46  | L     | 701 | PC1  | C23-C24-C25-C26 |
| 45  | M     | 603 | 3PE  | O21-C2-C3-O31   |
| 45  | N     | 403 | 3PE  | O21-C2-C3-O31   |
| 45  | Z     | 202 | 3PE  | O21-C2-C3-O31   |
| 45  | b     | 102 | 3PE  | O21-C2-C3-O31   |
| 46  | A     | 202 | PC1  | O21-C2-C3-O31   |
| 48  | Z     | 204 | PLC  | O2-C2-C3-O3     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 48  | g     | 202 | PLC  | O2-C2-C3-O3     |
| 53  | M     | 607 | CDL  | OA6-CA4-CA6-OA8 |
| 48  | L     | 703 | PLC  | C6B-C7B-C8B-C9B |
| 54  | O     | 401 | DGT  | O4'-C4'-C5'-O5' |
| 56  | P     | 501 | NDP  | C3B-C4B-C5B-O5B |
| 45  | J     | 201 | 3PE  | C35-C36-C37-C38 |
| 45  | Y     | 202 | 3PE  | C3A-C3B-C3C-C3D |
| 45  | Y     | 203 | 3PE  | C3F-C3G-C3H-C3I |
| 45  | b     | 101 | 3PE  | C37-C38-C39-C3A |
| 45  | J     | 201 | 3PE  | C36-C37-C38-C39 |
| 45  | b     | 101 | 3PE  | C2A-C2B-C2C-C2D |
| 45  | H     | 401 | 3PE  | C36-C37-C38-C39 |
| 53  | M     | 607 | CDL  | C75-C76-C77-C78 |
| 53  | i     | 202 | CDL  | CA7-C31-C32-C33 |
| 53  | M     | 607 | CDL  | C78-C79-C80-C81 |
| 56  | P     | 501 | NDP  | PN-O3-PA-O5B    |
| 46  | M     | 606 | PC1  | C32-C33-C34-C35 |
| 45  | d     | 201 | 3PE  | C22-C23-C24-C25 |
| 53  | M     | 607 | CDL  | C62-C63-C64-C65 |
| 57  | U     | 101 | EHZ  | C6-C7-C8-C9     |
| 53  | M     | 607 | CDL  | C35-C36-C37-C38 |
| 48  | J     | 203 | PLC  | C1B-C2B-C3B-C4B |
| 45  | Z     | 201 | 3PE  | C2F-C2G-C2H-C2I |
| 45  | Y     | 204 | 3PE  | C36-C37-C38-C39 |
| 46  | H     | 403 | PC1  | C3D-C3E-C3F-C3G |
| 45  | Y     | 204 | 3PE  | C28-C29-C2A-C2B |
| 53  | d     | 204 | CDL  | C11-C12-C13-C14 |
| 53  | d     | 204 | CDL  | CB2-C1-CA2-OA2  |
| 45  | b     | 101 | 3PE  | C2C-C2D-C2E-C2F |
| 48  | Z     | 204 | PLC  | OB-CB-O3-C3     |
| 45  | b     | 101 | 3PE  | O21-C21-C22-C23 |
| 46  | H     | 402 | PC1  | C32-C31-O31-C3  |
| 45  | Y     | 201 | 3PE  | O11-C1-C2-C3    |
| 45  | Y     | 205 | 3PE  | O11-C1-C2-C3    |
| 45  | Z     | 201 | 3PE  | O11-C1-C2-C3    |
| 45  | d     | 201 | 3PE  | O11-C1-C2-C3    |
| 46  | B     | 202 | PC1  | O11-C1-C2-C3    |
| 46  | q     | 202 | PC1  | O11-C1-C2-C3    |
| 48  | B     | 203 | PLC  | O3P-C1-C2-C3    |
| 48  | d     | 203 | PLC  | O3P-C1-C2-C3    |
| 53  | h     | 203 | CDL  | OA5-CA3-CA4-CA6 |
| 45  | N     | 402 | 3PE  | C23-C24-C25-C26 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 46  | Z     | 203 | PC1  | C34-C35-C36-C37 |
| 45  | I     | 203 | 3PE  | C28-C29-C2A-C2B |
| 45  | M     | 603 | 3PE  | C36-C37-C38-C39 |
| 48  | L     | 703 | PLC  | C2B-C3B-C4B-C5B |
| 53  | M     | 607 | CDL  | C17-C18-C19-C20 |
| 53  | d     | 204 | CDL  | C76-C77-C78-C79 |
| 46  | m     | 203 | PC1  | C39-C3A-C3B-C3C |
| 46  | Z     | 203 | PC1  | O22-C21-O21-C2  |
| 48  | B     | 203 | PLC  | O'-C'-O2-C2     |
| 53  | N     | 404 | CDL  | OA7-CA5-OA6-CA4 |
| 46  | g     | 201 | PC1  | C2C-C2D-C2E-C2F |
| 45  | N     | 403 | 3PE  | C2B-C2C-C2D-C2E |
| 45  | N     | 401 | 3PE  | C3-C2-O21-C21   |
| 53  | N     | 404 | CDL  | CA6-CA4-OA6-CA5 |
| 53  | X     | 201 | CDL  | CA5-C11-C12-C13 |
| 45  | b     | 101 | 3PE  | C27-C28-C29-C2A |
| 53  | i     | 202 | CDL  | OB7-CB5-OB6-CB4 |
| 45  | Y     | 201 | 3PE  | O11-C1-C2-O21   |
| 45  | Y     | 205 | 3PE  | O11-C1-C2-O21   |
| 45  | Z     | 201 | 3PE  | O11-C1-C2-O21   |
| 45  | b     | 101 | 3PE  | O11-C1-C2-O21   |
| 45  | f     | 101 | 3PE  | O11-C1-C2-O21   |
| 45  | r     | 201 | 3PE  | O11-C1-C2-O21   |
| 46  | I     | 204 | PC1  | O11-C1-C2-O21   |
| 48  | Y     | 208 | PLC  | O3P-C1-C2-O2    |
| 53  | N     | 404 | CDL  | C74-C75-C76-C77 |
| 45  | N     | 402 | 3PE  | C1-C2-C3-O31    |
| 45  | b     | 102 | 3PE  | C1-C2-C3-O31    |
| 45  | m     | 202 | 3PE  | C1-C2-C3-O31    |
| 48  | b     | 103 | PLC  | C1-C2-C3-O3     |
| 48  | g     | 202 | PLC  | C1-C2-C3-O3     |
| 45  | K     | 101 | 3PE  | C12-C11-O13-P   |
| 45  | N     | 402 | 3PE  | C12-C11-O13-P   |
| 45  | Y     | 202 | 3PE  | C12-C11-O13-P   |
| 45  | Y     | 204 | 3PE  | C12-C11-O13-P   |
| 45  | Y     | 205 | 3PE  | C12-C11-O13-P   |
| 45  | Y     | 206 | 3PE  | C12-C11-O13-P   |
| 45  | h     | 201 | 3PE  | C12-C11-O13-P   |
| 45  | m     | 201 | 3PE  | C12-C11-O13-P   |
| 45  | m     | 202 | 3PE  | C12-C11-O13-P   |
| 48  | Y     | 208 | PLC  | C5-C4-O4P-P     |
| 53  | i     | 202 | CDL  | CB7-C71-C72-C73 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 45  | L     | 702 | 3PE  | O21-C2-C3-O31   |
| 45  | Y     | 207 | 3PE  | O21-C2-C3-O31   |
| 45  | b     | 101 | 3PE  | O21-C2-C3-O31   |
| 45  | m     | 202 | 3PE  | O21-C2-C3-O31   |
| 48  | L     | 703 | PLC  | O2-C2-C3-O3     |
| 45  | Z     | 202 | 3PE  | C26-C27-C28-C29 |
| 45  | J     | 201 | 3PE  | C33-C34-C35-C36 |
| 45  | Y     | 206 | 3PE  | C22-C23-C24-C25 |
| 45  | b     | 102 | 3PE  | C3C-C3D-C3E-C3F |
| 46  | H     | 402 | PC1  | C2D-C2E-C2F-C2G |
| 45  | b     | 102 | 3PE  | C34-C35-C36-C37 |
| 53  | r     | 202 | CDL  | C12-C13-C14-C15 |
| 54  | O     | 401 | DGT  | C3'-C4'-C5'-O5' |
| 56  | P     | 501 | NDP  | O4B-C4B-C5B-O5B |
| 45  | I     | 203 | 3PE  | C2-C1-O11-P     |
| 45  | N     | 401 | 3PE  | C2-C1-O11-P     |
| 48  | Y     | 208 | PLC  | O4P-C4-C5-N     |
| 48  | b     | 103 | PLC  | O4P-C4-C5-N     |
| 45  | J     | 201 | 3PE  | C2-C3-O31-C31   |
| 45  | N     | 402 | 3PE  | C32-C33-C34-C35 |
| 46  | g     | 201 | PC1  | C22-C23-C24-C25 |
| 53  | r     | 202 | CDL  | CA7-C31-C32-C33 |
| 46  | H     | 402 | PC1  | O32-C31-O31-C3  |
| 53  | N     | 404 | CDL  | C56-C57-C58-C59 |
| 59  | o     | 201 | MYR  | C4-C5-C6-C7     |
| 45  | m     | 201 | 3PE  | C26-C27-C28-C29 |
| 45  | Y     | 204 | 3PE  | C2B-C2C-C2D-C2E |
| 45  | N     | 403 | 3PE  | C38-C39-C3A-C3B |
| 45  | h     | 201 | 3PE  | C26-C27-C28-C29 |
| 53  | r     | 202 | CDL  | CB7-C71-C72-C73 |
| 53  | h     | 203 | CDL  | C37-C38-C39-C40 |
| 45  | J     | 201 | 3PE  | O11-C1-C2-C3    |
| 45  | f     | 101 | 3PE  | O11-C1-C2-C3    |
| 46  | I     | 204 | PC1  | O11-C1-C2-C3    |
| 48  | J     | 203 | PLC  | O3P-C1-C2-C3    |
| 48  | L     | 703 | PLC  | O3P-C1-C2-C3    |
| 48  | Y     | 208 | PLC  | O3P-C1-C2-C3    |
| 45  | Y     | 203 | 3PE  | C35-C36-C37-C38 |
| 57  | T     | 101 | EHZ  | C18-C17-C20-O6  |
| 57  | T     | 101 | EHZ  | C19-C17-C20-O6  |
| 46  | g     | 201 | PC1  | C32-C33-C34-C35 |
| 46  | Z     | 203 | PC1  | C23-C24-C25-C26 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 46  | H     | 402 | PC1  | C26-C27-C28-C29 |
| 48  | d     | 203 | PLC  | C2-C1-O3P-P     |
| 57  | U     | 101 | EHZ  | C11-C10-S1-C9   |
| 48  | b     | 103 | PLC  | C1'-C2'-C3'-C4' |
| 48  | Z     | 204 | PLC  | C8B-C9B-CAA-CBA |
| 45  | J     | 201 | 3PE  | O11-C1-C2-O21   |
| 45  | m     | 201 | 3PE  | O11-C1-C2-O21   |
| 46  | B     | 202 | PC1  | O11-C1-C2-O21   |
| 46  | L     | 701 | PC1  | O11-C1-C2-O21   |
| 48  | B     | 203 | PLC  | O3P-C1-C2-O2    |
| 53  | X     | 201 | CDL  | OA5-CA3-CA4-OA6 |
| 53  | d     | 204 | CDL  | OA5-CA3-CA4-OA6 |
| 53  | h     | 203 | CDL  | OA5-CA3-CA4-OA6 |
| 53  | i     | 202 | CDL  | C54-C55-C56-C57 |
| 46  | H     | 402 | PC1  | O21-C21-C22-C23 |
| 53  | X     | 201 | CDL  | C63-C64-C65-C66 |
| 46  | H     | 402 | PC1  | C35-C36-C37-C38 |
| 46  | I     | 204 | PC1  | C22-C23-C24-C25 |
| 45  | J     | 202 | 3PE  | O21-C2-C3-O31   |
| 48  | b     | 103 | PLC  | O2-C2-C3-O3     |
| 53  | h     | 203 | CDL  | OB6-CB4-CB6-OB8 |
| 53  | i     | 202 | CDL  | OA6-CA4-CA6-OA8 |
| 45  | q     | 201 | 3PE  | C23-C24-C25-C26 |
| 48  | Y     | 208 | PLC  | C'-C1'-C2'-C3'  |
| 45  | A     | 201 | 3PE  | C1-C2-C3-O31    |
| 45  | Y     | 207 | 3PE  | C1-C2-C3-O31    |
| 45  | b     | 101 | 3PE  | C1-C2-C3-O31    |
| 46  | L     | 701 | PC1  | C1-C2-C3-O31    |
| 46  | d     | 202 | PC1  | C1-C2-C3-O31    |
| 53  | r     | 202 | CDL  | CA3-CA4-CA6-OA8 |
| 45  | I     | 203 | 3PE  | C2F-C2G-C2H-C2I |
| 53  | M     | 607 | CDL  | C44-C45-C46-C47 |
| 46  | h     | 202 | PC1  | C2B-C2C-C2D-C2E |
| 45  | b     | 101 | 3PE  | C31-C32-C33-C34 |
| 46  | h     | 202 | PC1  | C22-C23-C24-C25 |
| 46  | H     | 403 | PC1  | C31-C32-C33-C34 |
| 46  | I     | 204 | PC1  | C28-C29-C2A-C2B |
| 53  | X     | 201 | CDL  | C31-C32-C33-C34 |
| 45  | H     | 401 | 3PE  | C11-O13-P-O14   |
| 45  | I     | 203 | 3PE  | C11-O13-P-O12   |
| 45  | J     | 201 | 3PE  | C1-O11-P-O14    |
| 45  | J     | 201 | 3PE  | O13-C11-C12-N   |

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| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 45  | K     | 101 | 3PE  | C11-O13-P-O11 |
| 45  | K     | 101 | 3PE  | C11-O13-P-O14 |
| 45  | L     | 702 | 3PE  | O13-C11-C12-N |
| 45  | M     | 603 | 3PE  | C11-O13-P-O14 |
| 45  | M     | 603 | 3PE  | O13-C11-C12-N |
| 45  | M     | 604 | 3PE  | O13-C11-C12-N |
| 45  | N     | 402 | 3PE  | C1-O11-P-O12  |
| 45  | N     | 402 | 3PE  | C1-O11-P-O13  |
| 45  | N     | 402 | 3PE  | C1-O11-P-O14  |
| 45  | Y     | 202 | 3PE  | C11-O13-P-O12 |
| 45  | Y     | 204 | 3PE  | C1-O11-P-O12  |
| 45  | Y     | 207 | 3PE  | C1-O11-P-O13  |
| 45  | Y     | 207 | 3PE  | C1-O11-P-O14  |
| 45  | Y     | 207 | 3PE  | C11-O13-P-O14 |
| 45  | Y     | 207 | 3PE  | O13-C11-C12-N |
| 45  | Z     | 202 | 3PE  | O13-C11-C12-N |
| 45  | b     | 101 | 3PE  | C1-O11-P-O12  |
| 45  | b     | 101 | 3PE  | O13-C11-C12-N |
| 45  | b     | 102 | 3PE  | O13-C11-C12-N |
| 45  | f     | 101 | 3PE  | C1-O11-P-O14  |
| 45  | h     | 201 | 3PE  | C1-O11-P-O13  |
| 45  | m     | 201 | 3PE  | C11-O13-P-O11 |
| 45  | m     | 201 | 3PE  | C11-O13-P-O14 |
| 45  | m     | 202 | 3PE  | C1-O11-P-O12  |
| 46  | A     | 202 | PC1  | C1-O11-P-O14  |
| 46  | A     | 202 | PC1  | C1-O11-P-O13  |
| 46  | A     | 203 | PC1  | C11-C12-N-C15 |
| 46  | B     | 202 | PC1  | C11-O13-P-O12 |
| 46  | I     | 204 | PC1  | C11-O13-P-O12 |
| 46  | I     | 204 | PC1  | C11-O13-P-O14 |
| 46  | I     | 204 | PC1  | C11-O13-P-O11 |
| 46  | M     | 606 | PC1  | C1-O11-P-O13  |
| 46  | Z     | 203 | PC1  | C1-O11-P-O14  |
| 46  | Z     | 203 | PC1  | C1-O11-P-O13  |
| 46  | d     | 202 | PC1  | C11-O13-P-O14 |
| 46  | d     | 202 | PC1  | C11-O13-P-O11 |
| 46  | g     | 201 | PC1  | C11-O13-P-O14 |
| 46  | g     | 201 | PC1  | C11-O13-P-O11 |
| 46  | m     | 203 | PC1  | C1-O11-P-O12  |
| 46  | q     | 202 | PC1  | C1-O11-P-O14  |
| 48  | B     | 203 | PLC  | C4-O4P-P-O2P  |
| 48  | Z     | 204 | PLC  | C1-O3P-P-O4P  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 48  | b     | 103 | PLC  | C4-O4P-P-O3P    |
| 48  | d     | 203 | PLC  | C1-O3P-P-O4P    |
| 48  | d     | 203 | PLC  | C4-O4P-P-O1P    |
| 53  | N     | 404 | CDL  | CB2-OB2-PB2-OB4 |
| 53  | N     | 404 | CDL  | CB2-OB2-PB2-OB5 |
| 53  | N     | 404 | CDL  | CB3-OB5-PB2-OB2 |
| 53  | N     | 404 | CDL  | CB3-OB5-PB2-OB3 |
| 53  | N     | 404 | CDL  | CB3-OB5-PB2-OB4 |
| 53  | X     | 201 | CDL  | CA2-OA2-PA1-OA3 |
| 53  | X     | 201 | CDL  | CB2-OB2-PB2-OB3 |
| 53  | d     | 204 | CDL  | CA3-OA5-PA1-OA3 |
| 53  | d     | 204 | CDL  | CB3-OB5-PB2-OB2 |
| 53  | d     | 204 | CDL  | CB3-OB5-PB2-OB4 |
| 53  | h     | 203 | CDL  | CA2-OA2-PA1-OA5 |
| 53  | r     | 202 | CDL  | CB2-OB2-PB2-OB3 |
| 54  | O     | 401 | DGT  | C5'-O5'-PA-O3A  |
| 57  | U     | 101 | EHZ  | O5-C16-C17-C20  |
| 45  | N     | 401 | 3PE  | C38-C39-C3A-C3B |
| 46  | q     | 202 | PC1  | O21-C21-C22-C23 |
| 48  | O     | 403 | PLC  | C2-C1-O3P-P     |
| 50  | F     | 502 | FMN  | C4'-C5'-O5'-P   |
| 53  | d     | 204 | CDL  | C1-CB2-OB2-PB2  |
| 46  | Z     | 203 | PC1  | C29-C2A-C2B-C2C |
| 45  | Y     | 203 | 3PE  | C22-C23-C24-C25 |
| 45  | f     | 101 | 3PE  | C23-C24-C25-C26 |
| 45  | b     | 102 | 3PE  | C2B-C2C-C2D-C2E |
| 45  | N     | 403 | 3PE  | C22-C23-C24-C25 |
| 45  | Y     | 202 | 3PE  | C22-C23-C24-C25 |
| 48  | L     | 703 | PLC  | CB-C1B-C2B-C3B  |
| 53  | i     | 202 | CDL  | C52-C53-C54-C55 |
| 45  | d     | 201 | 3PE  | C34-C35-C36-C37 |
| 45  | Y     | 202 | 3PE  | C3-C2-O21-C21   |
| 45  | d     | 201 | 3PE  | C1-C2-O21-C21   |
| 45  | M     | 602 | 3PE  | C34-C35-C36-C37 |
| 45  | m     | 201 | 3PE  | O11-C1-C2-C3    |
| 46  | g     | 201 | PC1  | C25-C26-C27-C28 |
| 48  | J     | 203 | PLC  | C1'-C2'-C3'-C4' |
| 46  | A     | 203 | PC1  | O11-C1-C2-O21   |
| 48  | L     | 703 | PLC  | C1B-C2B-C3B-C4B |
| 45  | Y     | 203 | 3PE  | C23-C24-C25-C26 |
| 53  | h     | 203 | CDL  | C58-C59-C60-C61 |
| 45  | I     | 203 | 3PE  | C27-C28-C29-C2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 46  | L     | 701 | PC1  | C36-C37-C38-C39 |
| 46  | H     | 403 | PC1  | C2-C1-O11-P     |
| 45  | N     | 402 | 3PE  | O21-C2-C3-O31   |
| 46  | h     | 202 | PC1  | O21-C2-C3-O31   |
| 46  | q     | 202 | PC1  | O21-C2-C3-O31   |
| 53  | d     | 204 | CDL  | OB6-CB4-CB6-OB8 |
| 48  | L     | 703 | PLC  | C4B-C5B-C6B-C7B |
| 45  | r     | 201 | 3PE  | C36-C37-C38-C39 |
| 45  | A     | 201 | 3PE  | C23-C24-C25-C26 |
| 59  | o     | 201 | MYR  | C10-C11-C12-C13 |
| 54  | O     | 401 | DGT  | PA-O3A-PB-O1B   |
| 45  | b     | 101 | 3PE  | C2B-C2C-C2D-C2E |
| 53  | M     | 607 | CDL  | C59-C60-C61-C62 |
| 56  | P     | 501 | NDP  | C3D-C4D-C5D-O5D |
| 45  | Z     | 202 | 3PE  | C24-C25-C26-C27 |
| 46  | A     | 203 | PC1  | C11-C12-N-C13   |
| 46  | H     | 402 | PC1  | C11-C12-N-C13   |
| 53  | d     | 204 | CDL  | C31-C32-C33-C34 |
| 53  | X     | 201 | CDL  | CB2-C1-CA2-OA2  |
| 57  | T     | 101 | EHZ  | C5-C6-C7-O1     |
| 53  | r     | 202 | CDL  | C18-C19-C20-C21 |
| 48  | g     | 202 | PLC  | C2-C1-O3P-P     |
| 53  | h     | 203 | CDL  | C32-C33-C34-C35 |
| 45  | Y     | 204 | 3PE  | C3D-C3E-C3F-C3G |
| 53  | M     | 607 | CDL  | C74-C75-C76-C77 |
| 45  | M     | 605 | 3PE  | O21-C21-C22-C23 |
| 53  | r     | 202 | CDL  | C17-C18-C19-C20 |
| 59  | o     | 201 | MYR  | C9-C10-C11-C12  |
| 46  | d     | 202 | PC1  | C23-C24-C25-C26 |
| 45  | q     | 201 | 3PE  | C2A-C2B-C2C-C2D |
| 45  | h     | 201 | 3PE  | C23-C24-C25-C26 |
| 53  | N     | 404 | CDL  | C14-C15-C16-C17 |
| 53  | M     | 607 | CDL  | C34-C35-C36-C37 |
| 45  | L     | 702 | 3PE  | C3F-C3G-C3H-C3I |
| 46  | B     | 202 | PC1  | C3D-C3E-C3F-C3G |
| 45  | h     | 201 | 3PE  | C32-C33-C34-C35 |
| 45  | Z     | 201 | 3PE  | C2A-C2B-C2C-C2D |
| 46  | I     | 204 | PC1  | C26-C27-C28-C29 |
| 46  | d     | 202 | PC1  | C3B-C3C-C3D-C3E |
| 46  | A     | 203 | PC1  | C11-C12-N-C14   |
| 48  | L     | 703 | PLC  | C3B-C4B-C5B-C6B |
| 45  | A     | 201 | 3PE  | C22-C23-C24-C25 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 45  | Y     | 205 | 3PE  | C2C-C2D-C2E-C2F |
| 45  | d     | 201 | 3PE  | C3-C2-O21-C21   |
| 46  | H     | 403 | PC1  | C3-C2-O21-C21   |
| 53  | X     | 201 | CDL  | CA3-CA4-OA6-CA5 |
| 46  | I     | 204 | PC1  | C33-C34-C35-C36 |
| 45  | b     | 101 | 3PE  | C3A-C3B-C3C-C3D |
| 46  | M     | 606 | PC1  | C34-C35-C36-C37 |
| 48  | b     | 103 | PLC  | C2-C3-O3-CB     |
| 45  | N     | 403 | 3PE  | C35-C36-C37-C38 |
| 53  | M     | 607 | CDL  | C40-C41-C42-C43 |
| 46  | H     | 402 | PC1  | C11-C12-N-C15   |
| 45  | h     | 201 | 3PE  | C22-C23-C24-C25 |
| 53  | N     | 404 | CDL  | C24-C25-C26-C27 |
| 45  | M     | 602 | 3PE  | C37-C38-C39-C3A |
| 48  | O     | 403 | PLC  | C1B-CB-O3-C3    |
| 46  | g     | 201 | PC1  | C34-C35-C36-C37 |
| 45  | b     | 101 | 3PE  | C39-C3A-C3B-C3C |
| 45  | M     | 604 | 3PE  | O21-C2-C3-O31   |
| 45  | N     | 403 | 3PE  | C26-C27-C28-C29 |
| 45  | Z     | 202 | 3PE  | C27-C28-C29-C2A |
| 53  | X     | 201 | CDL  | C36-C37-C38-C39 |
| 46  | H     | 402 | PC1  | C11-C12-N-C14   |
| 45  | N     | 401 | 3PE  | C37-C38-C39-C3A |
| 58  | i     | 201 | CHD  | C22-C23-C24-O26 |
| 45  | K     | 101 | 3PE  | C36-C37-C38-C39 |
| 46  | L     | 701 | PC1  | C37-C38-C39-C3A |
| 45  | L     | 702 | 3PE  | C36-C37-C38-C39 |
| 48  | O     | 403 | PLC  | OB-CB-O3-C3     |
| 46  | B     | 202 | PC1  | C28-C29-C2A-C2B |
| 53  | h     | 203 | CDL  | C56-C57-C58-C59 |
| 46  | B     | 202 | PC1  | C3B-C3C-C3D-C3E |
| 45  | d     | 201 | 3PE  | C3A-C3B-C3C-C3D |
| 53  | X     | 201 | CDL  | C62-C63-C64-C65 |
| 45  | d     | 201 | 3PE  | C2F-C2G-C2H-C2I |
| 58  | i     | 201 | CHD  | C22-C23-C24-O25 |
| 45  | m     | 202 | 3PE  | C2-C1-O11-P     |
| 46  | q     | 202 | PC1  | O22-C21-C22-C23 |
| 46  | L     | 701 | PC1  | O22-C21-O21-C2  |
| 45  | N     | 403 | 3PE  | O22-C21-C22-C23 |
| 45  | N     | 401 | 3PE  | C33-C34-C35-C36 |
| 46  | I     | 204 | PC1  | C2B-C2C-C2D-C2E |
| 57  | U     | 101 | EHZ  | O3-C12-C13-C14  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 46  | Z     | 203 | PC1  | C3B-C3C-C3D-C3E |
| 53  | N     | 404 | CDL  | C57-C58-C59-C60 |
| 45  | A     | 201 | 3PE  | O11-C1-C2-O21   |
| 45  | Y     | 206 | 3PE  | O11-C1-C2-O21   |
| 45  | Y     | 203 | 3PE  | C39-C3A-C3B-C3C |
| 48  | Y     | 208 | PLC  | C7'-C8'-C9'-CA' |
| 53  | h     | 203 | CDL  | C63-C64-C65-C66 |
| 45  | M     | 604 | 3PE  | C31-C32-C33-C34 |
| 45  | d     | 201 | 3PE  | C26-C27-C28-C29 |
| 45  | K     | 101 | 3PE  | C38-C39-C3A-C3B |
| 45  | I     | 203 | 3PE  | O11-C1-C2-C3    |
| 46  | A     | 203 | PC1  | O11-C1-C2-C3    |
| 45  | f     | 101 | 3PE  | C2D-C2E-C2F-C2G |
| 45  | Y     | 205 | 3PE  | C21-C22-C23-C24 |
| 45  | N     | 402 | 3PE  | O31-C31-C32-C33 |
| 53  | M     | 607 | CDL  | C12-C11-CA5-OA6 |
| 46  | Z     | 203 | PC1  | C27-C28-C29-C2A |
| 48  | b     | 103 | PLC  | C2B-C3B-C4B-C5B |
| 53  | N     | 404 | CDL  | C75-C76-C77-C78 |
| 56  | P     | 501 | NDP  | O4D-C4D-C5D-O5D |
| 45  | Z     | 202 | 3PE  | C33-C34-C35-C36 |
| 48  | d     | 203 | PLC  | C2B-C1B-CB-O3   |
| 45  | K     | 101 | 3PE  | C3D-C3E-C3F-C3G |
| 46  | M     | 606 | PC1  | C24-C25-C26-C27 |
| 45  | L     | 702 | 3PE  | C34-C35-C36-C37 |
| 46  | g     | 201 | PC1  | C27-C28-C29-C2A |
| 53  | i     | 202 | CDL  | C56-C57-C58-C59 |
| 45  | N     | 402 | 3PE  | O21-C21-C22-C23 |
| 48  | J     | 203 | PLC  | C4-C5-N-C8      |
| 45  | L     | 702 | 3PE  | C1-C2-O21-C21   |
| 45  | L     | 702 | 3PE  | C3-C2-O21-C21   |
| 46  | H     | 403 | PC1  | C1-C2-O21-C21   |
| 53  | N     | 404 | CDL  | C34-C35-C36-C37 |
| 46  | M     | 606 | PC1  | C33-C34-C35-C36 |
| 45  | q     | 201 | 3PE  | C2B-C2C-C2D-C2E |
| 45  | Y     | 202 | 3PE  | C3E-C3F-C3G-C3H |
| 45  | f     | 101 | 3PE  | C26-C27-C28-C29 |
| 53  | i     | 202 | CDL  | C35-C36-C37-C38 |
| 45  | m     | 201 | 3PE  | C28-C29-C2A-C2B |
| 45  | M     | 605 | 3PE  | C2-C1-O11-P     |
| 45  | Y     | 202 | 3PE  | C2-C1-O11-P     |
| 53  | h     | 203 | CDL  | OB5-CB3-CB4-OB6 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 45  | q     | 201 | 3PE  | C39-C3A-C3B-C3C |
| 48  | Y     | 208 | PLC  | C2'-C3'-C4'-C5' |
| 57  | U     | 101 | EHZ  | N1-C12-C13-C14  |
| 45  | m     | 201 | 3PE  | C2B-C2C-C2D-C2E |
| 53  | M     | 607 | CDL  | C24-C25-C26-C27 |
| 57  | U     | 101 | EHZ  | C15-C16-C17-C18 |
| 48  | B     | 203 | PLC  | OB-CB-O3-C3     |
| 45  | H     | 401 | 3PE  | C38-C39-C3A-C3B |
| 53  | X     | 201 | CDL  | OA6-CA4-CA6-OA8 |
| 53  | i     | 202 | CDL  | OB6-CB4-CB6-OB8 |
| 53  | X     | 201 | CDL  | C72-C71-CB7-OB8 |
| 53  | h     | 203 | CDL  | OB7-CB5-OB6-CB4 |
| 45  | Y     | 204 | 3PE  | C2A-C2B-C2C-C2D |
| 45  | A     | 201 | 3PE  | O11-C1-C2-C3    |
| 53  | M     | 607 | CDL  | C16-C17-C18-C19 |
| 46  | A     | 202 | PC1  | C11-C12-N-C14   |
| 46  | I     | 204 | PC1  | C11-C12-N-C13   |
| 46  | I     | 204 | PC1  | C11-C12-N-C14   |
| 53  | N     | 404 | CDL  | C18-C19-C20-C21 |
| 53  | i     | 202 | CDL  | C12-C11-CA5-OA6 |
| 53  | M     | 607 | CDL  | C15-C16-C17-C18 |
| 45  | Y     | 207 | 3PE  | C2F-C2G-C2H-C2I |
| 46  | h     | 202 | PC1  | C23-C24-C25-C26 |
| 45  | J     | 202 | 3PE  | O31-C31-C32-C33 |
| 53  | N     | 404 | CDL  | C36-C37-C38-C39 |
| 46  | L     | 701 | PC1  | C22-C21-O21-C2  |
| 48  | O     | 403 | PLC  | O'-C'-O2-C2     |
| 45  | f     | 101 | 3PE  | C33-C34-C35-C36 |
| 45  | q     | 201 | 3PE  | C2C-C2D-C2E-C2F |
| 53  | h     | 203 | CDL  | C54-C55-C56-C57 |
| 45  | q     | 201 | 3PE  | C37-C38-C39-C3A |
| 53  | h     | 203 | CDL  | C52-C51-CB5-OB6 |
| 48  | B     | 203 | PLC  | C1B-CB-O3-C3    |
| 45  | N     | 403 | 3PE  | C21-C22-C23-C24 |
| 53  | X     | 201 | CDL  | C84-C85-C86-C87 |
| 45  | L     | 702 | 3PE  | O21-C21-C22-C23 |
| 45  | Y     | 201 | 3PE  | O31-C31-C32-C33 |
| 45  | Y     | 205 | 3PE  | C27-C28-C29-C2A |
| 45  | m     | 201 | 3PE  | C2A-C2B-C2C-C2D |
| 46  | A     | 202 | PC1  | C11-C12-N-C13   |
| 45  | b     | 101 | 3PE  | O22-C21-C22-C23 |
| 45  | b     | 101 | 3PE  | O31-C31-C32-C33 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 45  | f     | 101 | 3PE  | O21-C21-C22-C23 |
| 45  | M     | 604 | 3PE  | O11-C1-C2-O21   |
| 45  | b     | 102 | 3PE  | C36-C37-C38-C39 |
| 45  | f     | 101 | 3PE  | C2A-C2B-C2C-C2D |
| 53  | X     | 201 | CDL  | C60-C61-C62-C63 |
| 45  | Y     | 205 | 3PE  | C2B-C2C-C2D-C2E |
| 53  | h     | 203 | CDL  | C51-CB5-OB6-CB4 |
| 48  | J     | 203 | PLC  | C3B-C4B-C5B-C6B |
| 53  | i     | 202 | CDL  | C11-C12-C13-C14 |
| 45  | Y     | 205 | 3PE  | C36-C37-C38-C39 |
| 45  | Y     | 205 | 3PE  | C2-C1-O11-P     |
| 53  | h     | 203 | CDL  | C1-CB2-OB2-PB2  |
| 45  | m     | 201 | 3PE  | O21-C21-C22-C23 |
| 48  | Y     | 208 | PLC  | O2-C'-C1'-C2'   |
| 53  | X     | 201 | CDL  | C52-C51-CB5-OB6 |
| 53  | d     | 204 | CDL  | C72-C71-CB7-OB8 |
| 45  | N     | 402 | 3PE  | C29-C2A-C2B-C2C |
| 53  | X     | 201 | CDL  | C74-C75-C76-C77 |
| 45  | N     | 403 | 3PE  | C1-C2-C3-O31    |
| 48  | Y     | 208 | PLC  | C1-C2-C3-O3     |
| 46  | I     | 204 | PC1  | C11-C12-N-C15   |
| 45  | J     | 202 | 3PE  | C23-C24-C25-C26 |
| 53  | N     | 404 | CDL  | OA6-CA4-CA6-OA8 |
| 53  | r     | 202 | CDL  | OB6-CB4-CB6-OB8 |
| 45  | Y     | 207 | 3PE  | C3F-C3G-C3H-C3I |
| 45  | Y     | 202 | 3PE  | C32-C33-C34-C35 |
| 48  | g     | 202 | PLC  | C2'-C3'-C4'-C5' |
| 45  | A     | 201 | 3PE  | O31-C31-C32-C33 |
| 45  | Y     | 201 | 3PE  | O21-C21-C22-C23 |
| 45  | Y     | 205 | 3PE  | O31-C31-C32-C33 |
| 53  | X     | 201 | CDL  | CA7-C31-C32-C33 |
| 53  | M     | 607 | CDL  | C41-C42-C43-C44 |
| 46  | h     | 202 | PC1  | C27-C28-C29-C2A |
| 53  | X     | 201 | CDL  | C73-C74-C75-C76 |
| 45  | M     | 603 | 3PE  | C27-C28-C29-C2A |
| 45  | f     | 101 | 3PE  | C35-C36-C37-C38 |
| 46  | L     | 701 | PC1  | C3A-C3B-C3C-C3D |
| 46  | A     | 202 | PC1  | C11-C12-N-C15   |
| 46  | m     | 203 | PC1  | C23-C24-C25-C26 |
| 45  | M     | 603 | 3PE  | C22-C23-C24-C25 |
| 45  | Y     | 203 | 3PE  | C2B-C2C-C2D-C2E |
| 53  | X     | 201 | CDL  | C75-C76-C77-C78 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 46  | A     | 202 | PC1  | O21-C21-C22-C23 |
| 45  | Y     | 204 | 3PE  | C3B-C3C-C3D-C3E |
| 53  | N     | 404 | CDL  | CB4-CB3-OB5-PB2 |
| 53  | h     | 203 | CDL  | C52-C51-CB5-OB7 |
| 48  | J     | 203 | PLC  | O2-C'-C1'-C2'   |
| 45  | N     | 403 | 3PE  | C32-C33-C34-C35 |
| 45  | Y     | 205 | 3PE  | C39-C3A-C3B-C3C |
| 45  | L     | 702 | 3PE  | O22-C21-C22-C23 |
| 53  | X     | 201 | CDL  | C72-C71-CB7-OB9 |
| 45  | M     | 605 | 3PE  | C2D-C2E-C2F-C2G |
| 45  | b     | 101 | 3PE  | O32-C31-C32-C33 |
| 45  | f     | 101 | 3PE  | O22-C21-C22-C23 |
| 53  | d     | 204 | CDL  | C72-C71-CB7-OB9 |
| 48  | b     | 103 | PLC  | C7'-C8'-C9'-CA' |
| 45  | H     | 401 | 3PE  | C3C-C3D-C3E-C3F |
| 48  | O     | 403 | PLC  | C1'-C'-O2-C2    |
| 48  | Z     | 204 | PLC  | C2B-C1B-CB-O3   |
| 45  | q     | 201 | 3PE  | C3E-C3F-C3G-C3H |
| 53  | h     | 203 | CDL  | C55-C56-C57-C58 |
| 45  | Y     | 201 | 3PE  | O32-C31-C32-C33 |
| 45  | Y     | 205 | 3PE  | O32-C31-C32-C33 |
| 45  | m     | 201 | 3PE  | O22-C21-C22-C23 |
| 46  | A     | 202 | PC1  | O22-C21-O21-C2  |
| 53  | X     | 201 | CDL  | C52-C51-CB5-OB7 |
| 45  | M     | 602 | 3PE  | O31-C31-C32-C33 |
| 45  | Z     | 202 | 3PE  | C37-C38-C39-C3A |
| 45  | d     | 201 | 3PE  | C23-C24-C25-C26 |
| 53  | i     | 202 | CDL  | C12-C11-CA5-OA7 |
| 45  | Y     | 205 | 3PE  | C24-C25-C26-C27 |
| 45  | H     | 401 | 3PE  | C39-C3A-C3B-C3C |
| 45  | A     | 201 | 3PE  | O32-C31-C32-C33 |
| 45  | J     | 202 | 3PE  | C2B-C2C-C2D-C2E |
| 45  | Z     | 202 | 3PE  | O31-C31-C32-C33 |
| 45  | Y     | 206 | 3PE  | O11-C1-C2-C3    |
| 53  | r     | 202 | CDL  | C72-C73-C74-C75 |
| 45  | J     | 201 | 3PE  | O21-C21-C22-C23 |
| 45  | m     | 201 | 3PE  | C21-C22-C23-C24 |
| 46  | d     | 202 | PC1  | C38-C39-C3A-C3B |
| 46  | B     | 202 | PC1  | C2A-C2B-C2C-C2D |
| 53  | X     | 201 | CDL  | C56-C57-C58-C59 |
| 45  | I     | 203 | 3PE  | C29-C2A-C2B-C2C |
| 57  | T     | 101 | EHZ  | C5-C6-C7-C8     |

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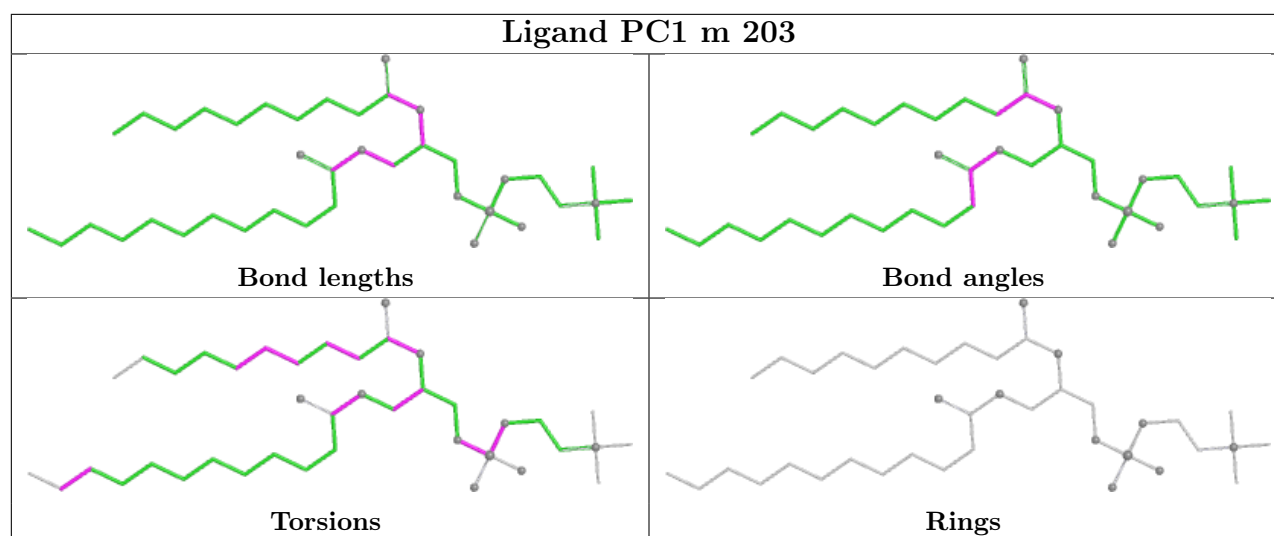
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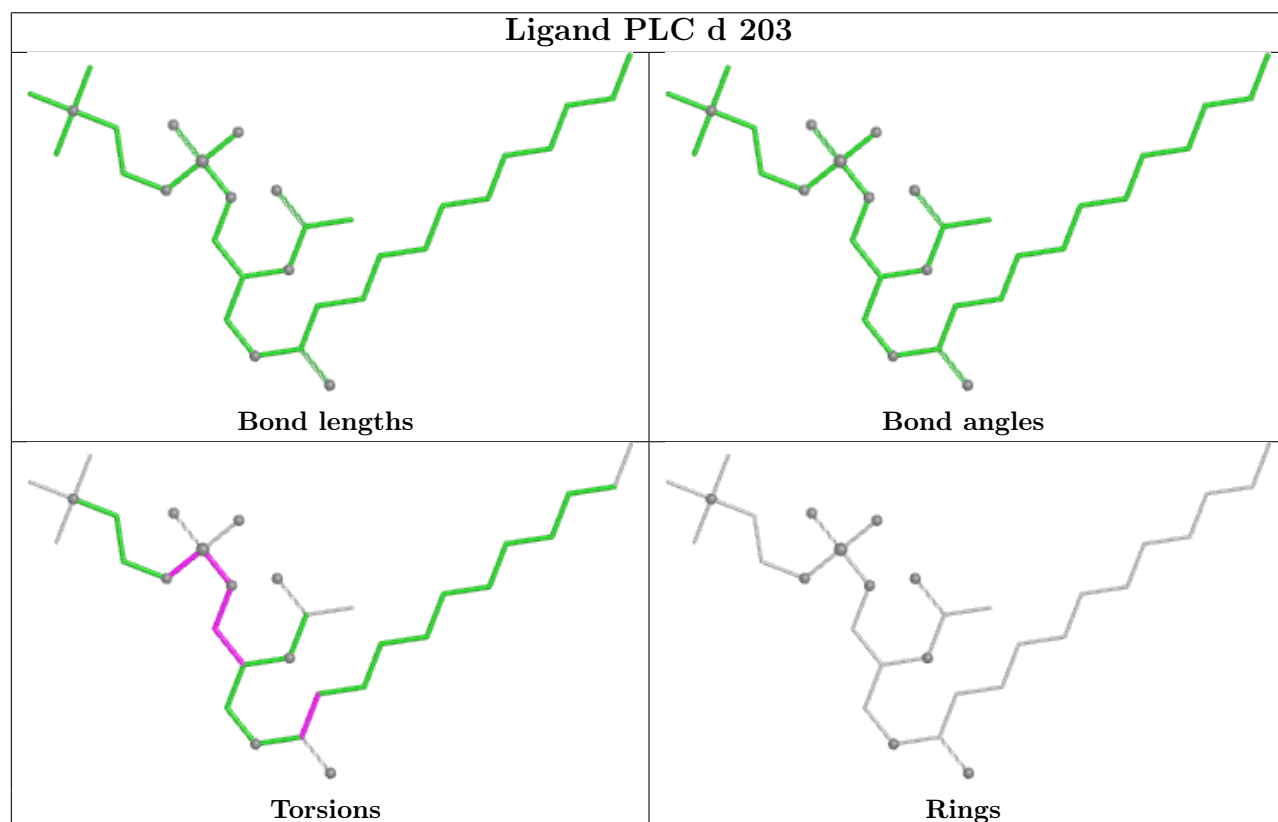
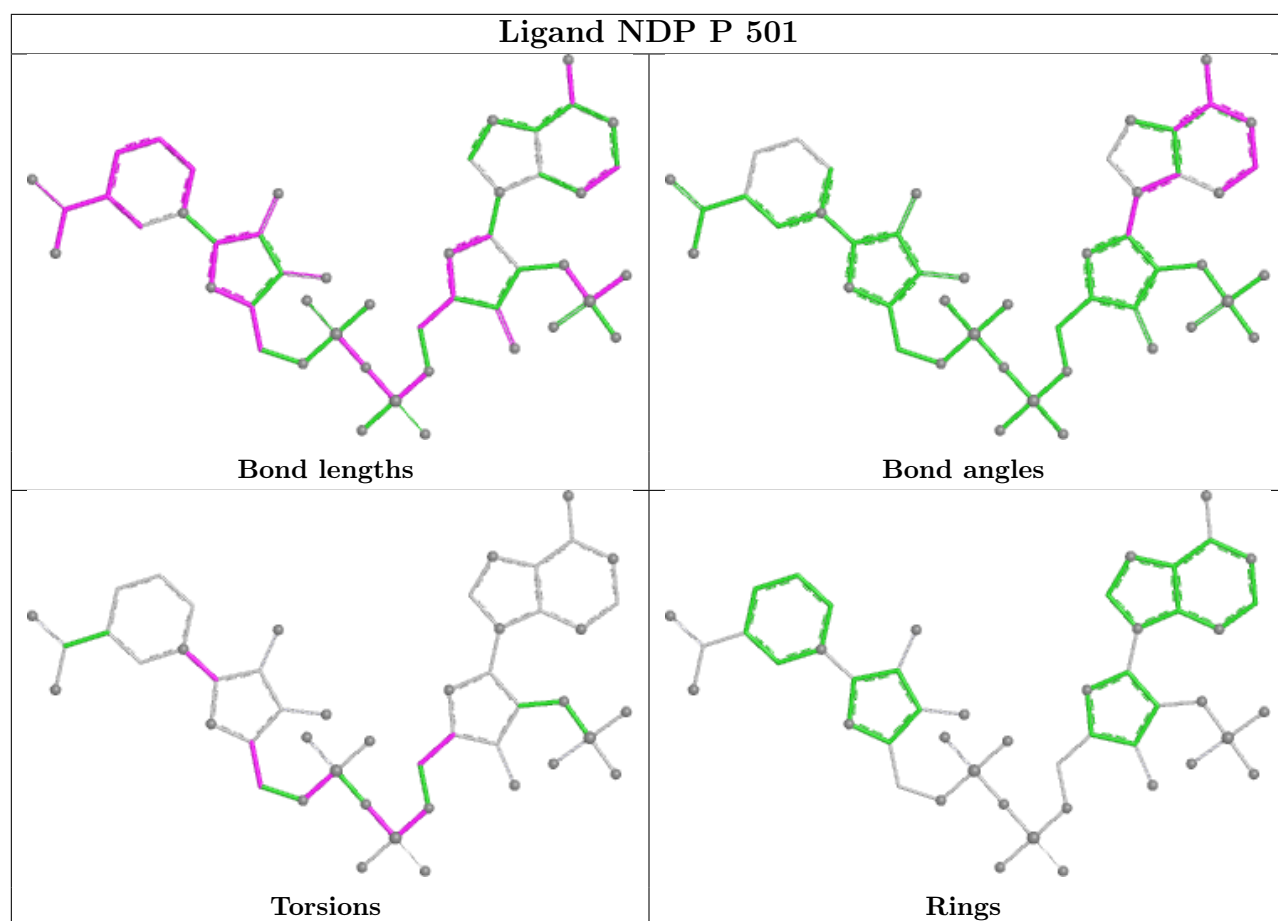
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 46  | A     | 202 | PC1  | O22-C21-C22-C23 |
| 45  | d     | 201 | 3PE  | C21-C22-C23-C24 |
| 45  | b     | 101 | 3PE  | C35-C36-C37-C38 |
| 45  | M     | 604 | 3PE  | C34-C35-C36-C37 |
| 45  | d     | 201 | 3PE  | O21-C21-C22-C23 |
| 46  | B     | 202 | PC1  | O21-C21-C22-C23 |
| 45  | Y     | 201 | 3PE  | O22-C21-C22-C23 |
| 48  | Y     | 208 | PLC  | O'-C'-C1'-C2'   |

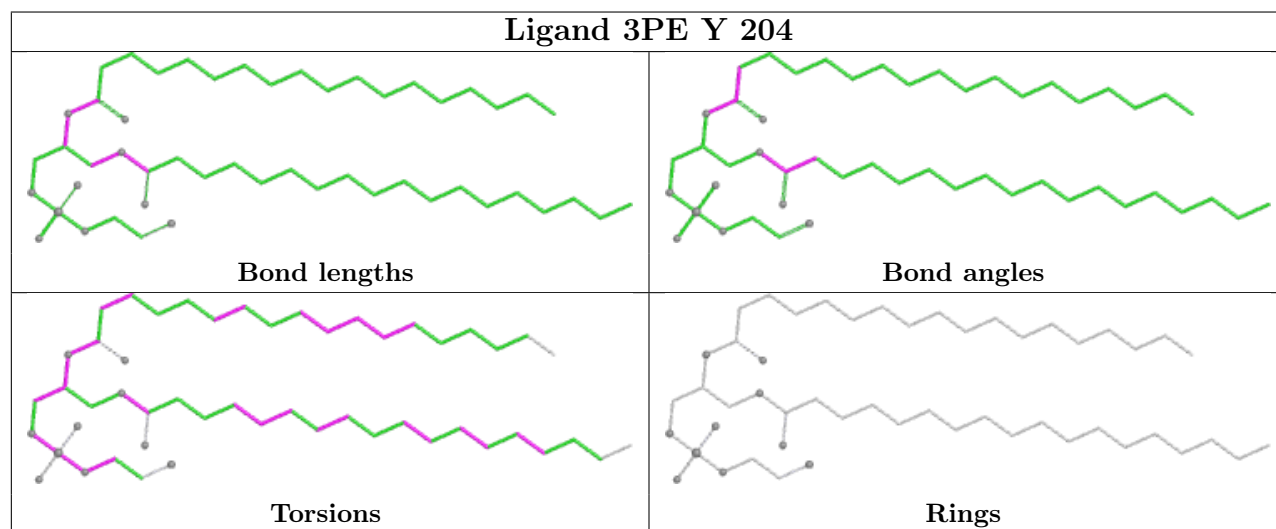
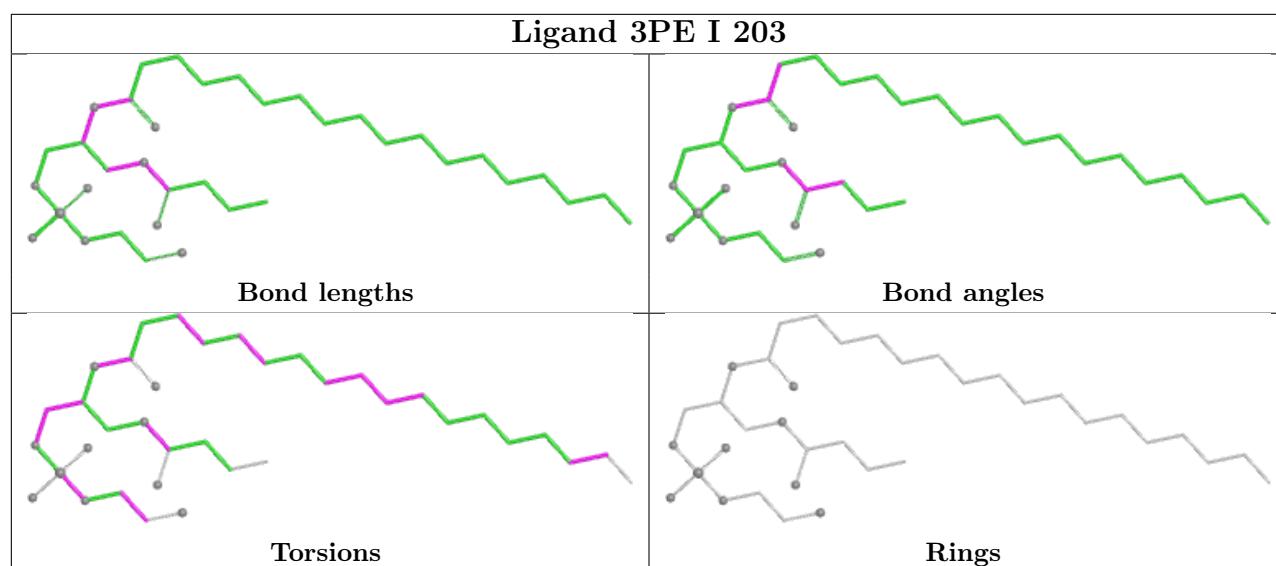
There are no ring outliers.

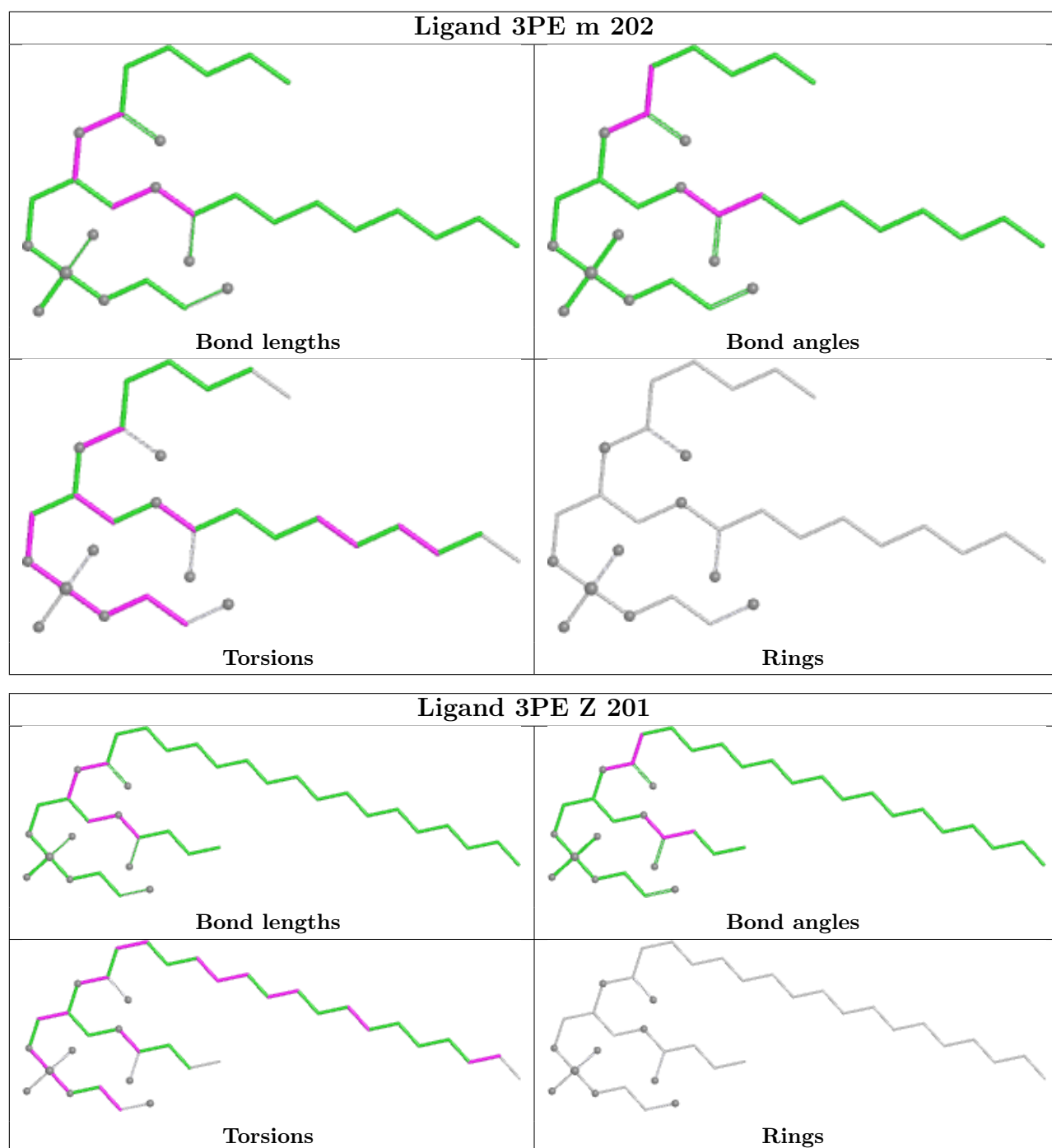
No monomer is involved in short contacts.

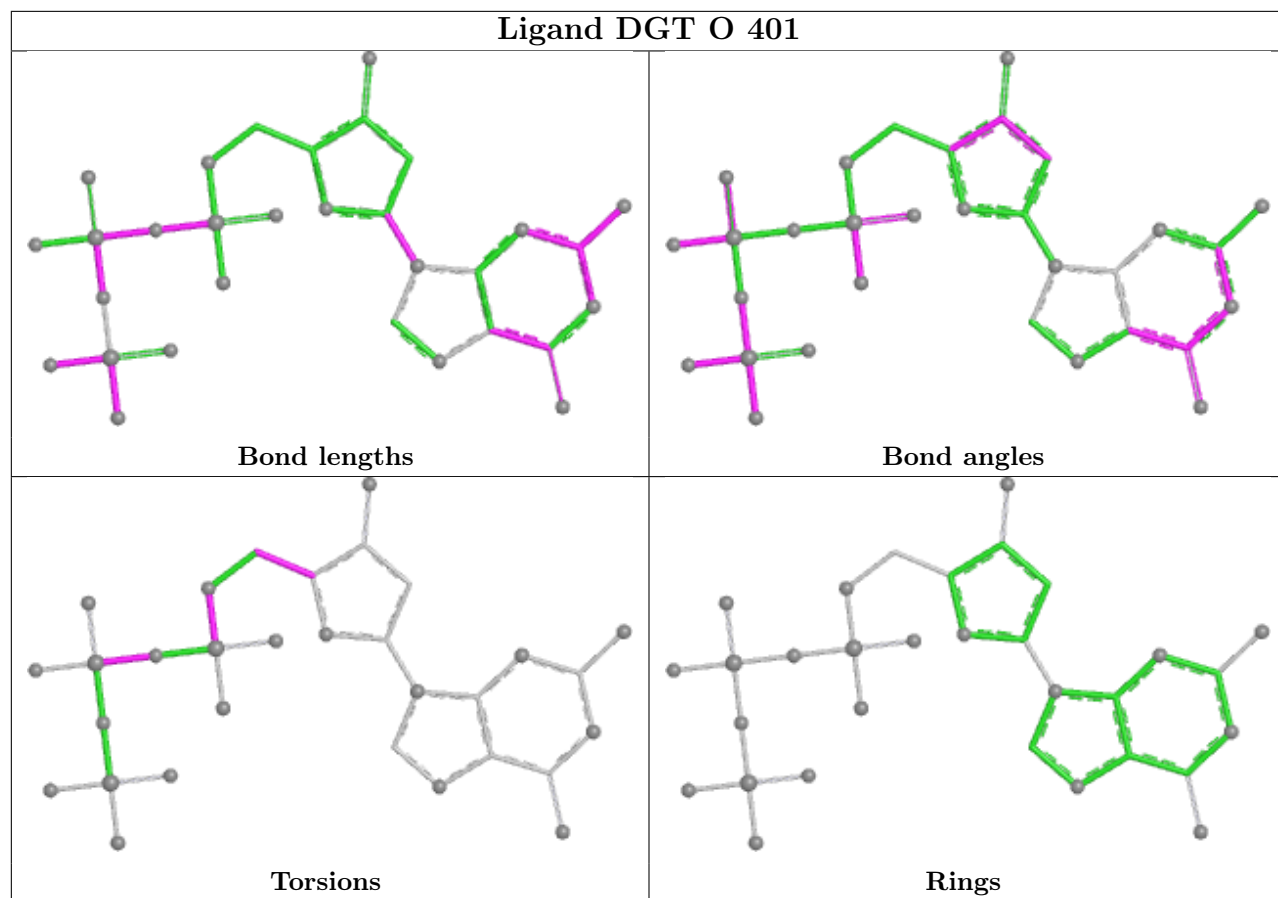
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

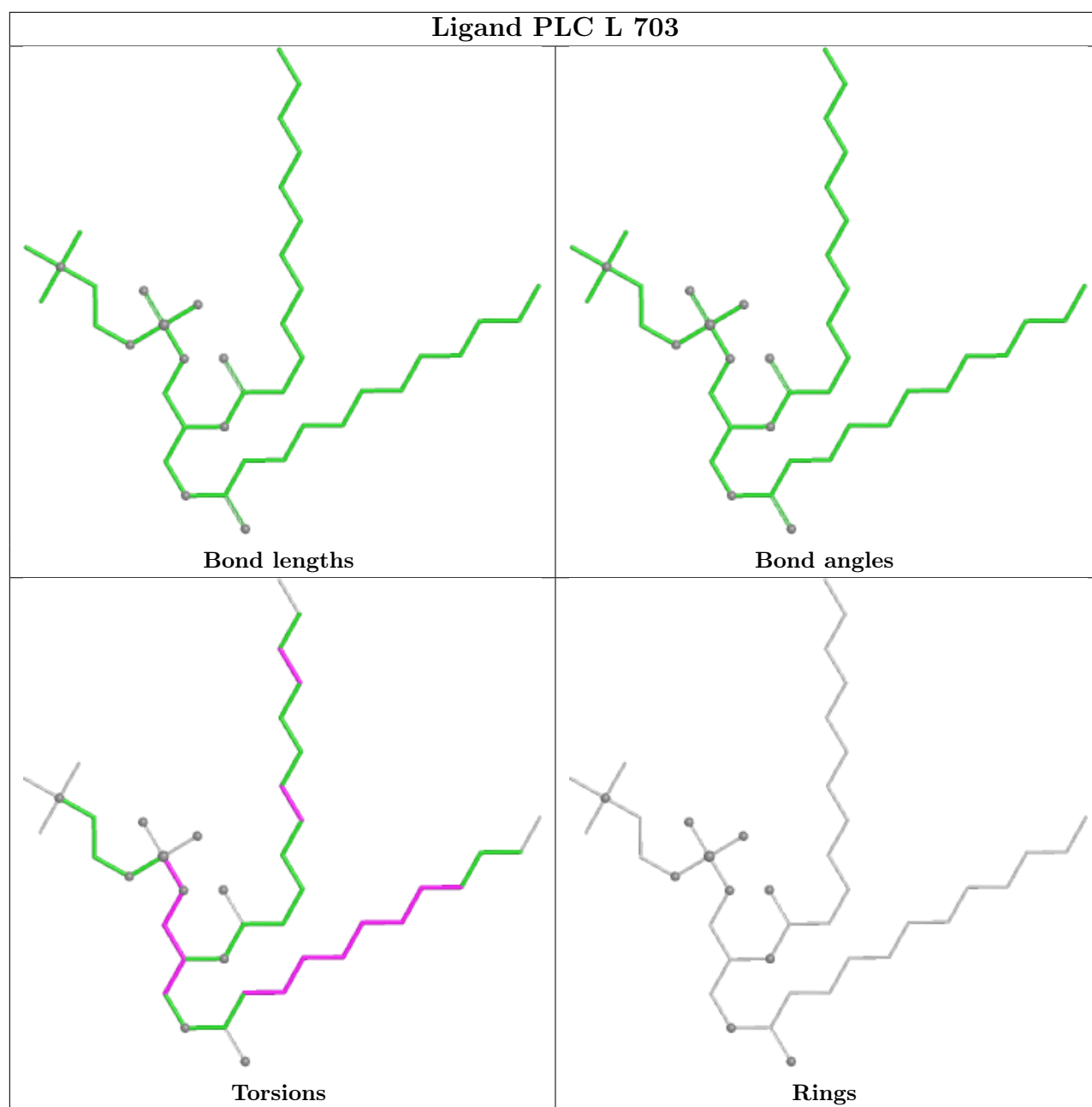




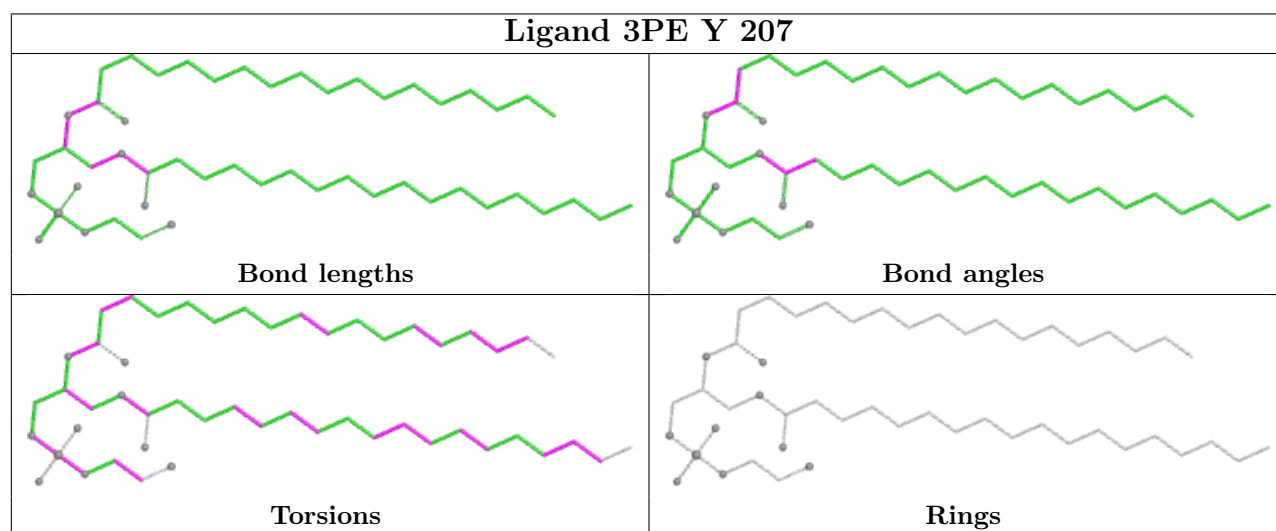
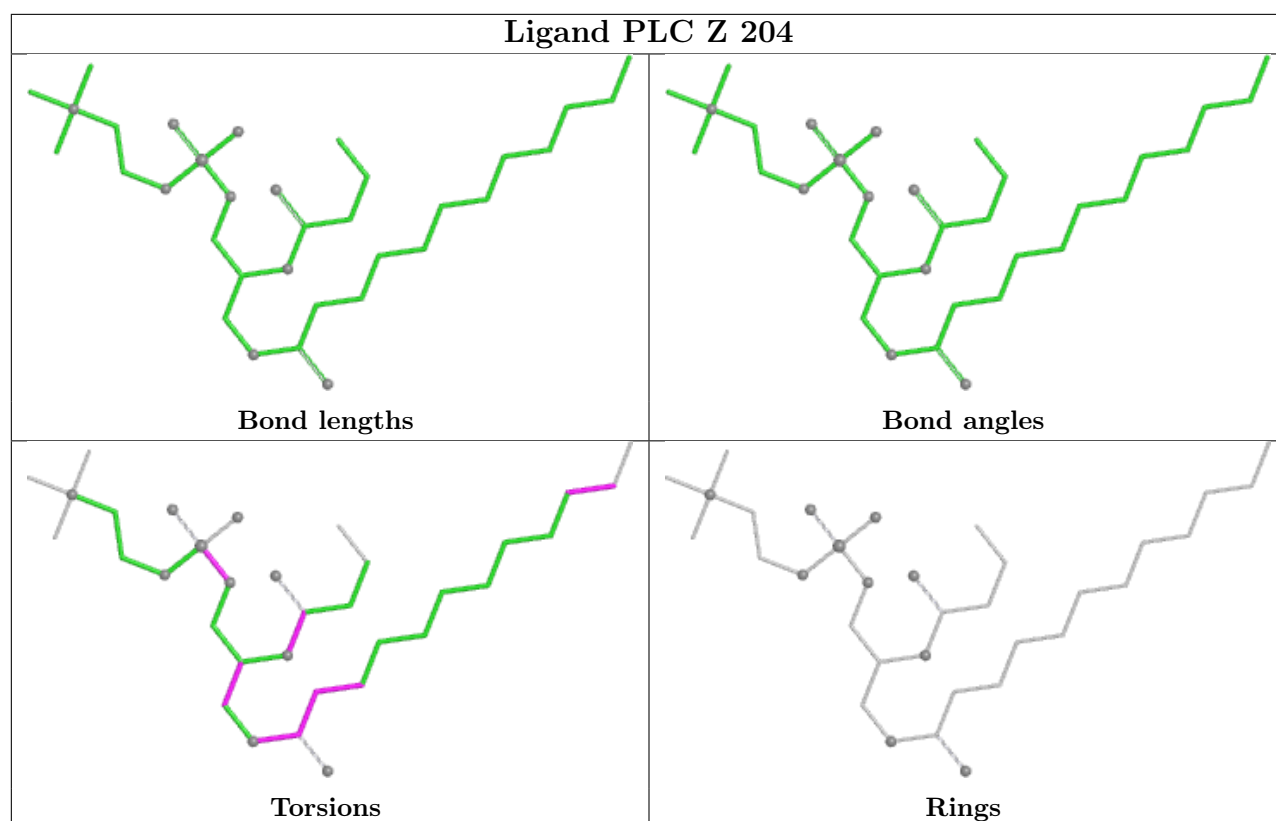


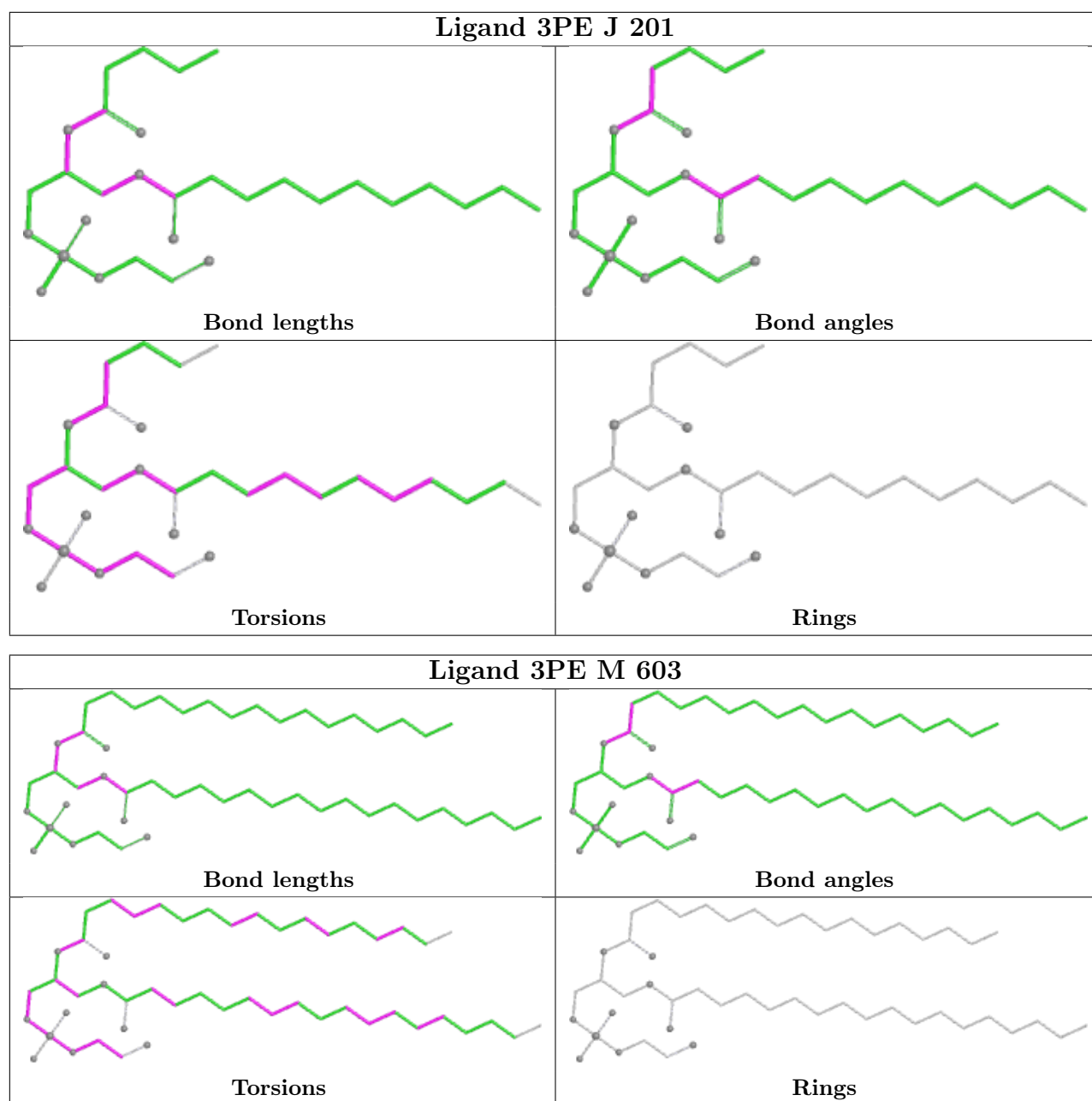


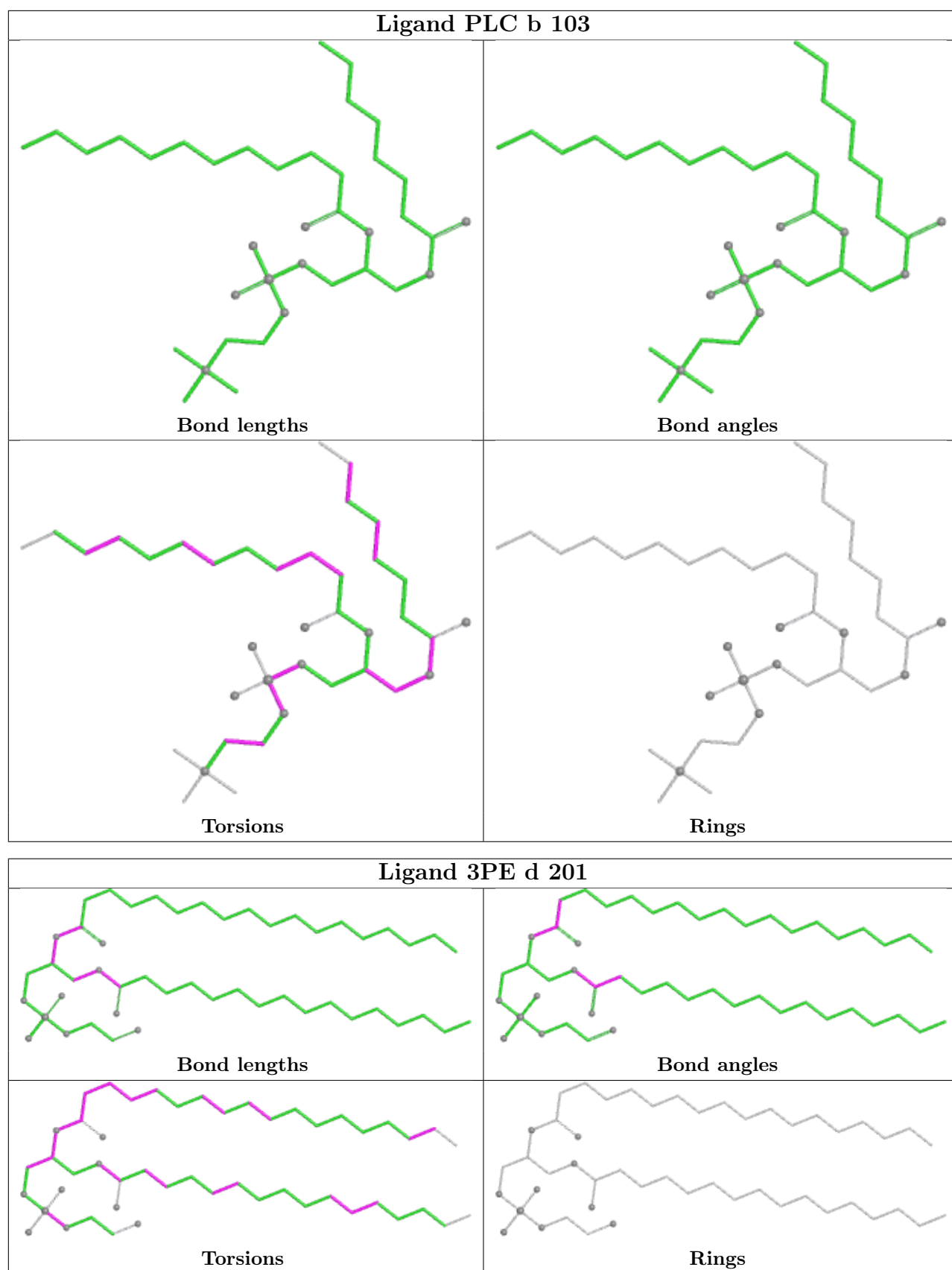


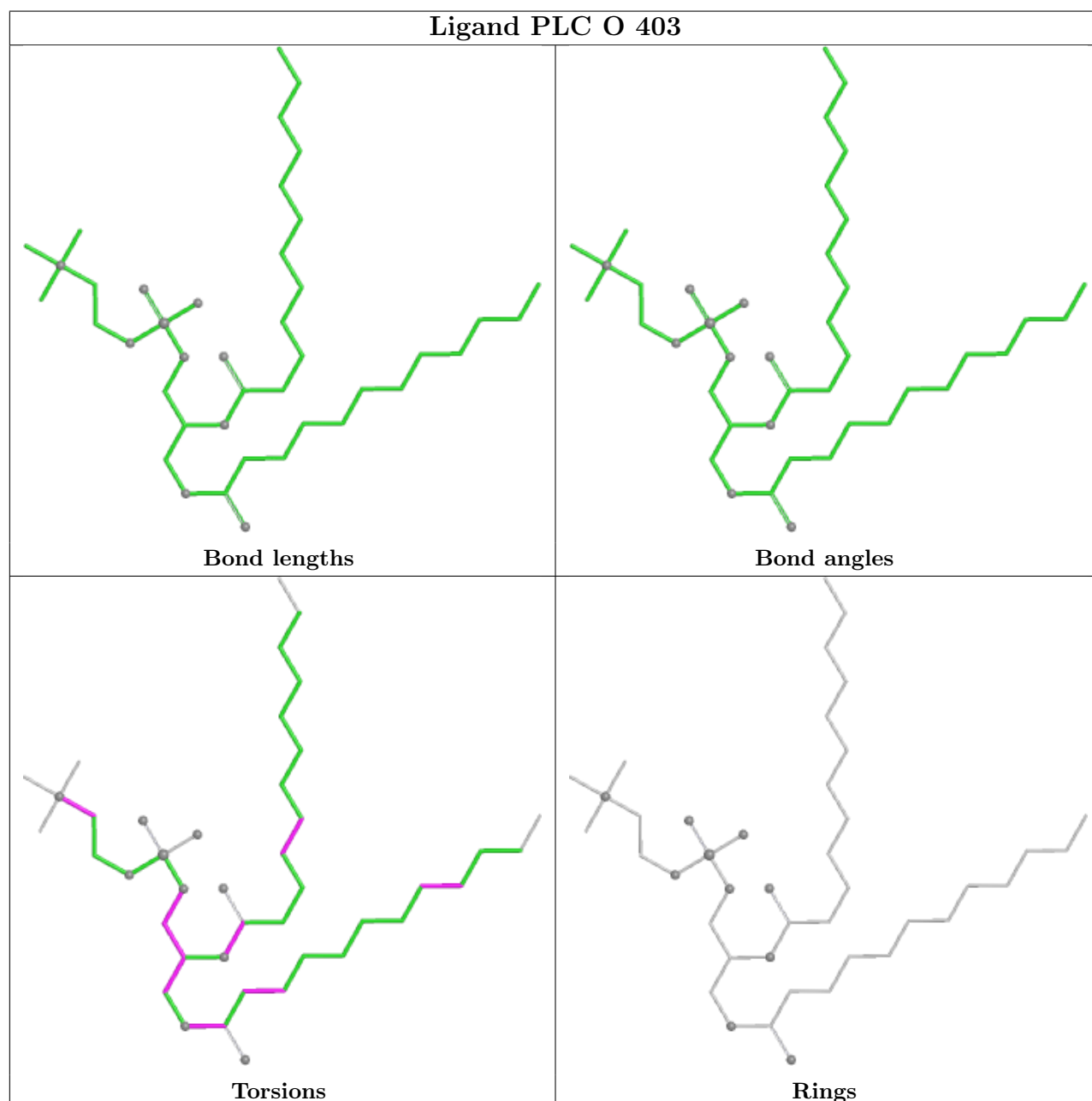
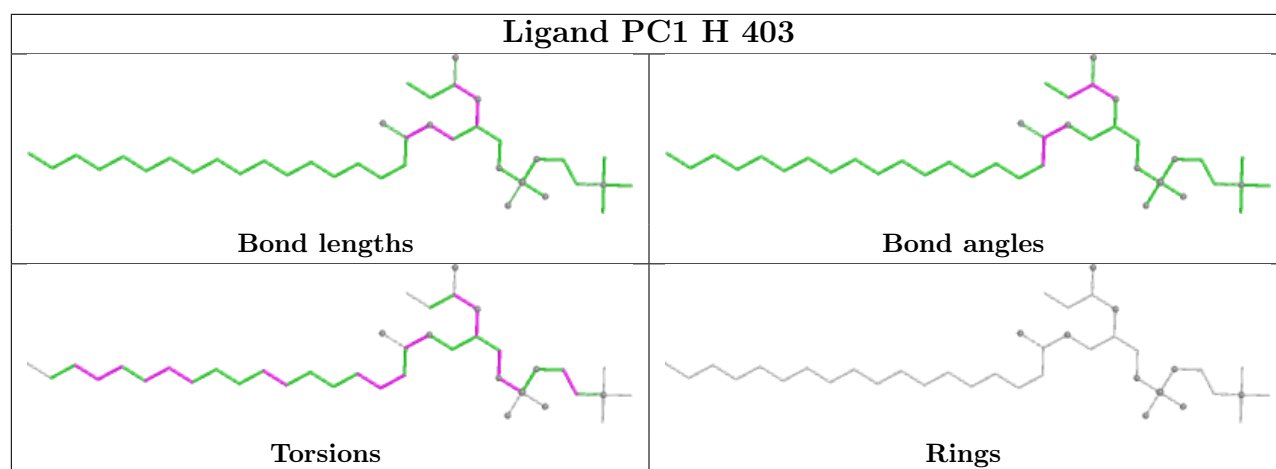


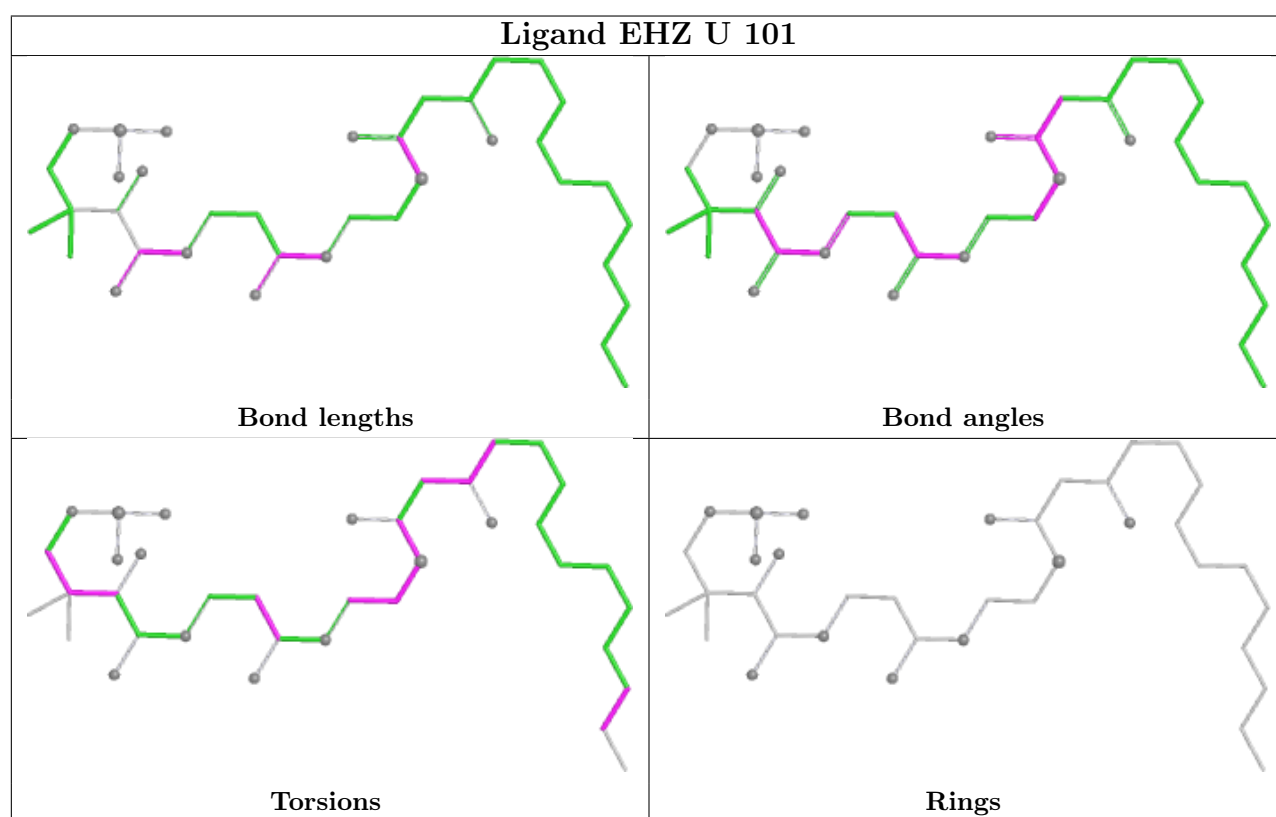
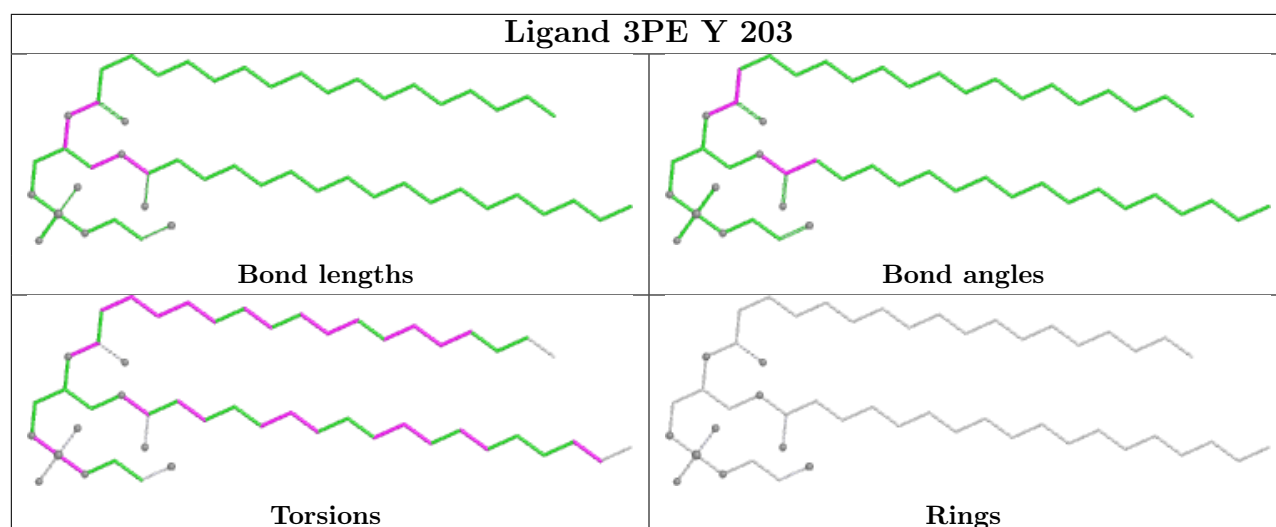


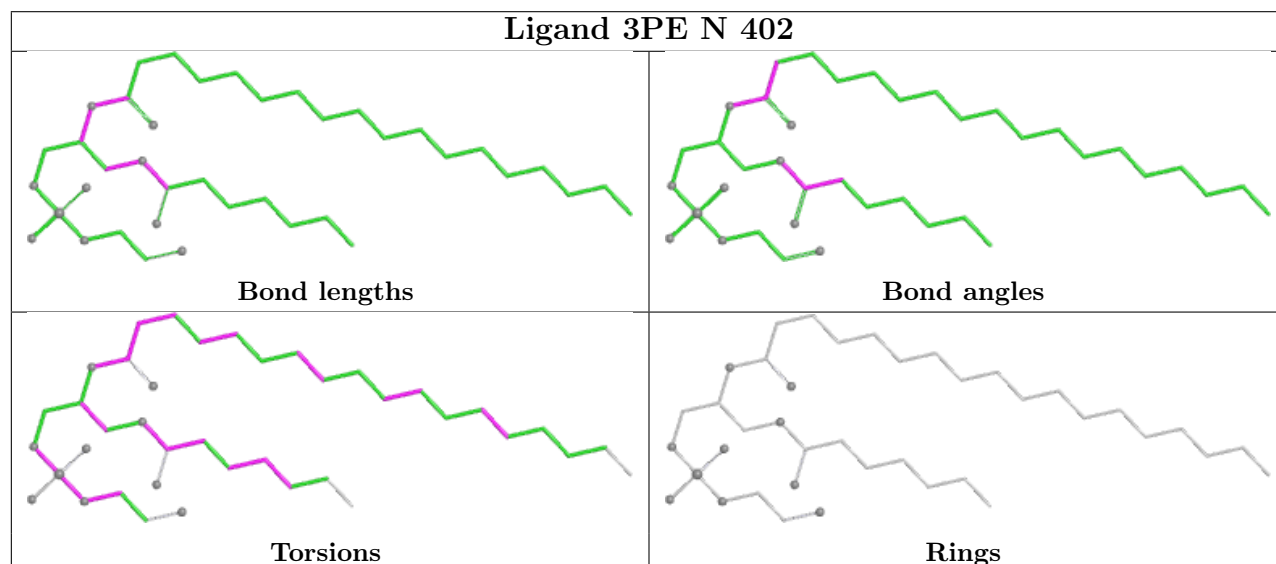
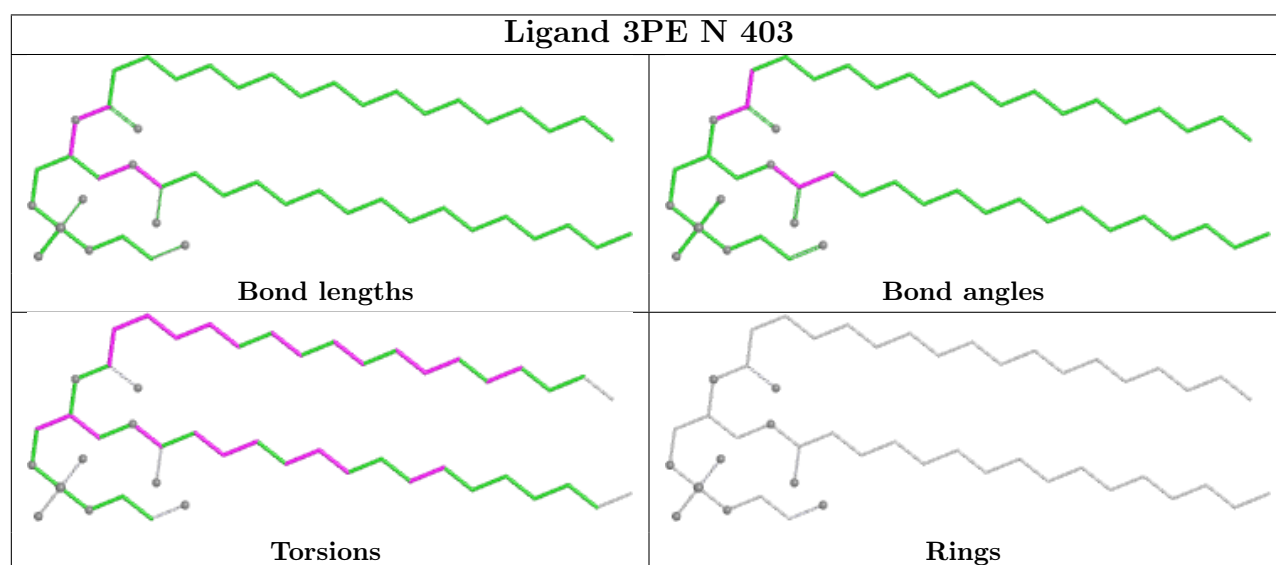
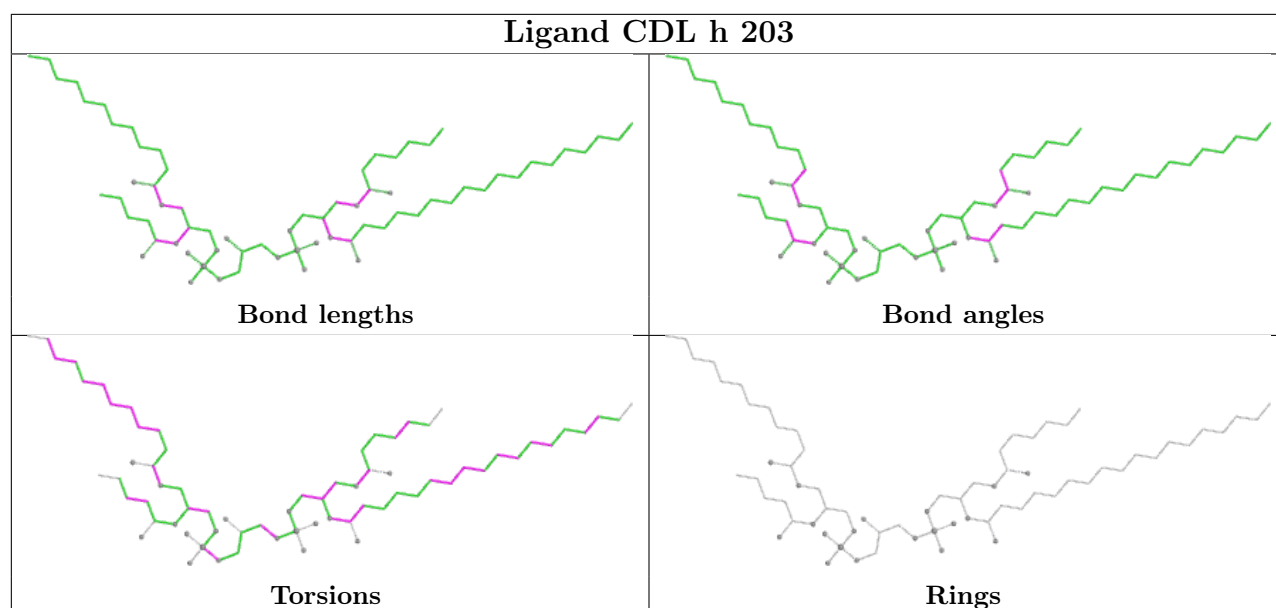


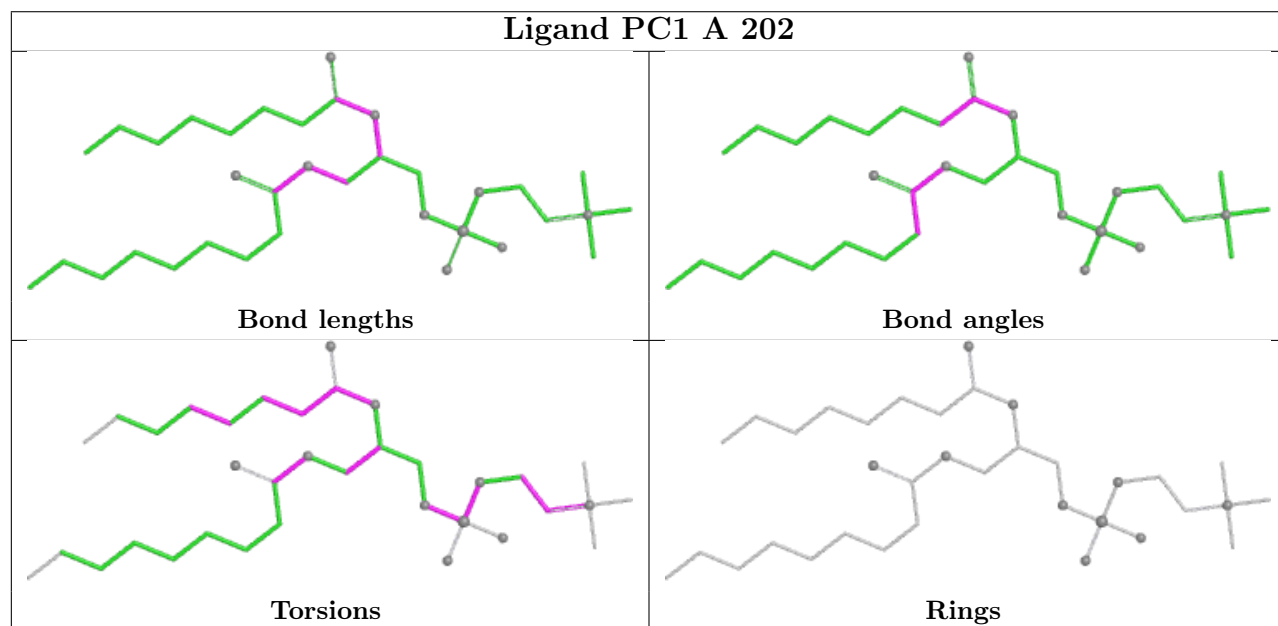
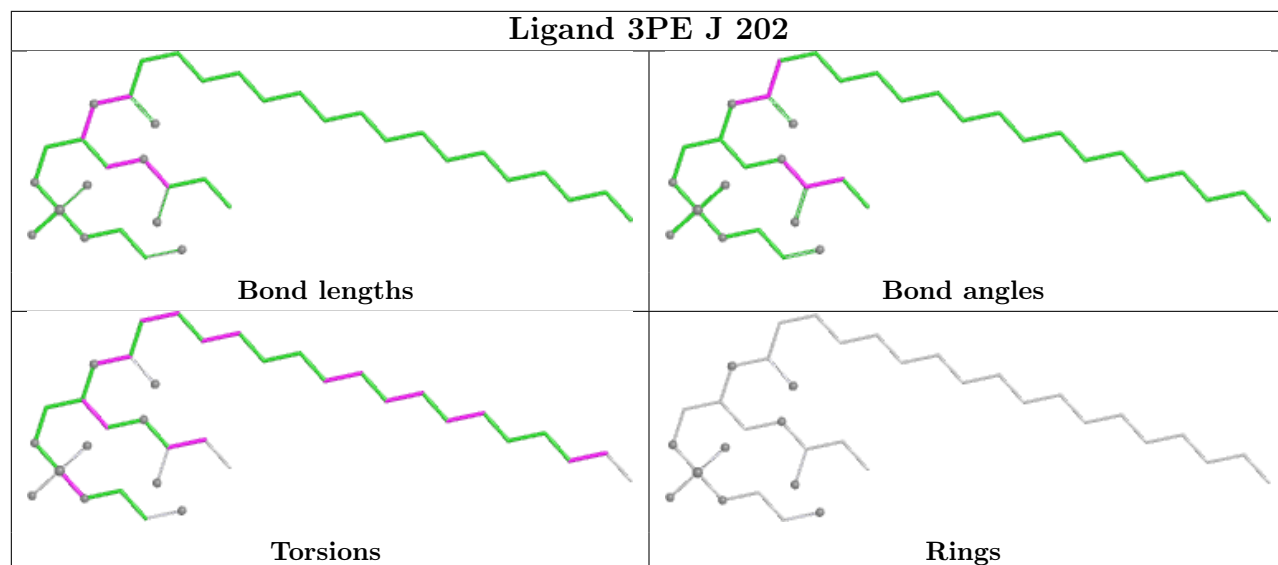


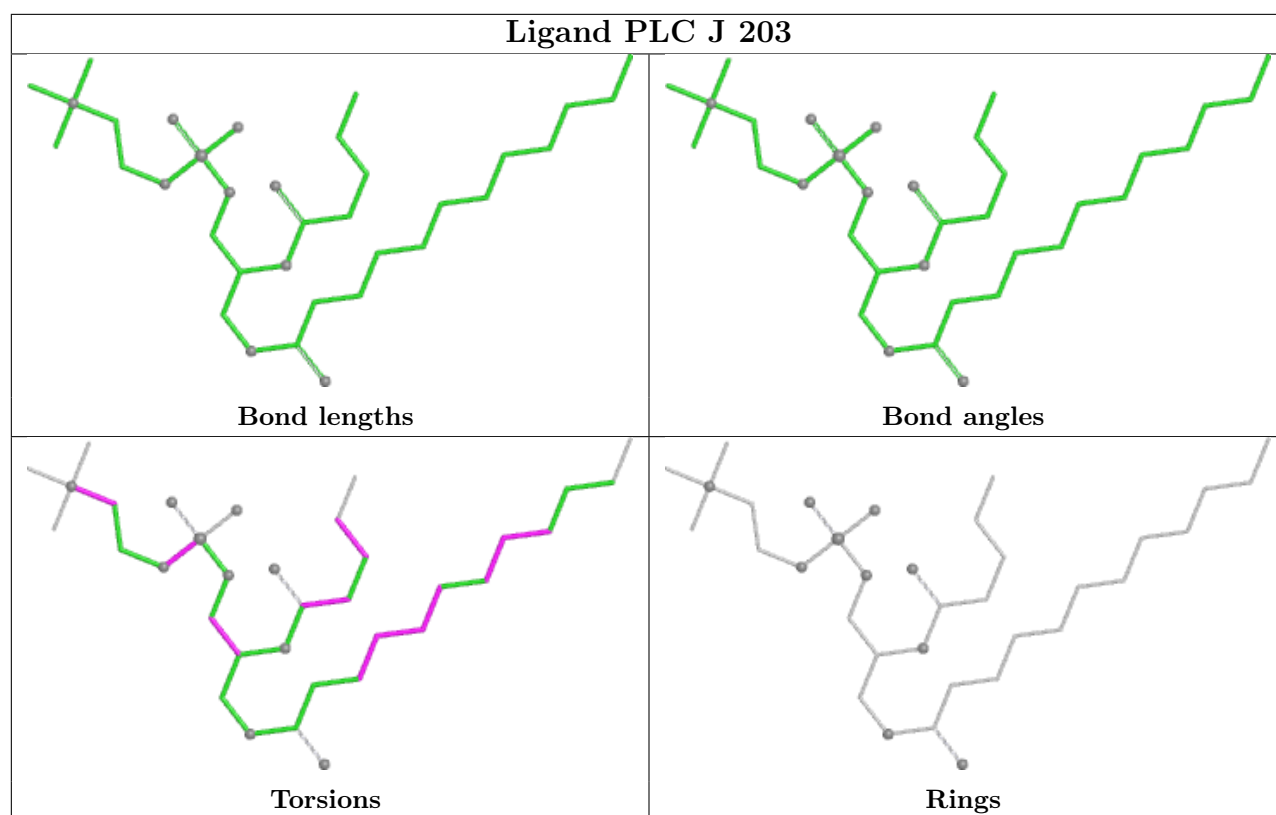
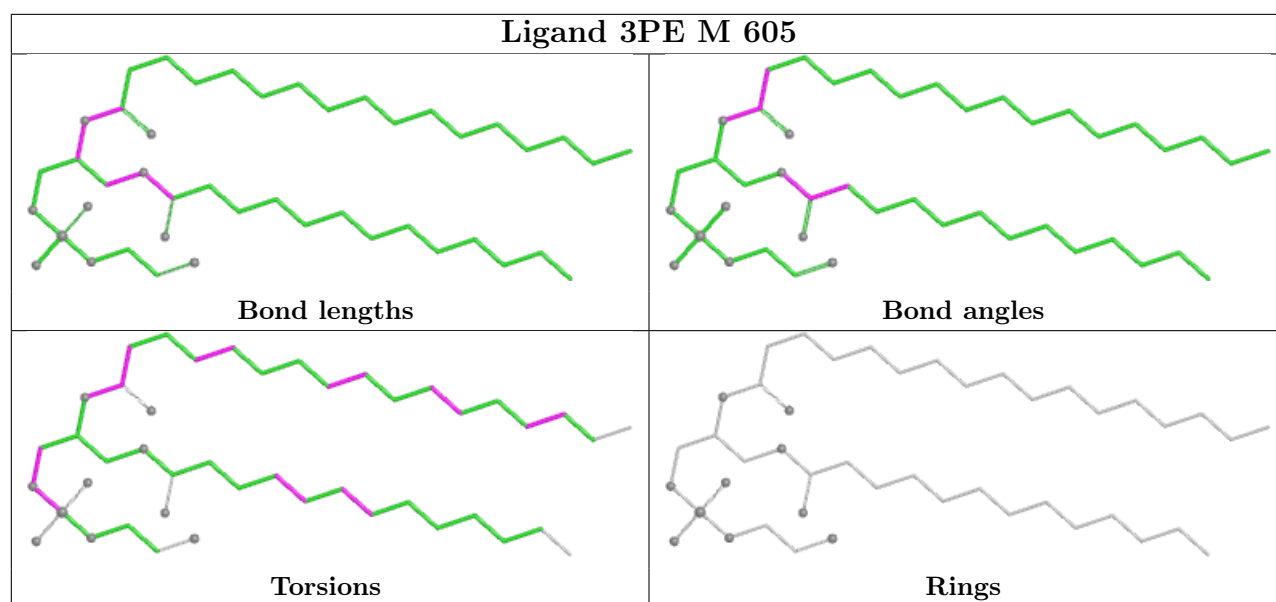




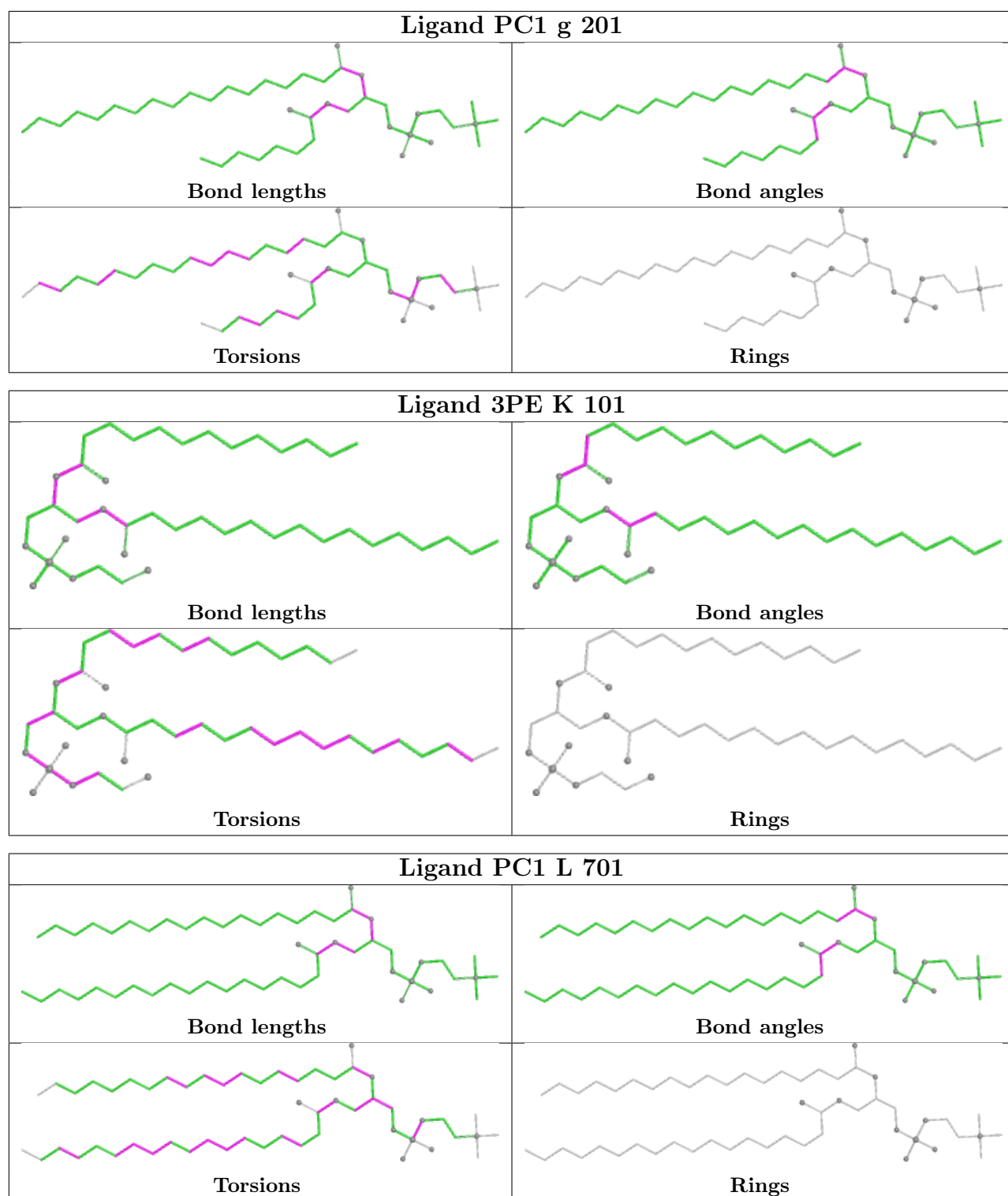




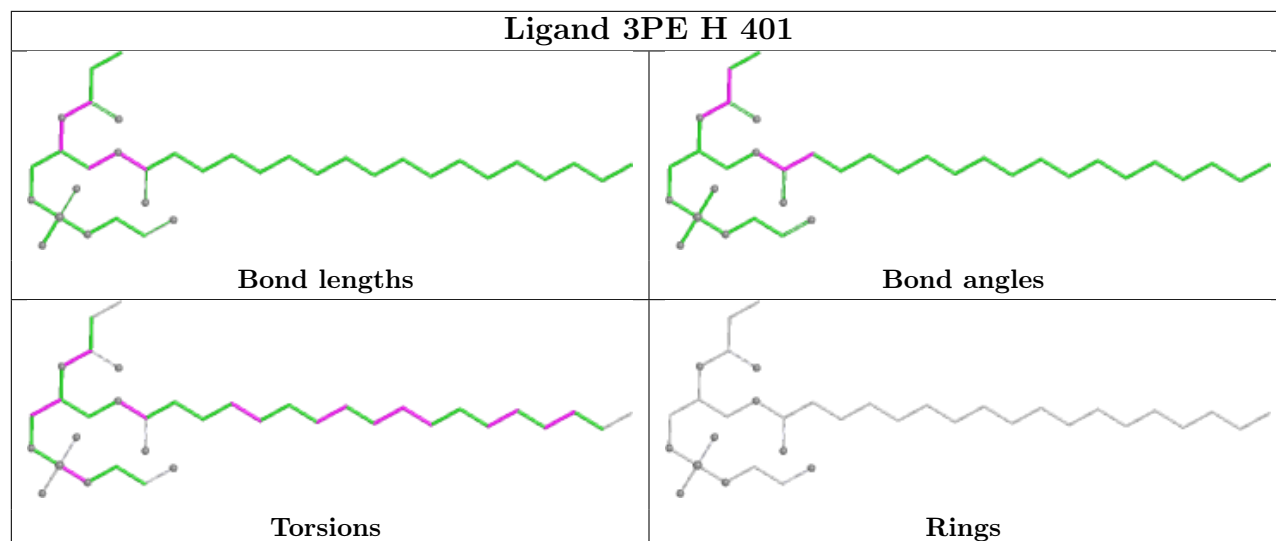




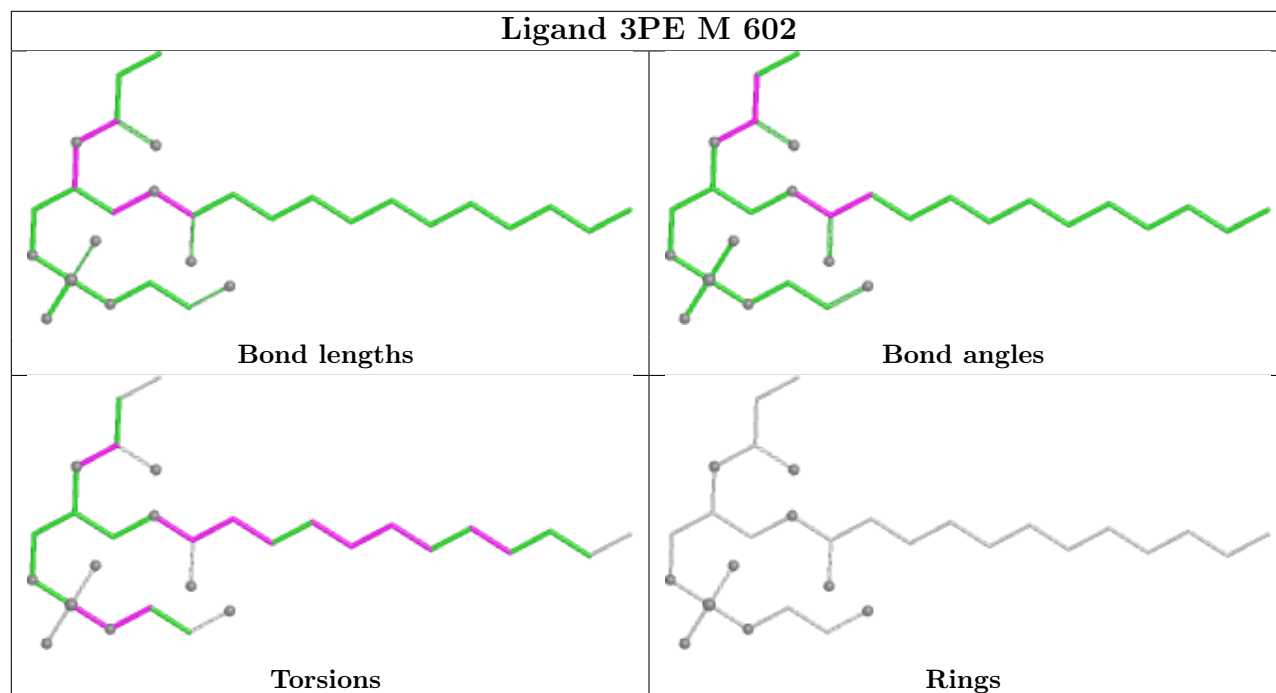




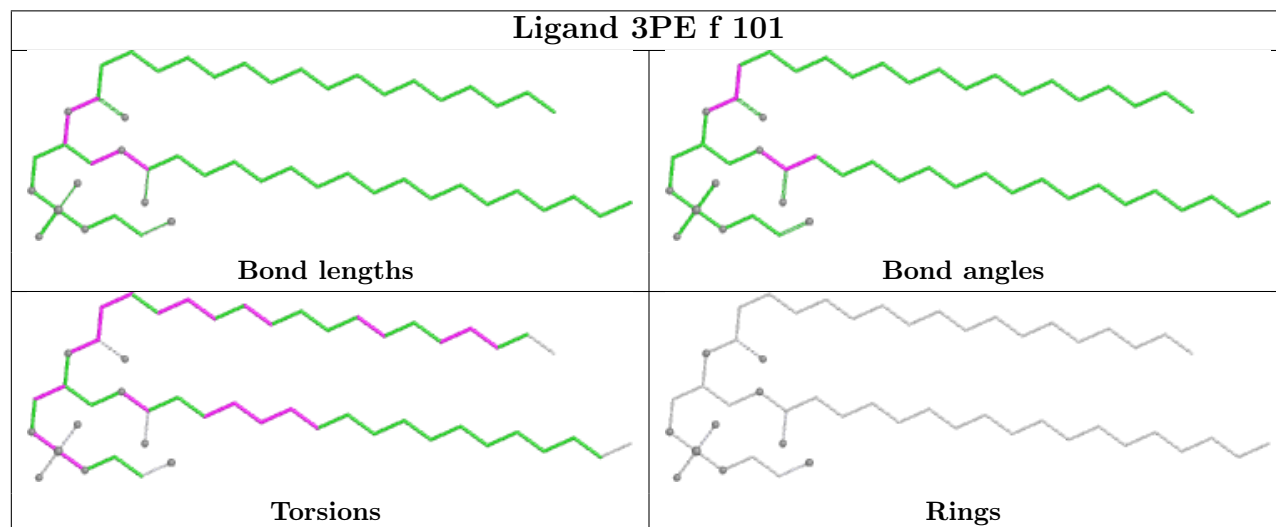
## Ligand 3PE H 401



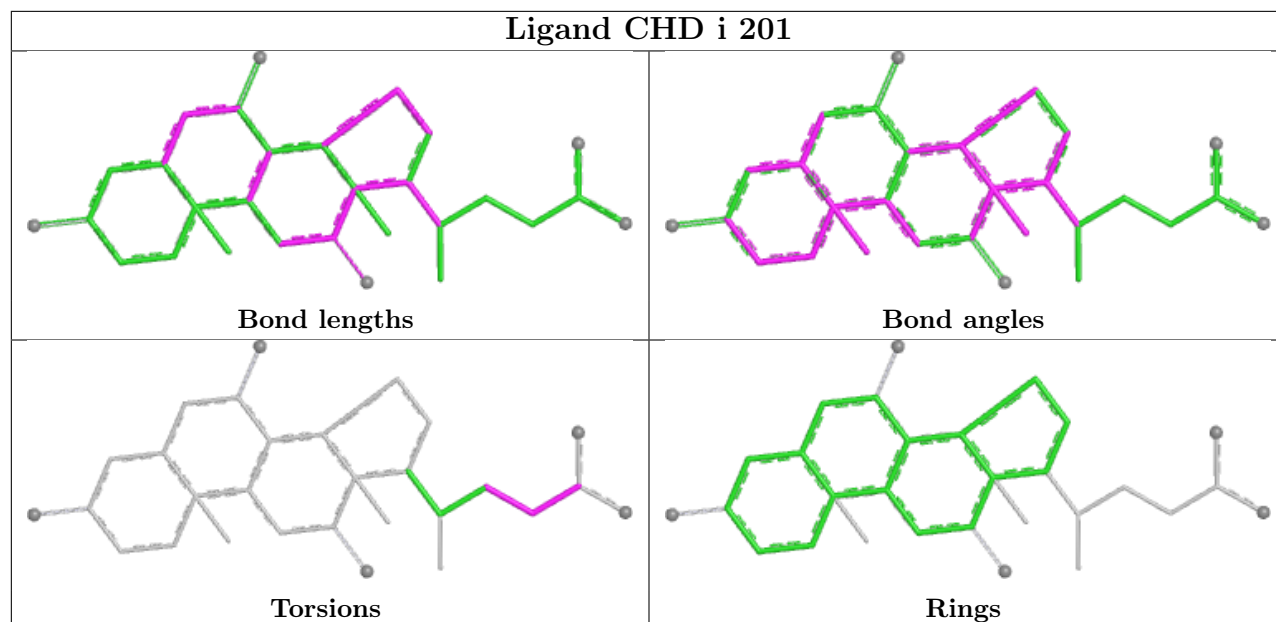
## Ligand 3PE M 602



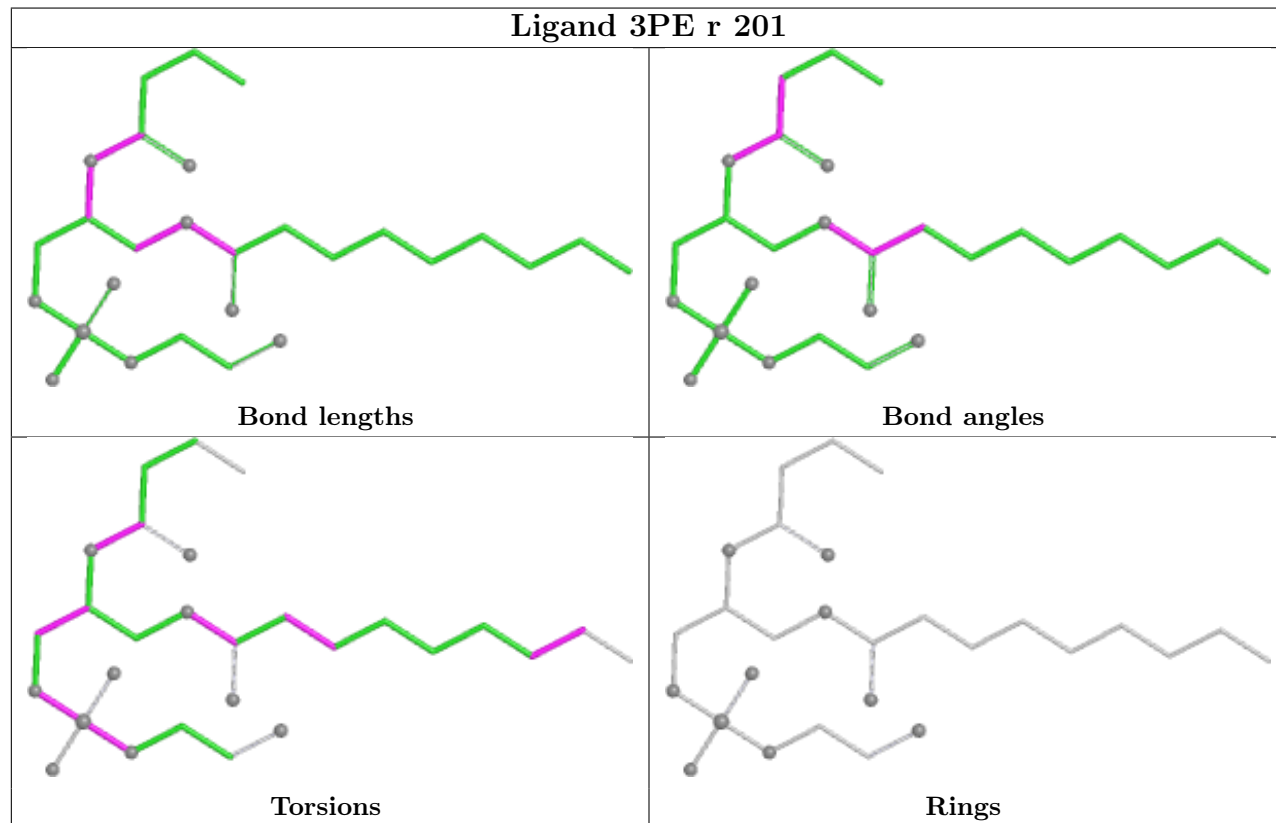
## Ligand 3PE f 101

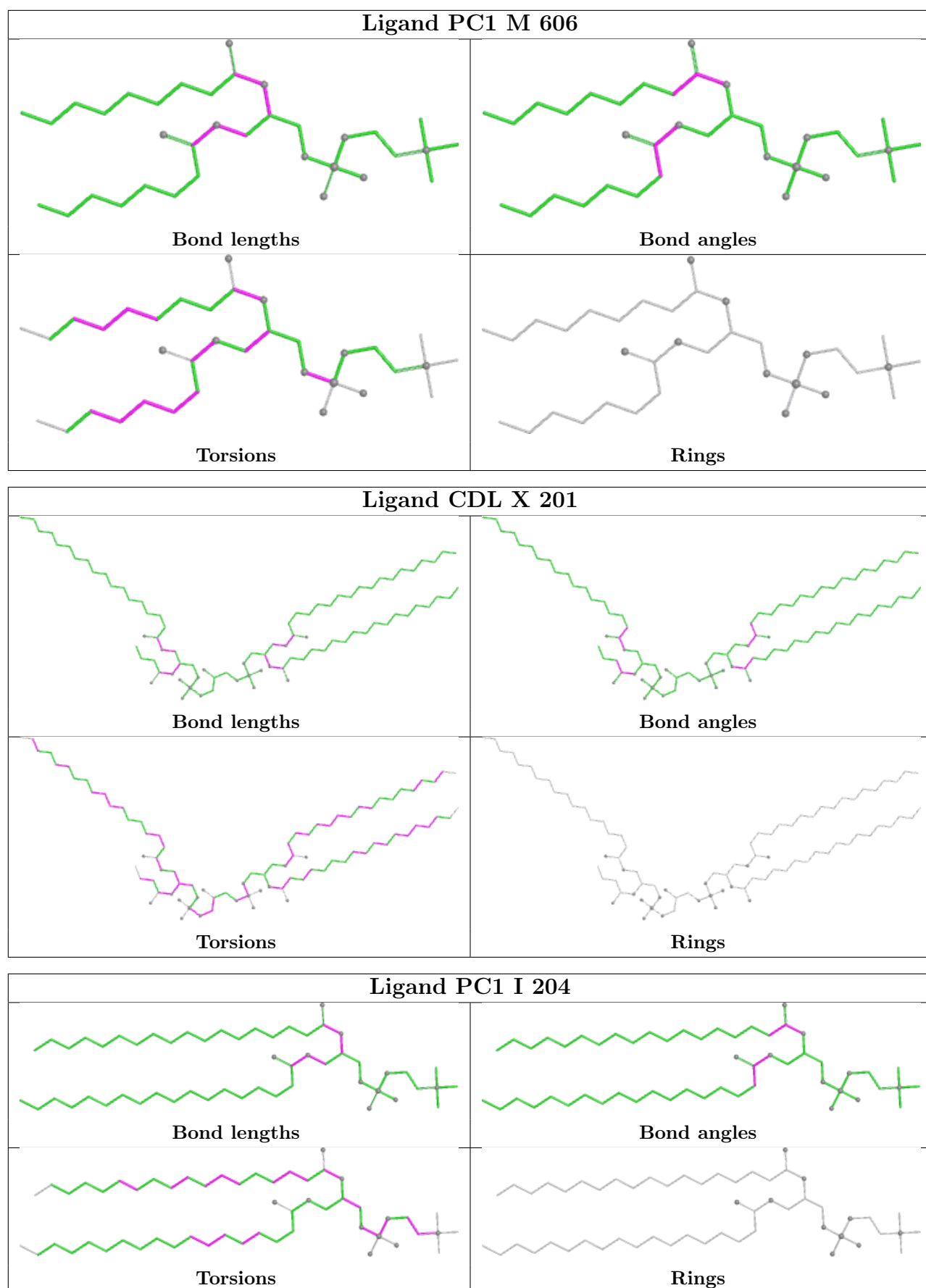


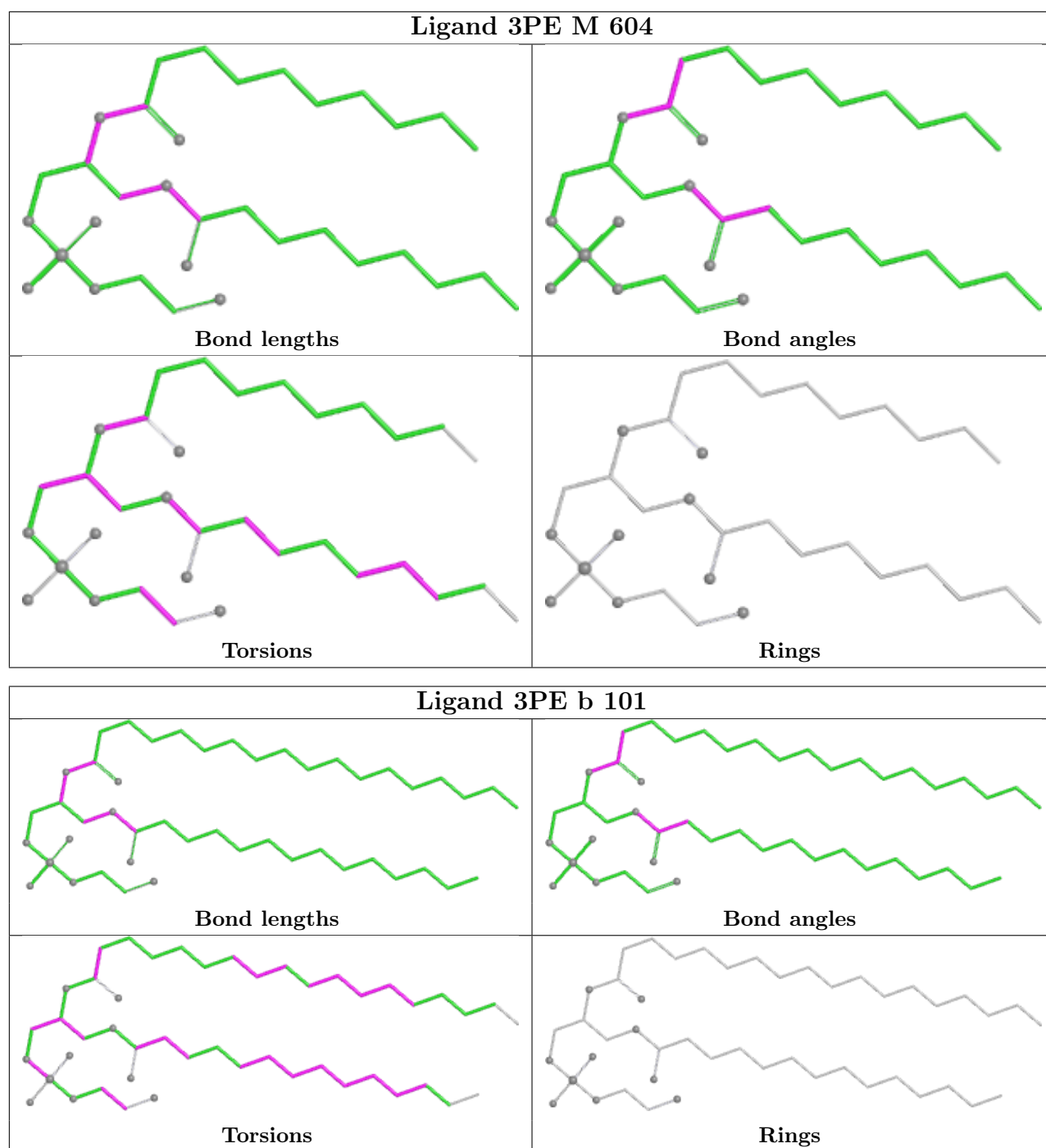
## Ligand CHD i 201

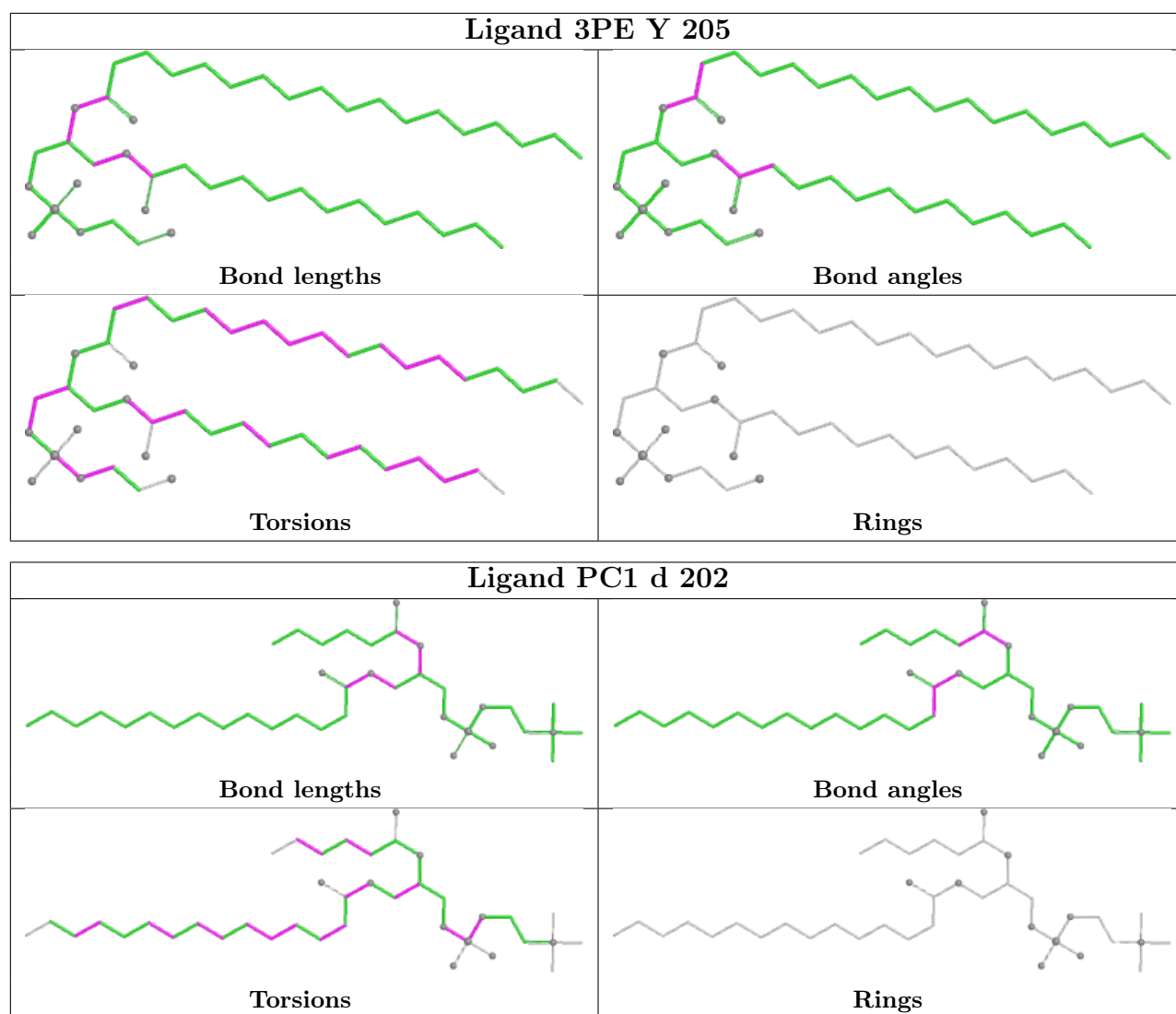


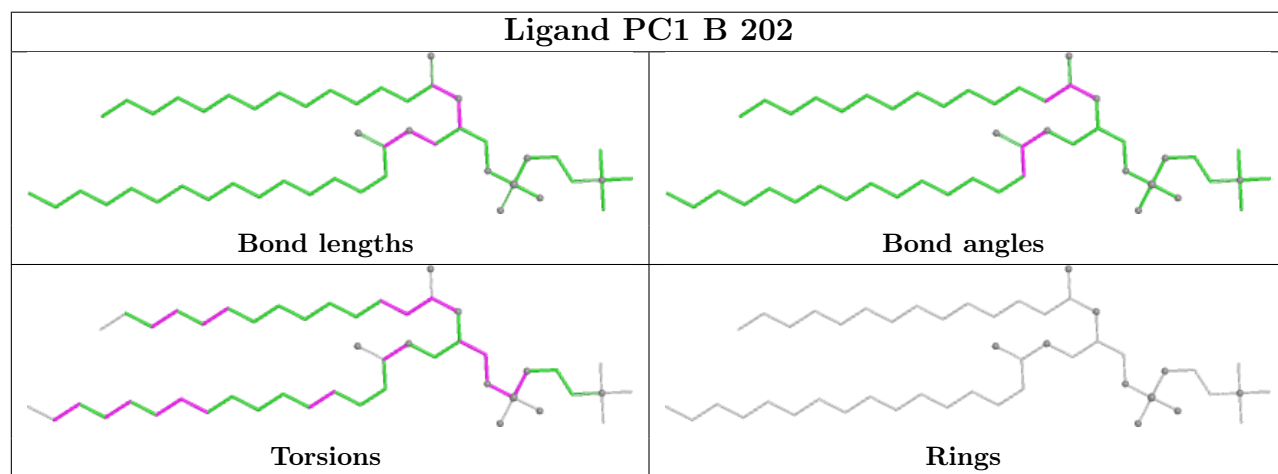
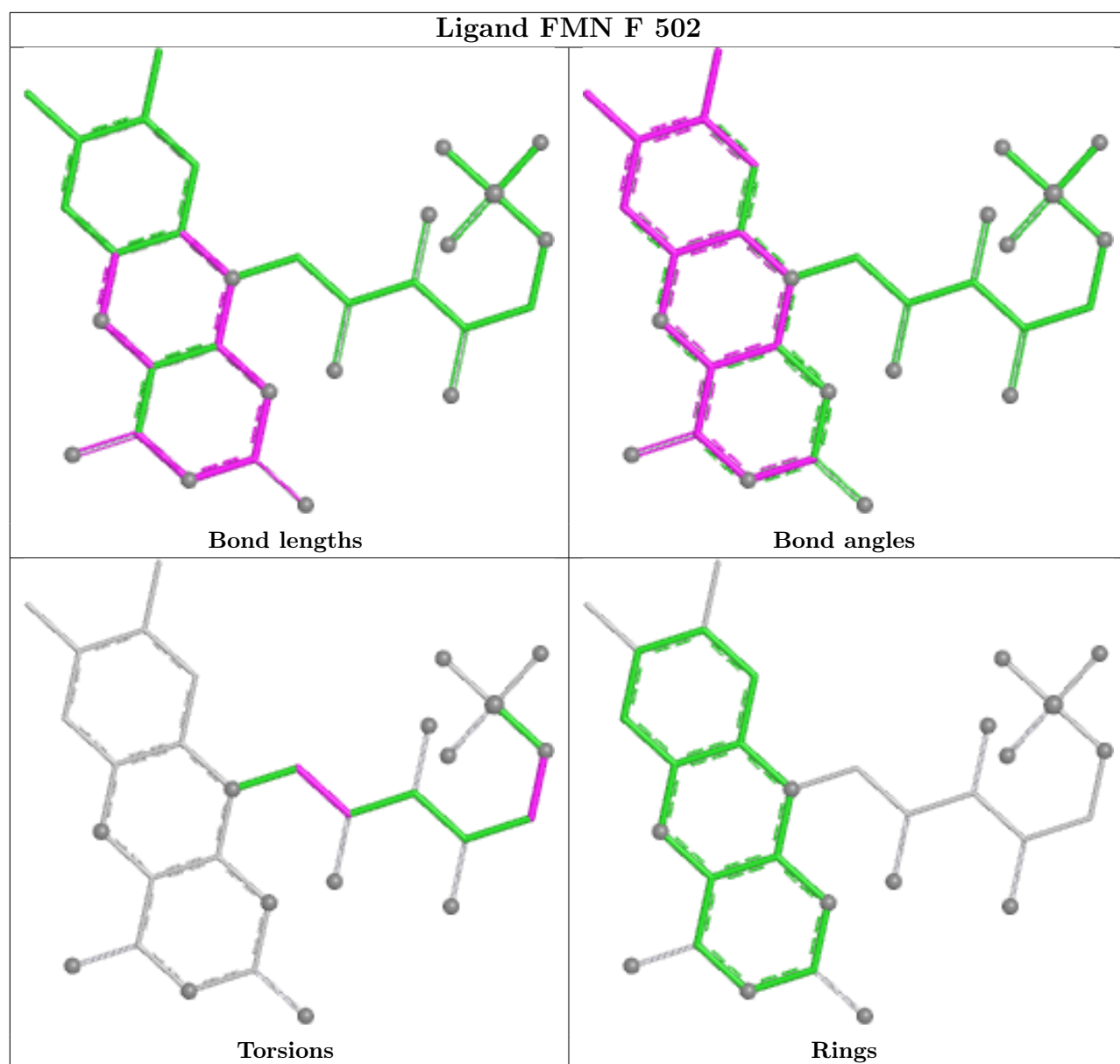
## Ligand 3PE r 201

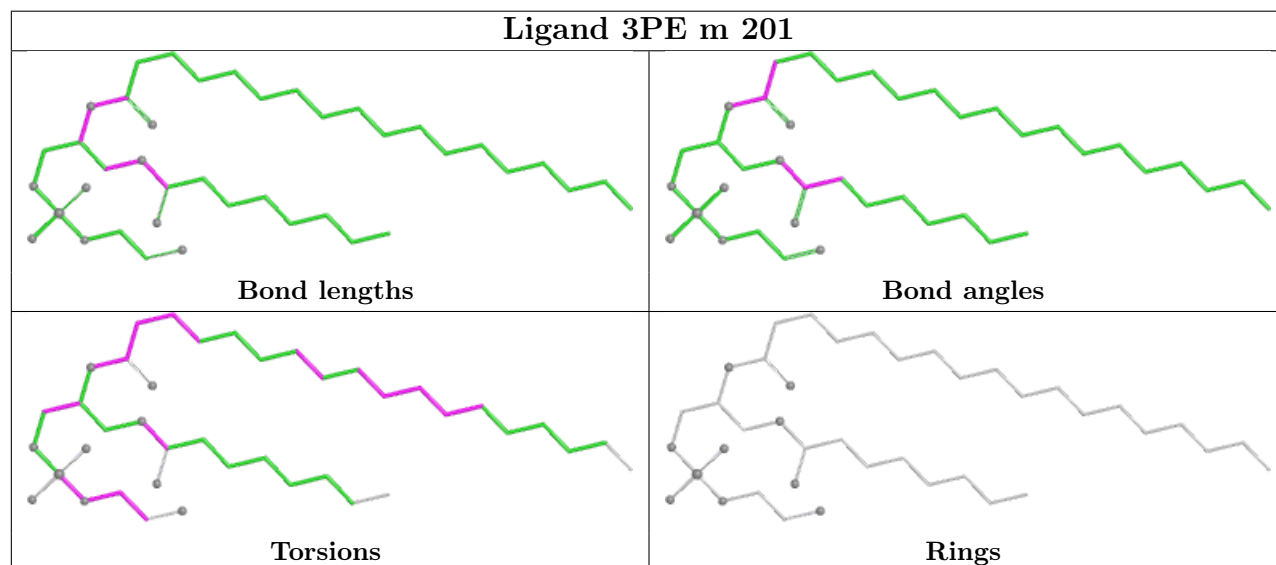
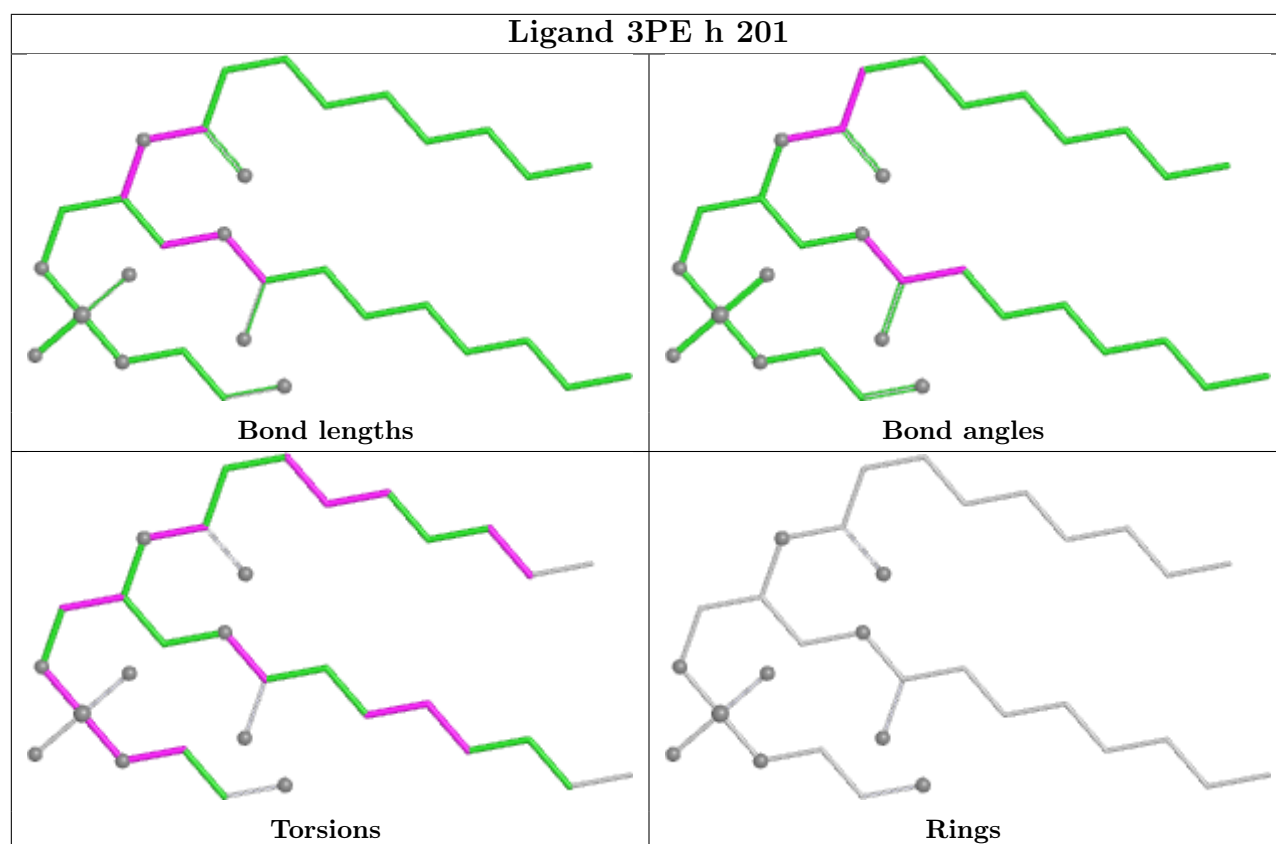




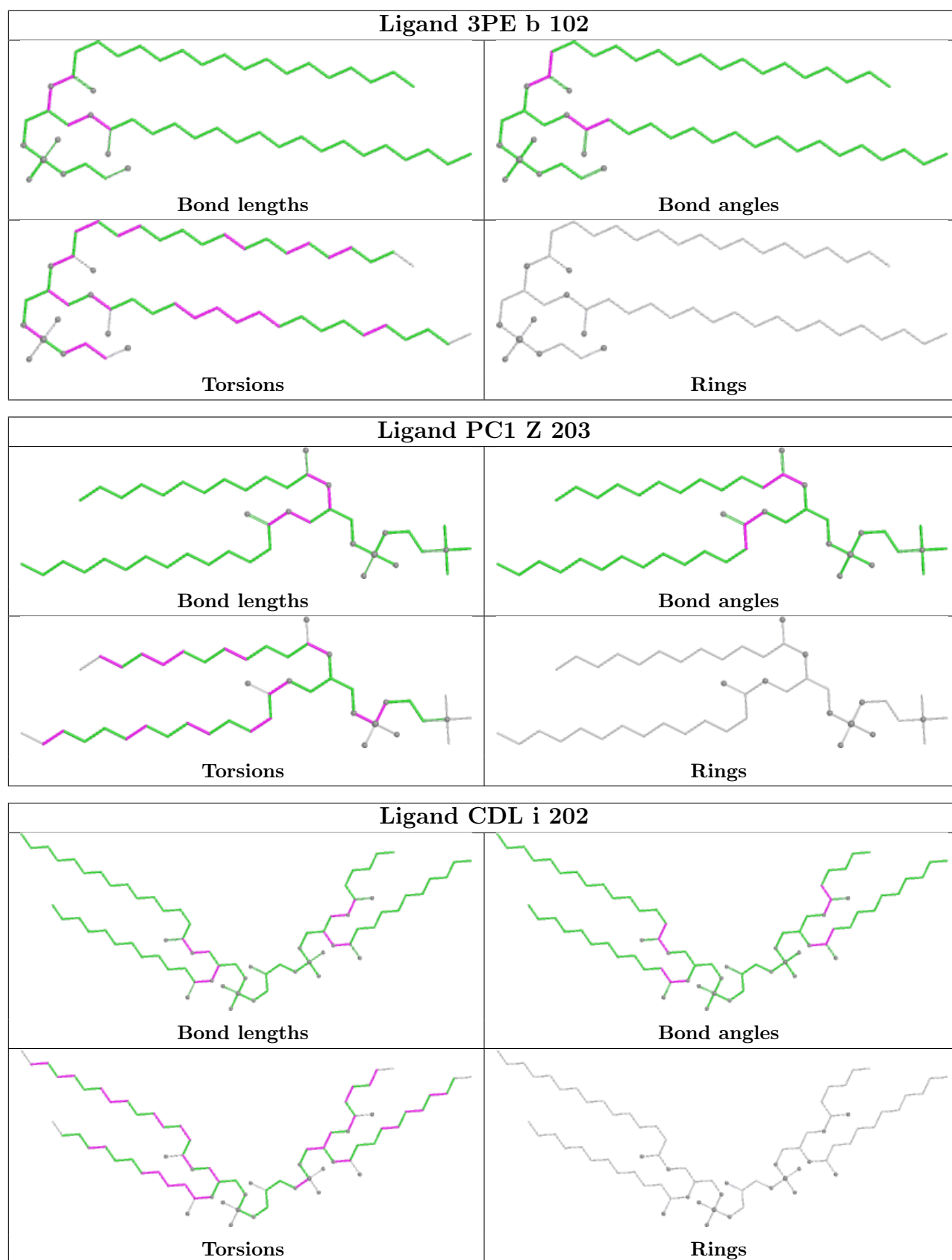


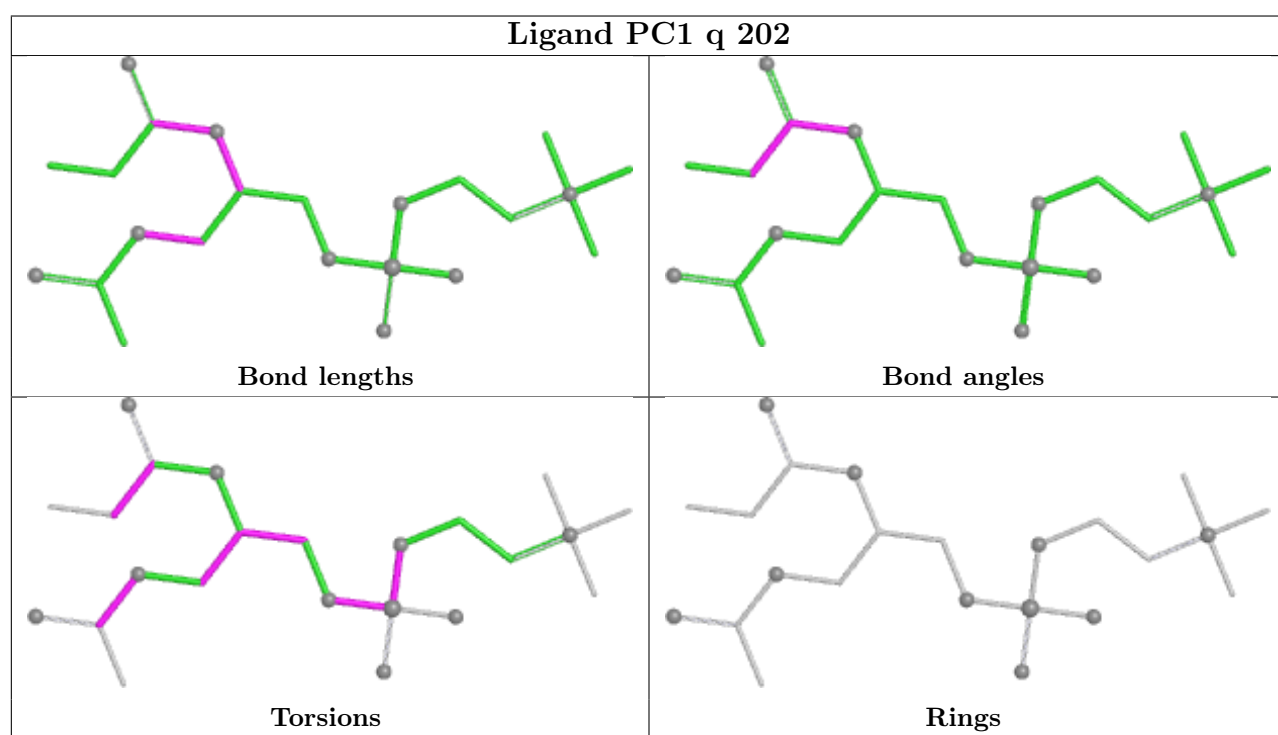
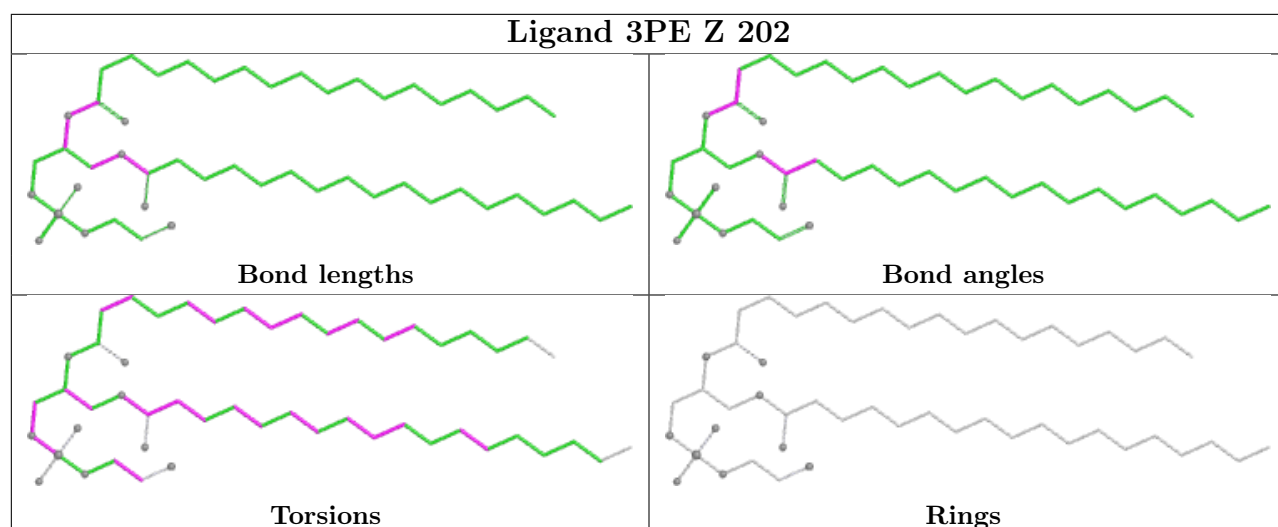


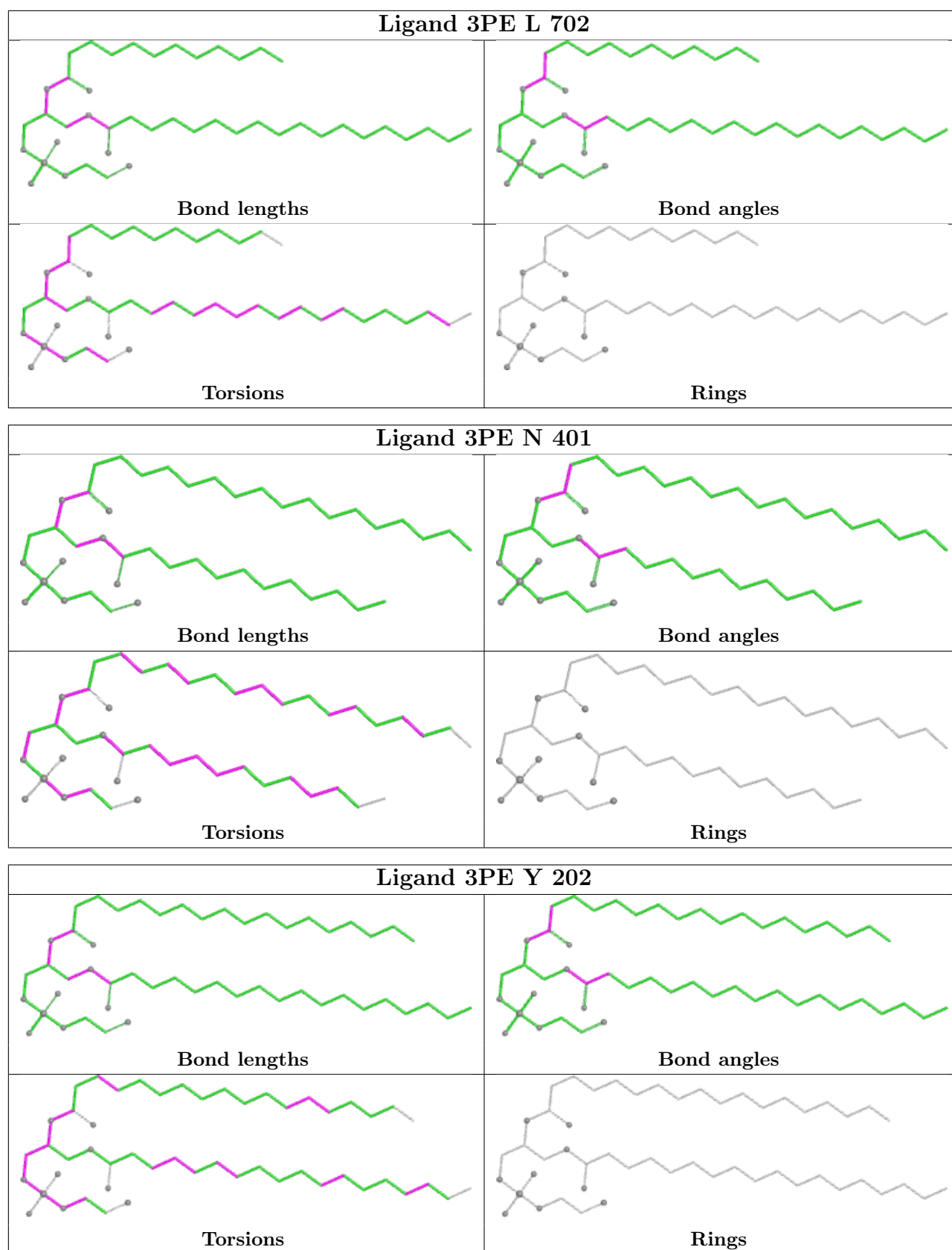


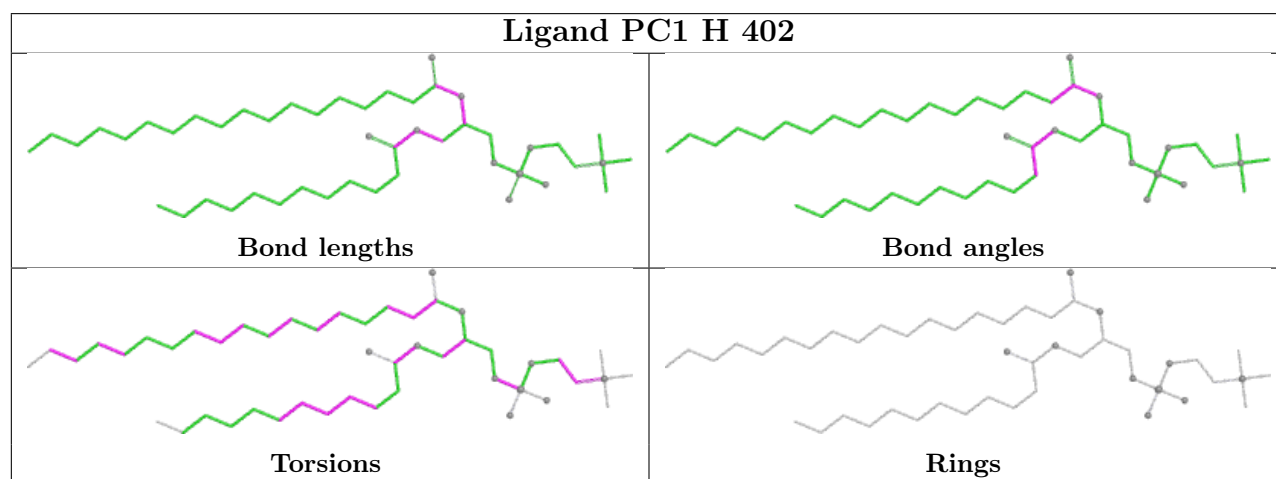
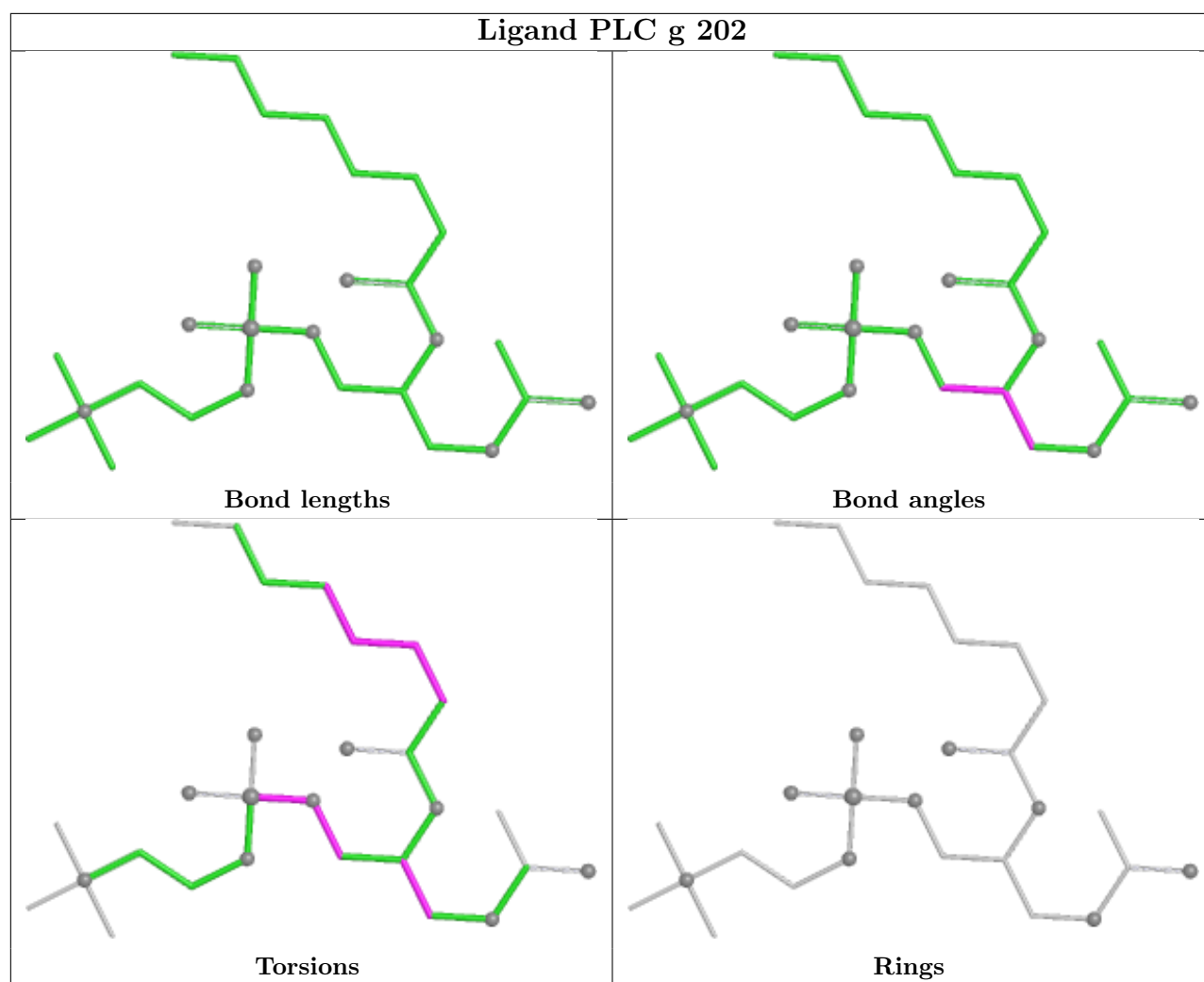


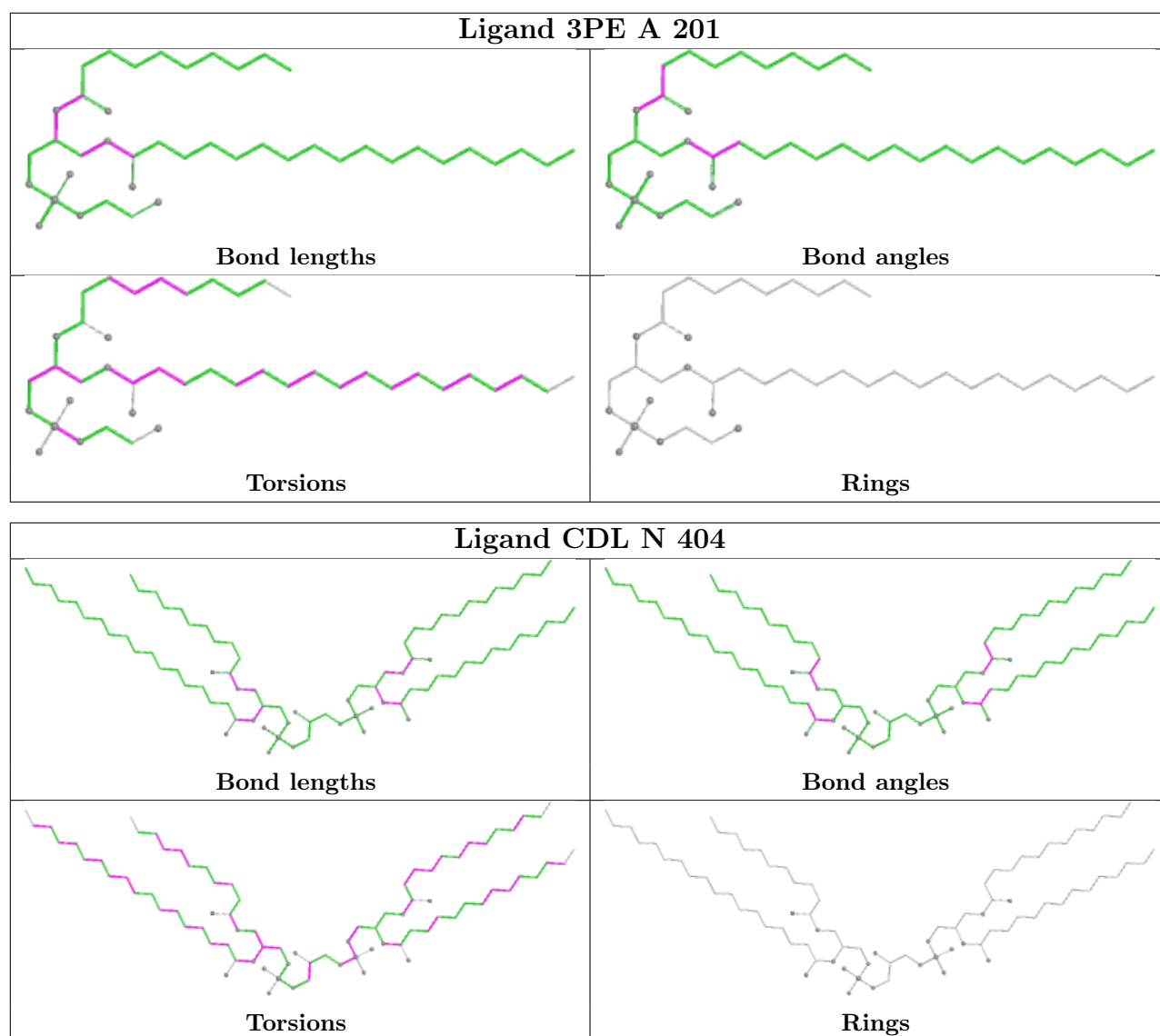




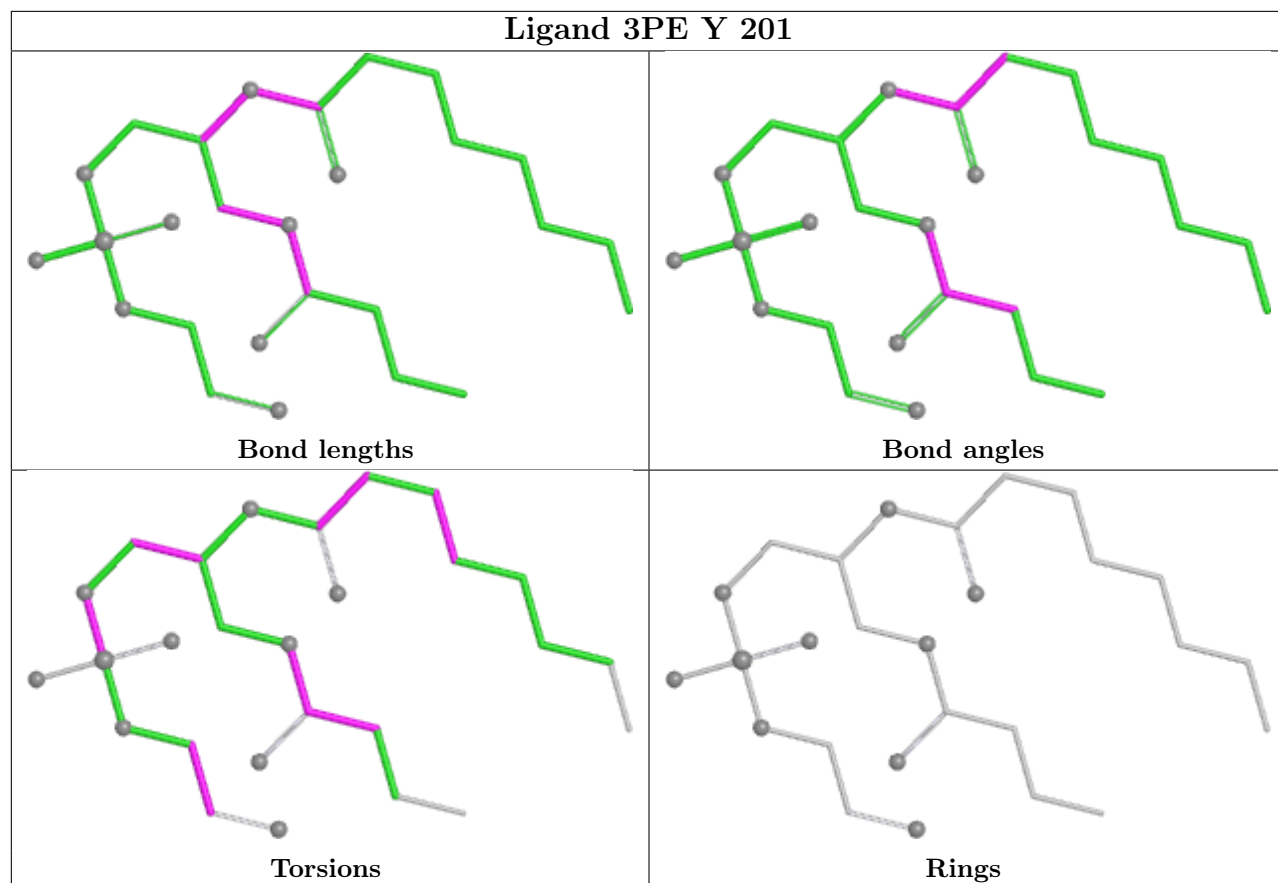




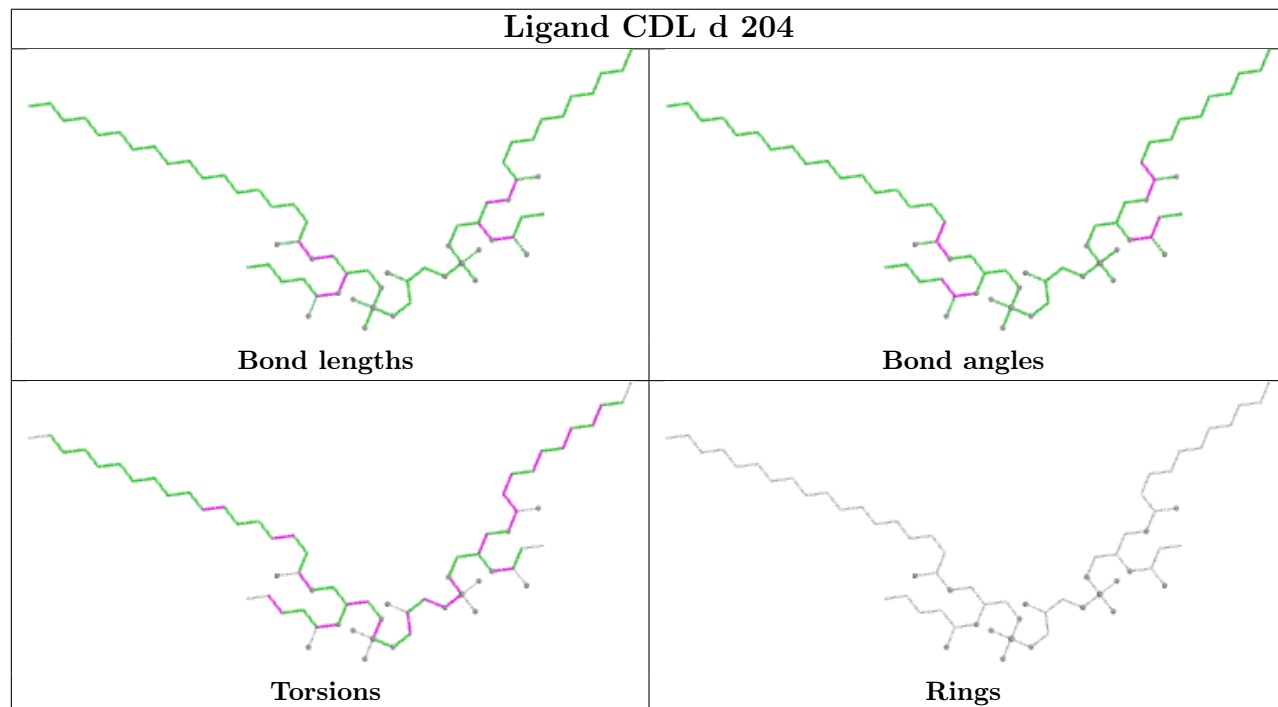


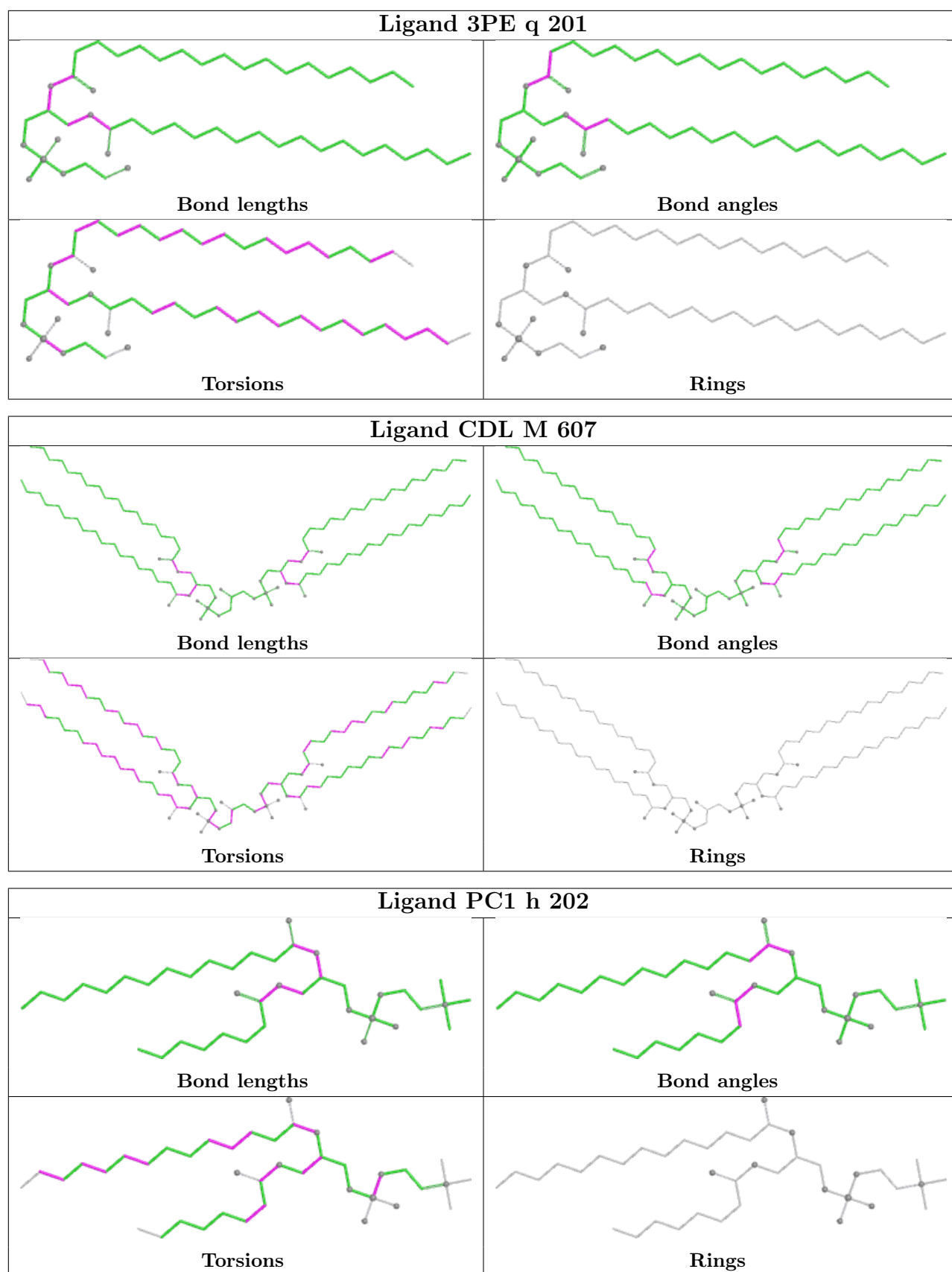


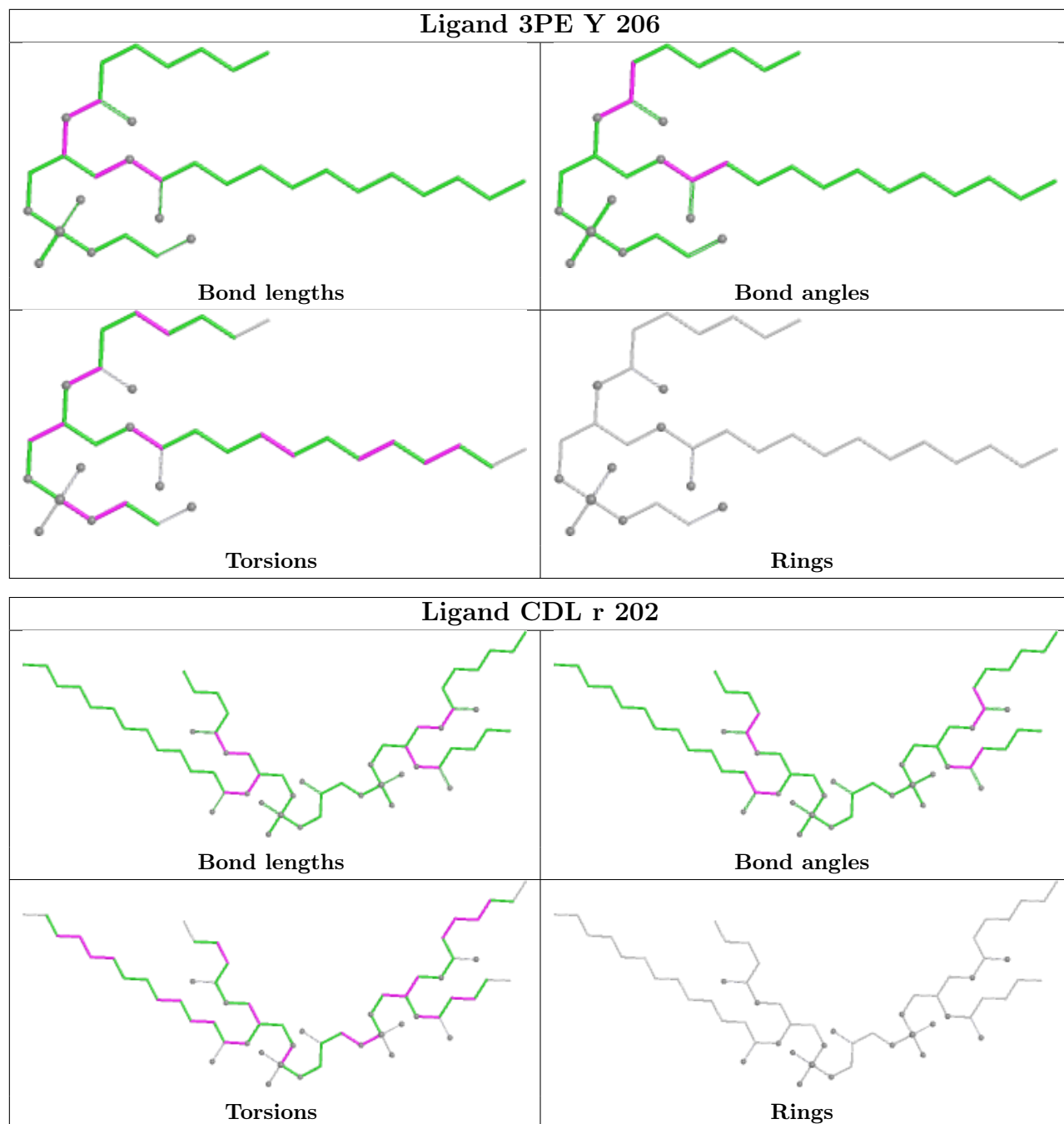
## Ligand 3PE Y 201



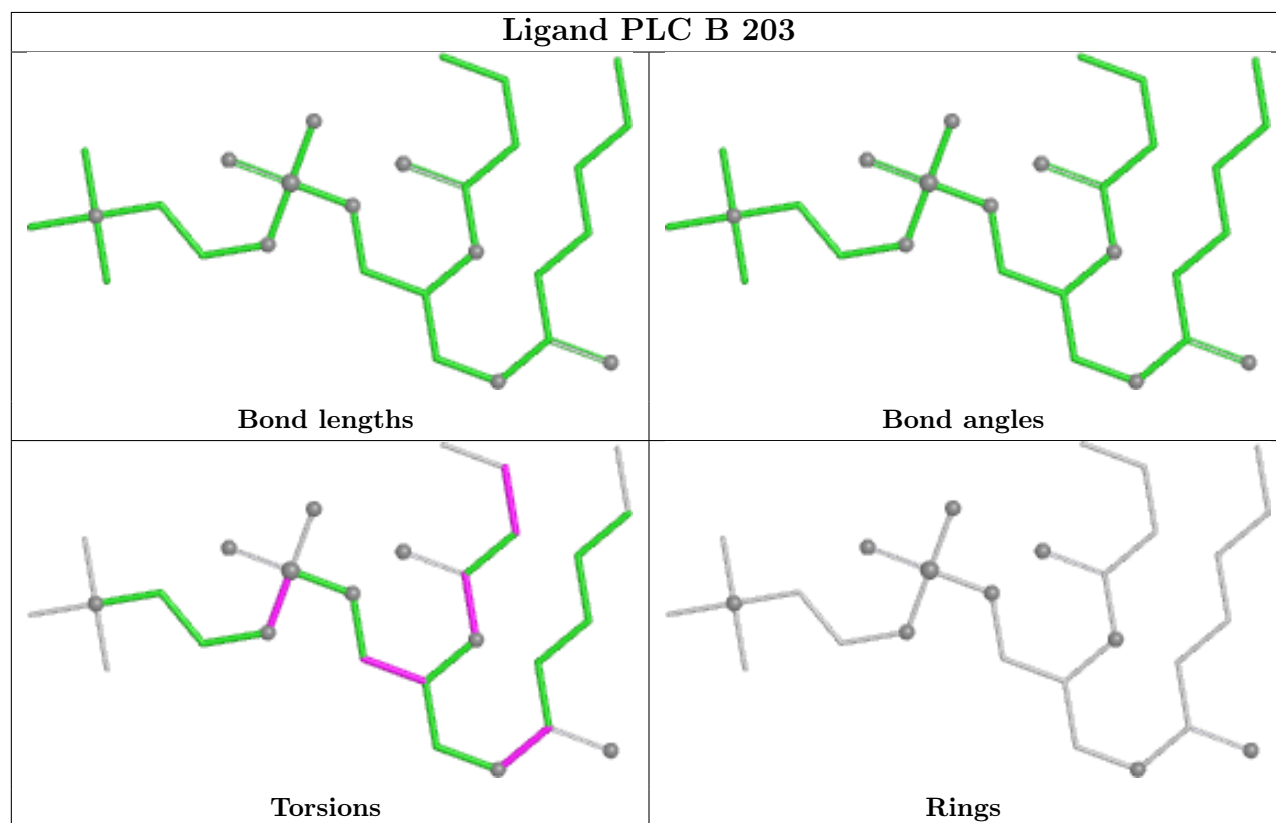
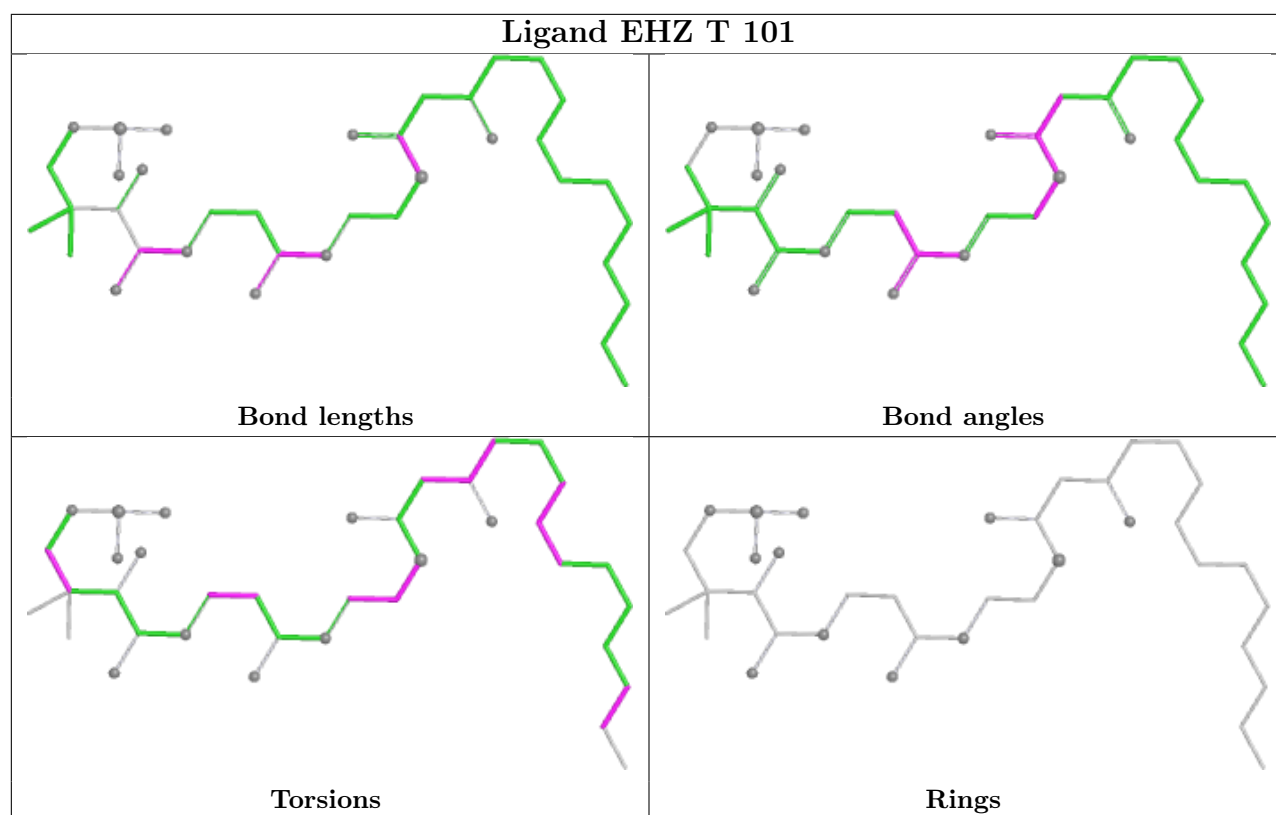
## Ligand CDL d 204

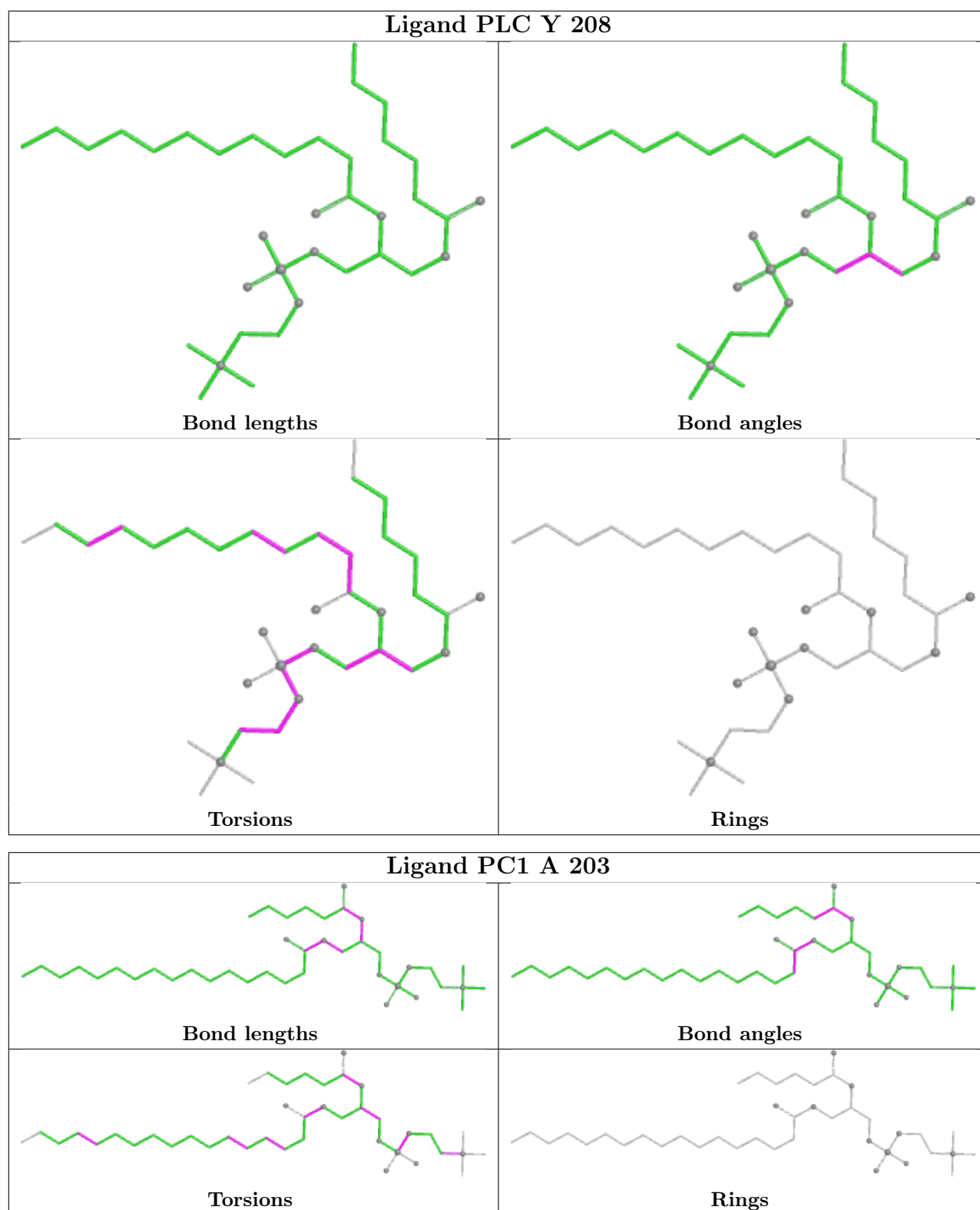












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

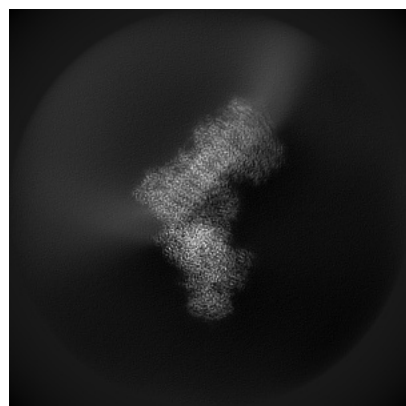
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18068. These allow visual inspection of the internal detail of the map and identification of artifacts.

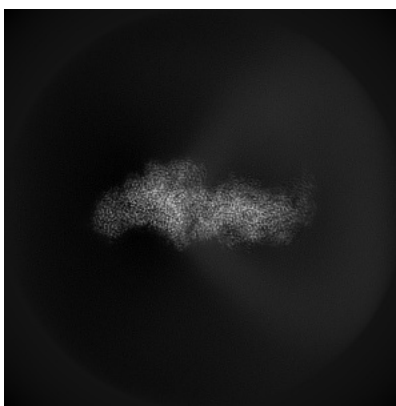
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

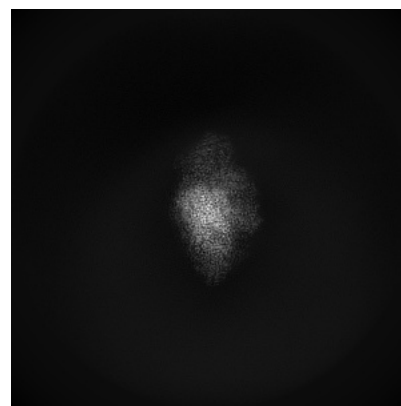
#### 6.1.1 Primary map



X

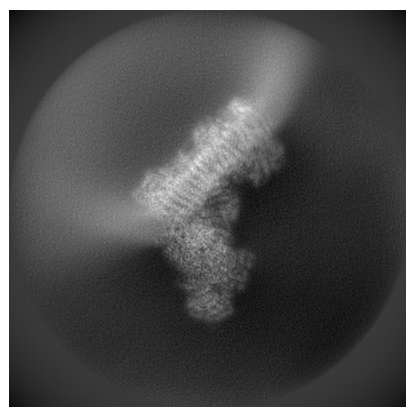


Y

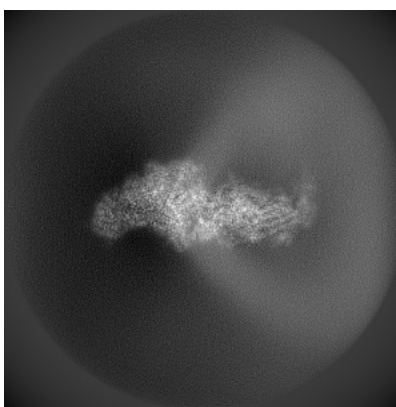


Z

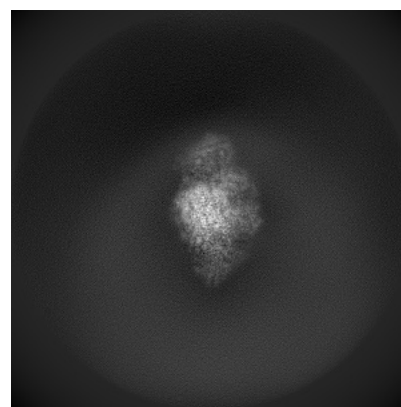
#### 6.1.2 Raw map



X



Y

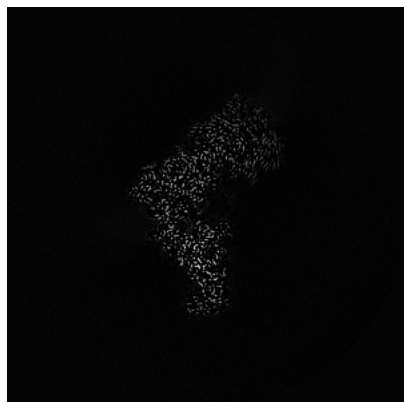


Z

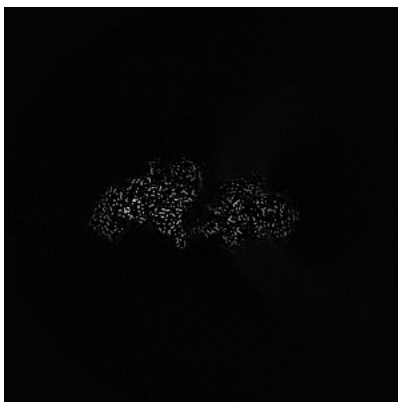
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

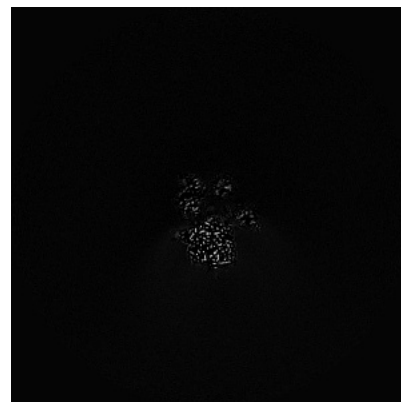
### 6.2.1 Primary map



X Index: 240

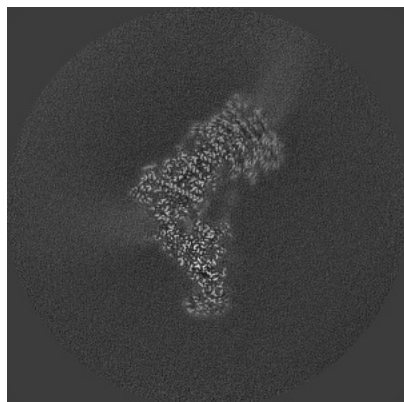


Y Index: 240

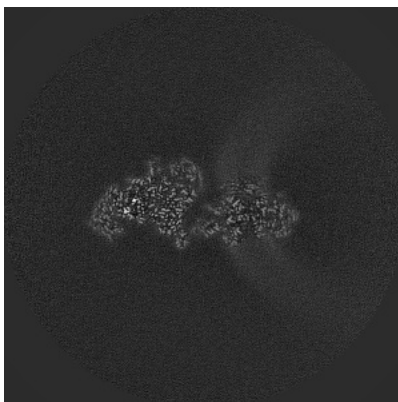


Z Index: 240

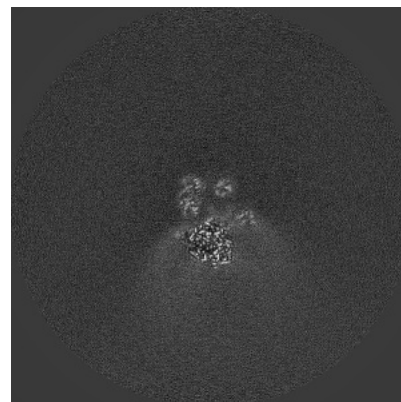
### 6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

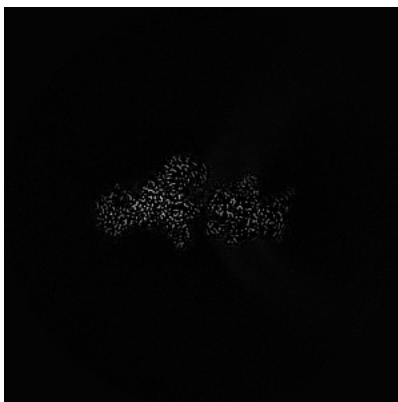
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 236

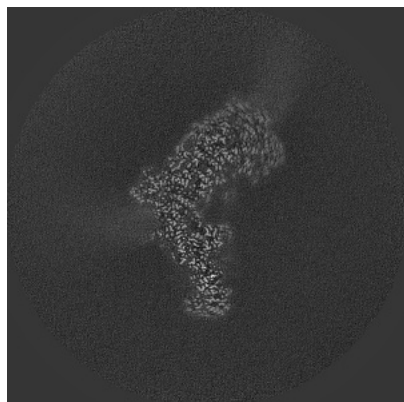


Y Index: 228

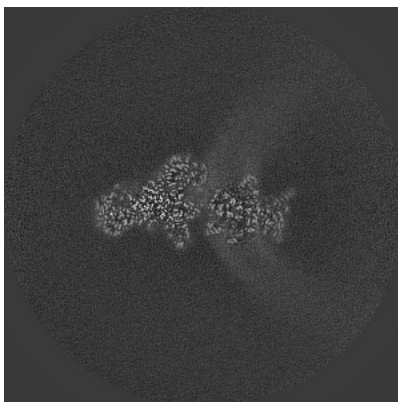


Z Index: 198

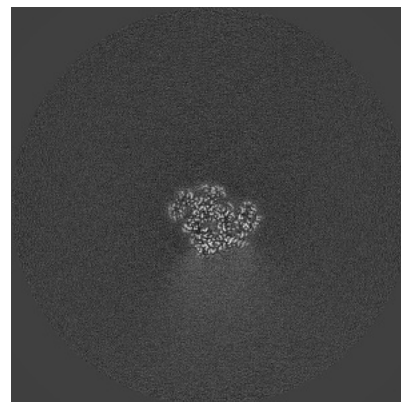
### 6.3.2 Raw map



X Index: 236



Y Index: 228

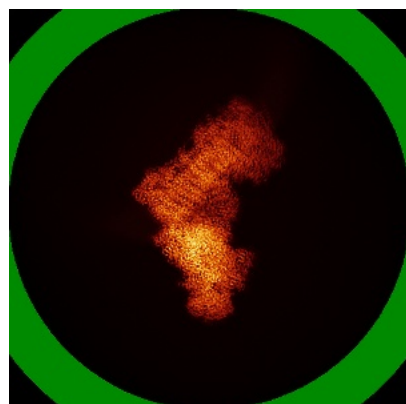


Z Index: 211

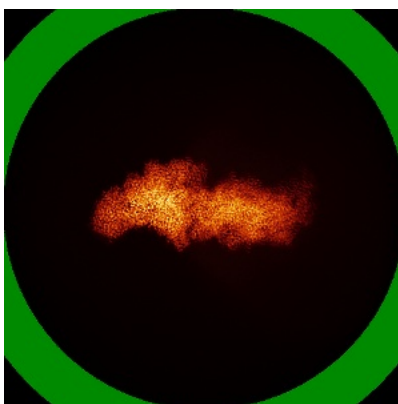
The images above show the largest variance slices of the map in three orthogonal directions.

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

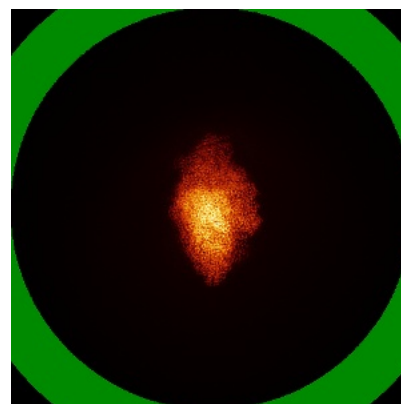
### 6.4.1 Primary map



X

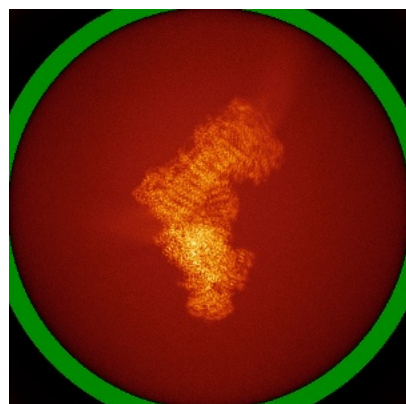


Y

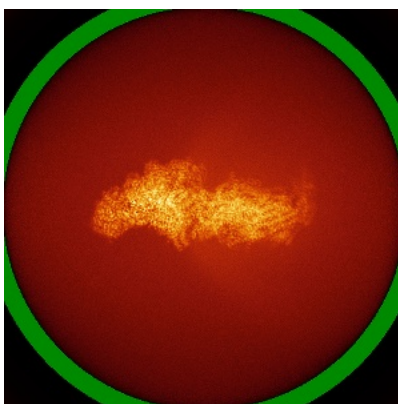


Z

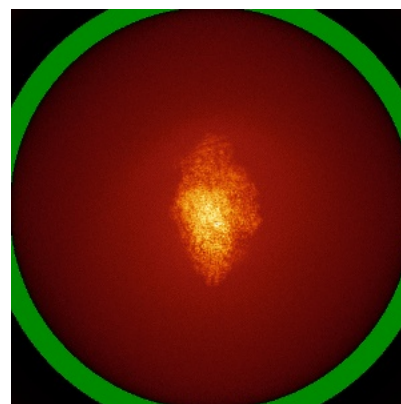
### 6.4.2 Raw map



X



Y



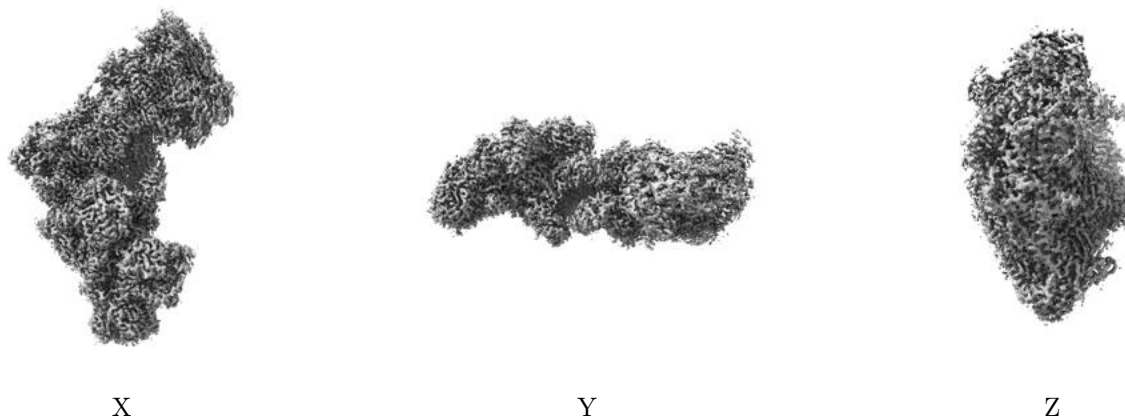
Z

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



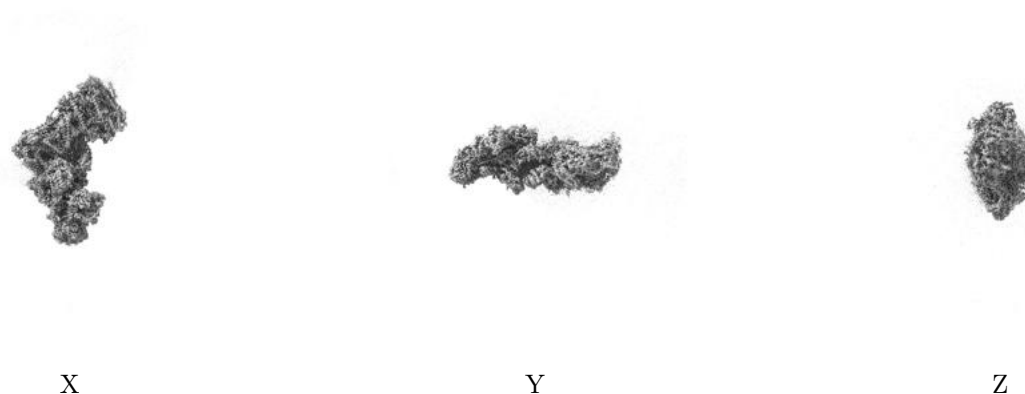
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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



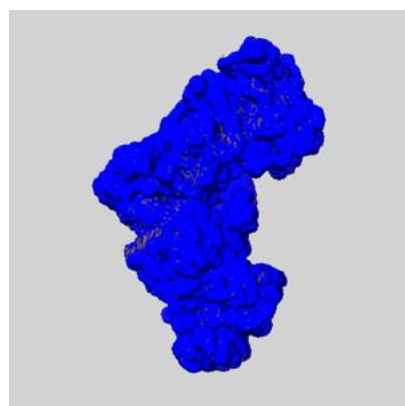
## 6.6 Mask visualisation [i](#)

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

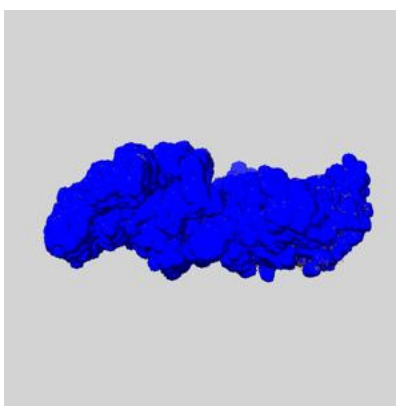
A mask typically either:

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

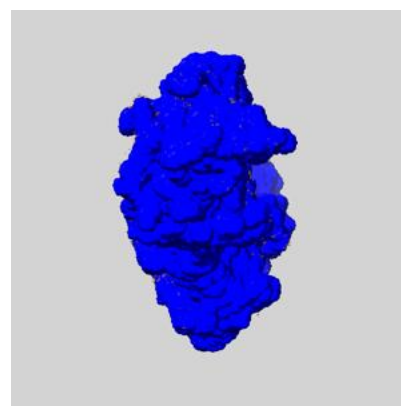
### 6.6.1 emd\_18068\_msk\_1.map [i](#)



X



Y

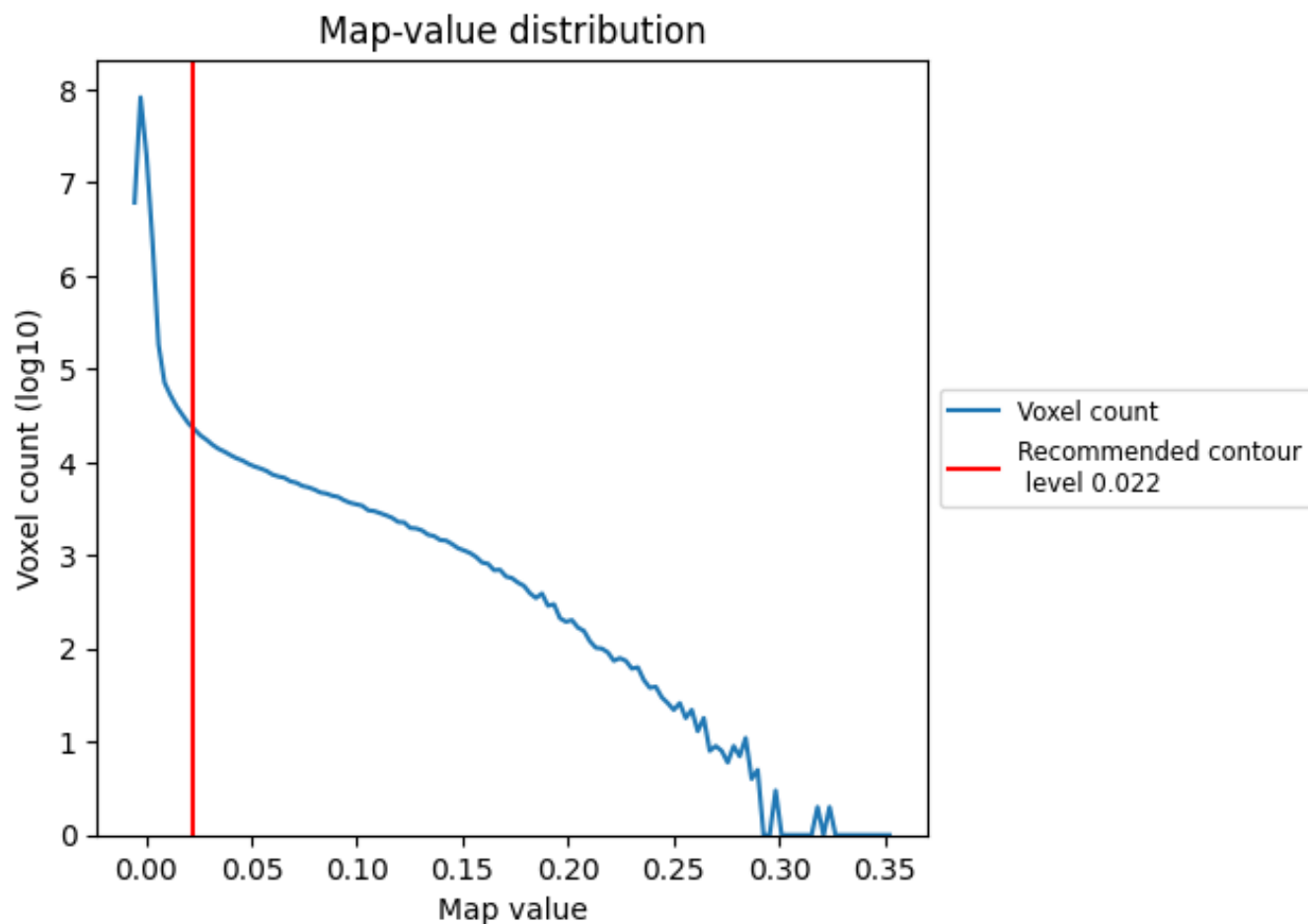


Z

## 7 Map analysis [i](#)

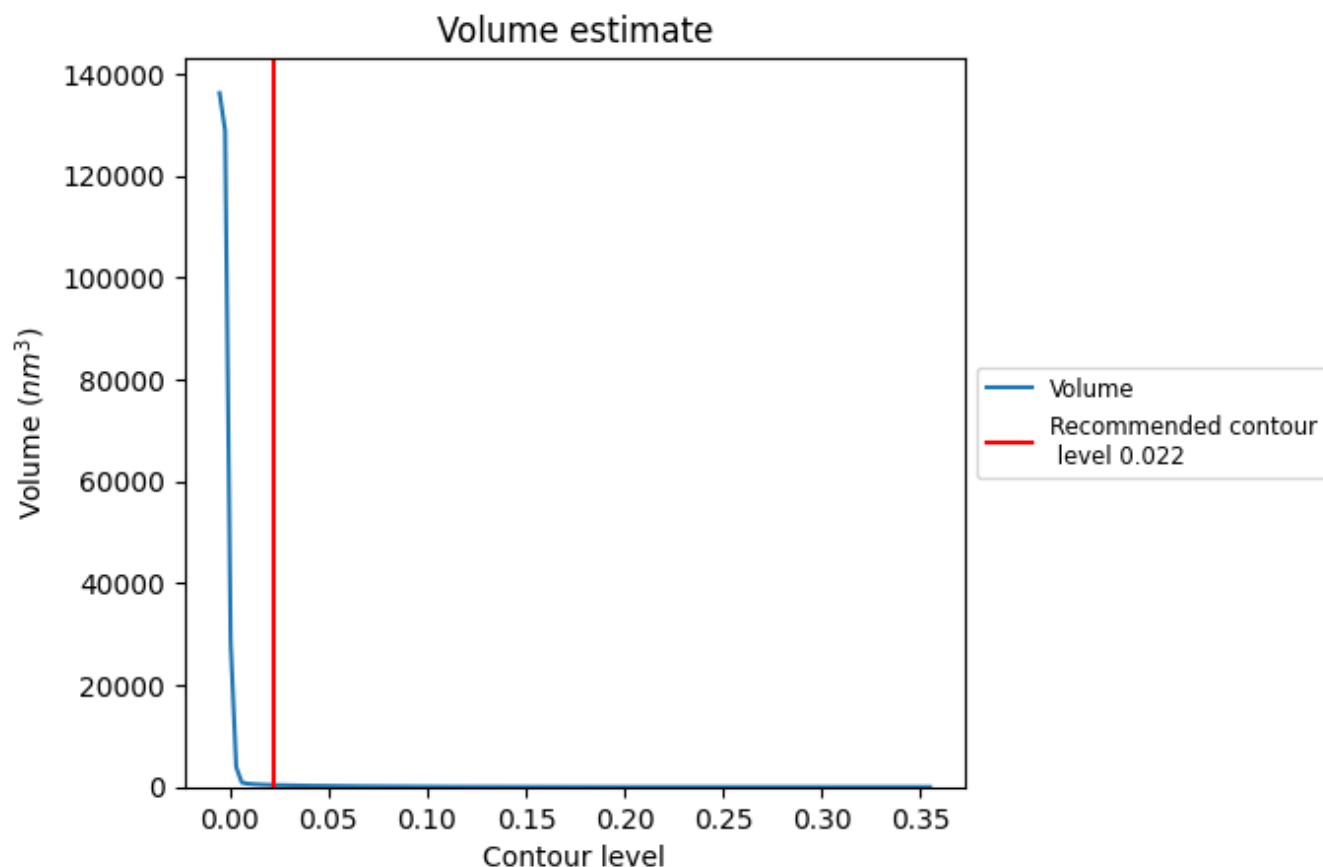
This section contains the results of statistical analysis of the map.

### 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.

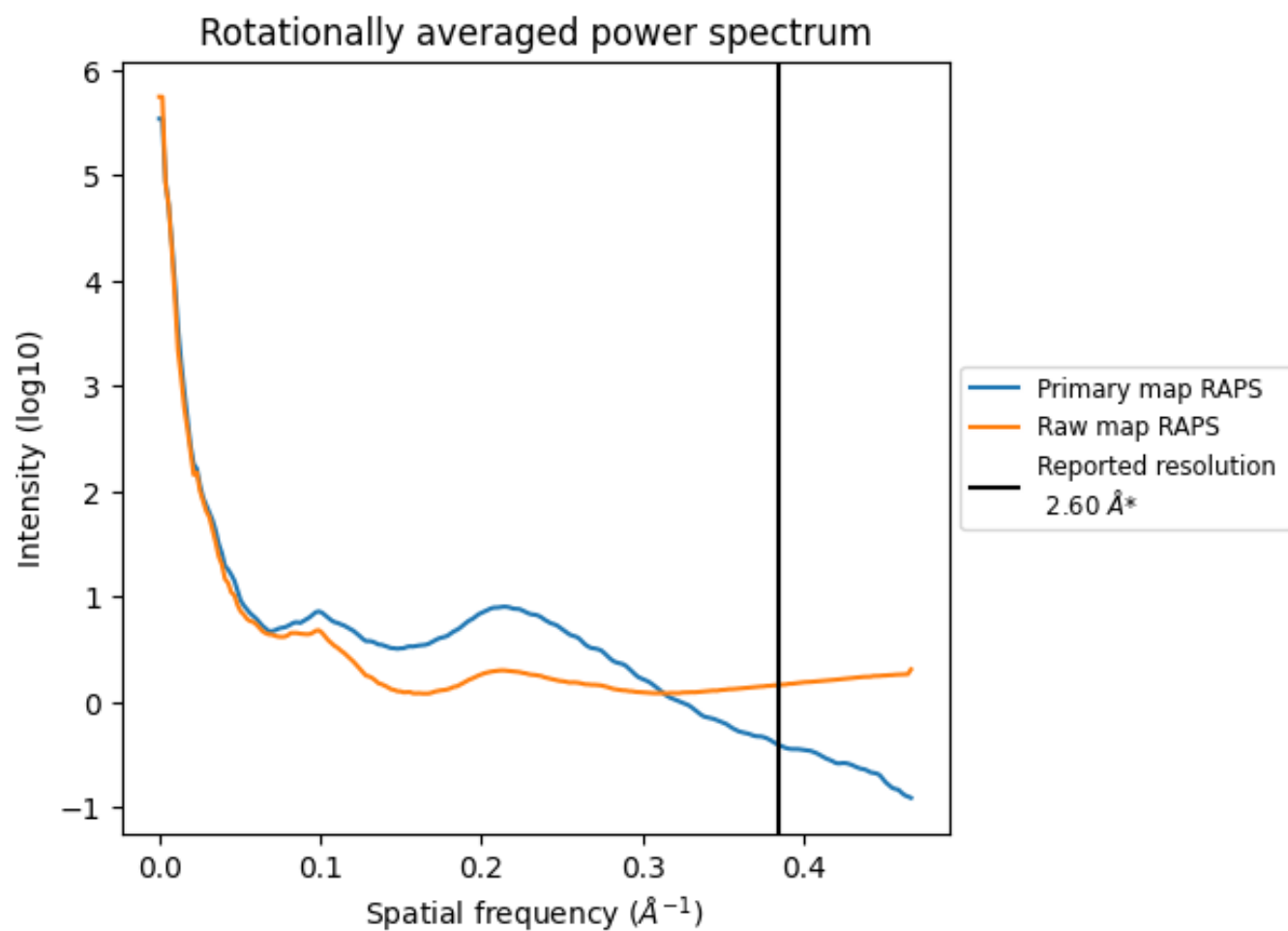
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 378  $\text{nm}^3$ ; this corresponds to an approximate mass of 341 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

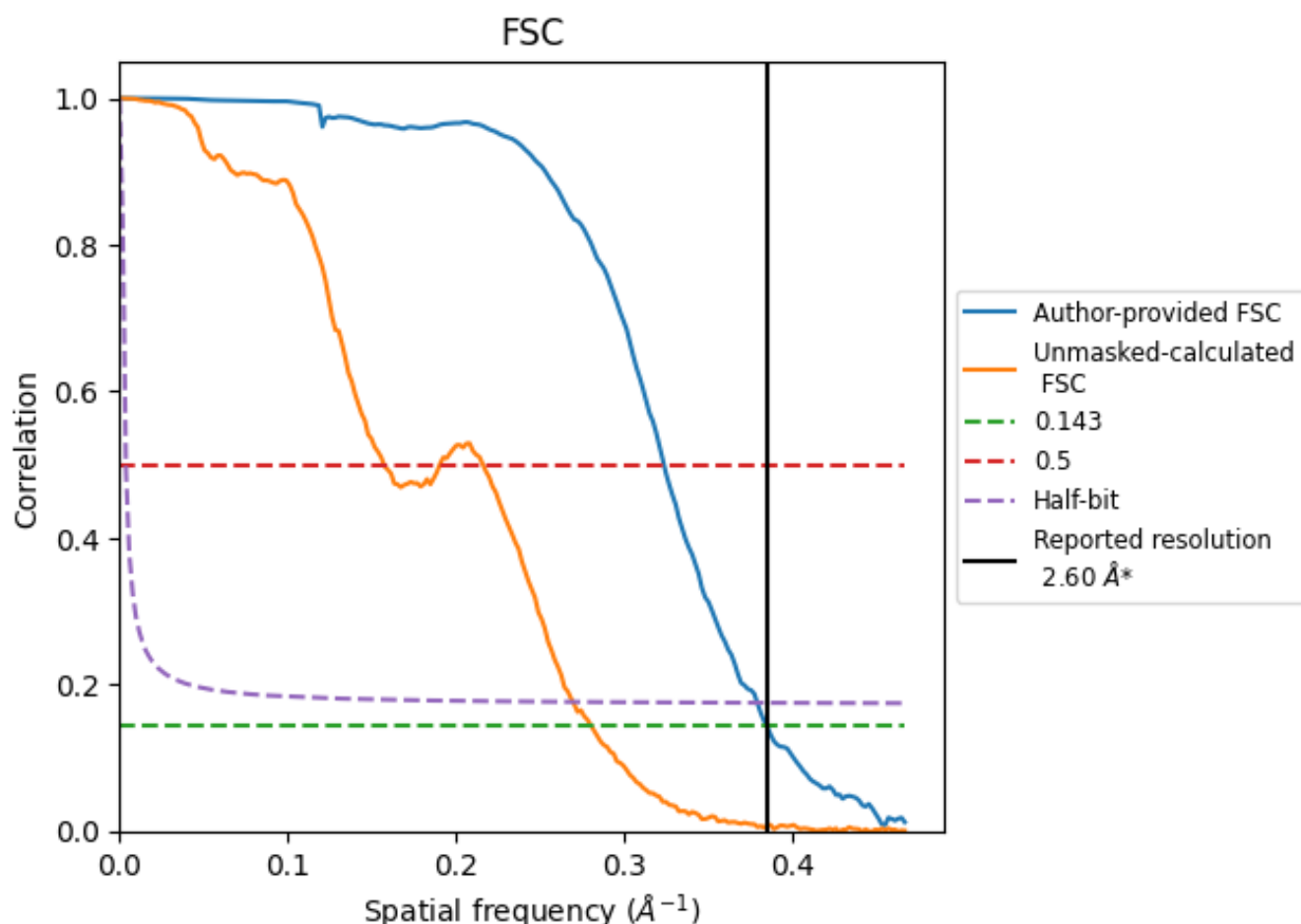


\*Reported resolution corresponds to spatial frequency of 0.385 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



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

## 8.2 Resolution estimates [i](#)

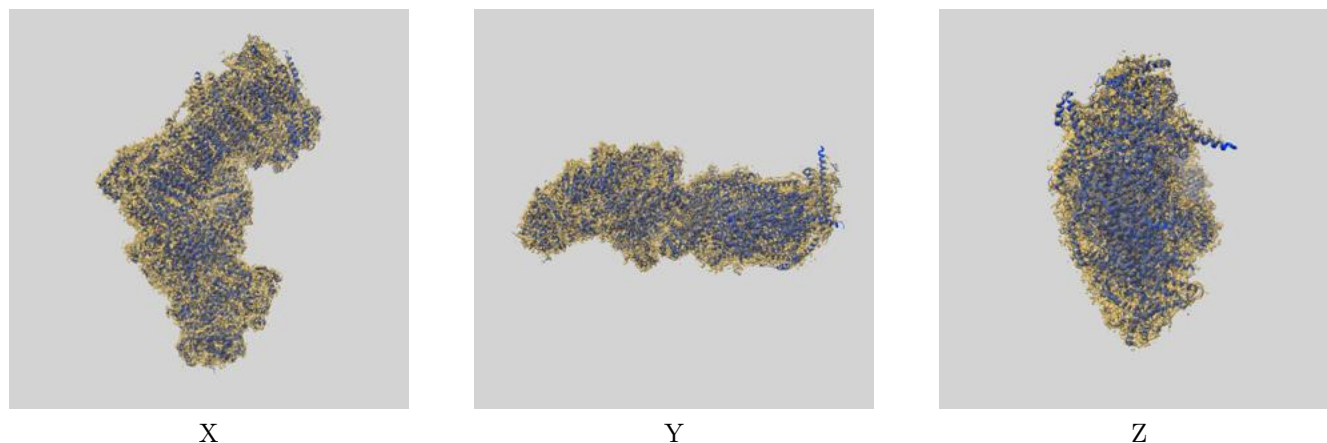
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.60                               | -    | -        |
| Author-provided FSC curve | 2.60                               | 3.09 | 2.64     |
| Unmasked-calculated*      | 3.57                               | 6.37 | 3.71     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.57 differs from the reported value 2.6 by more than 10 %

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

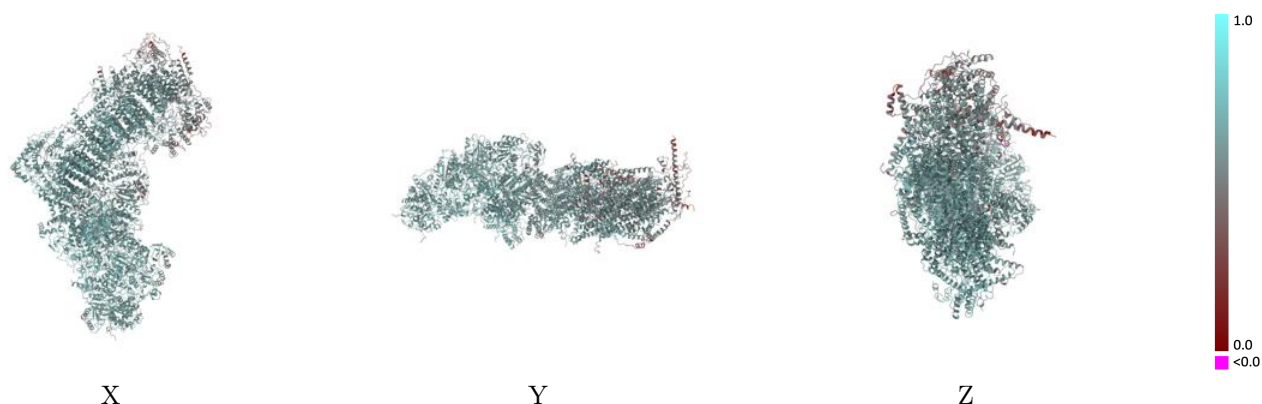
This section contains information regarding the fit between EMDB map EMD-18068 and PDB model 8Q1Y. Per-residue inclusion information can be found in section 3 on page 22.

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



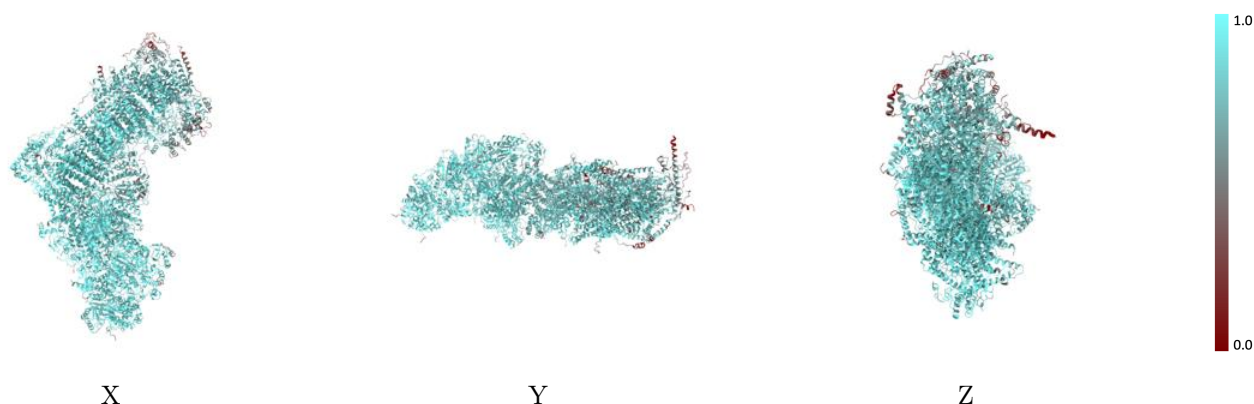
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

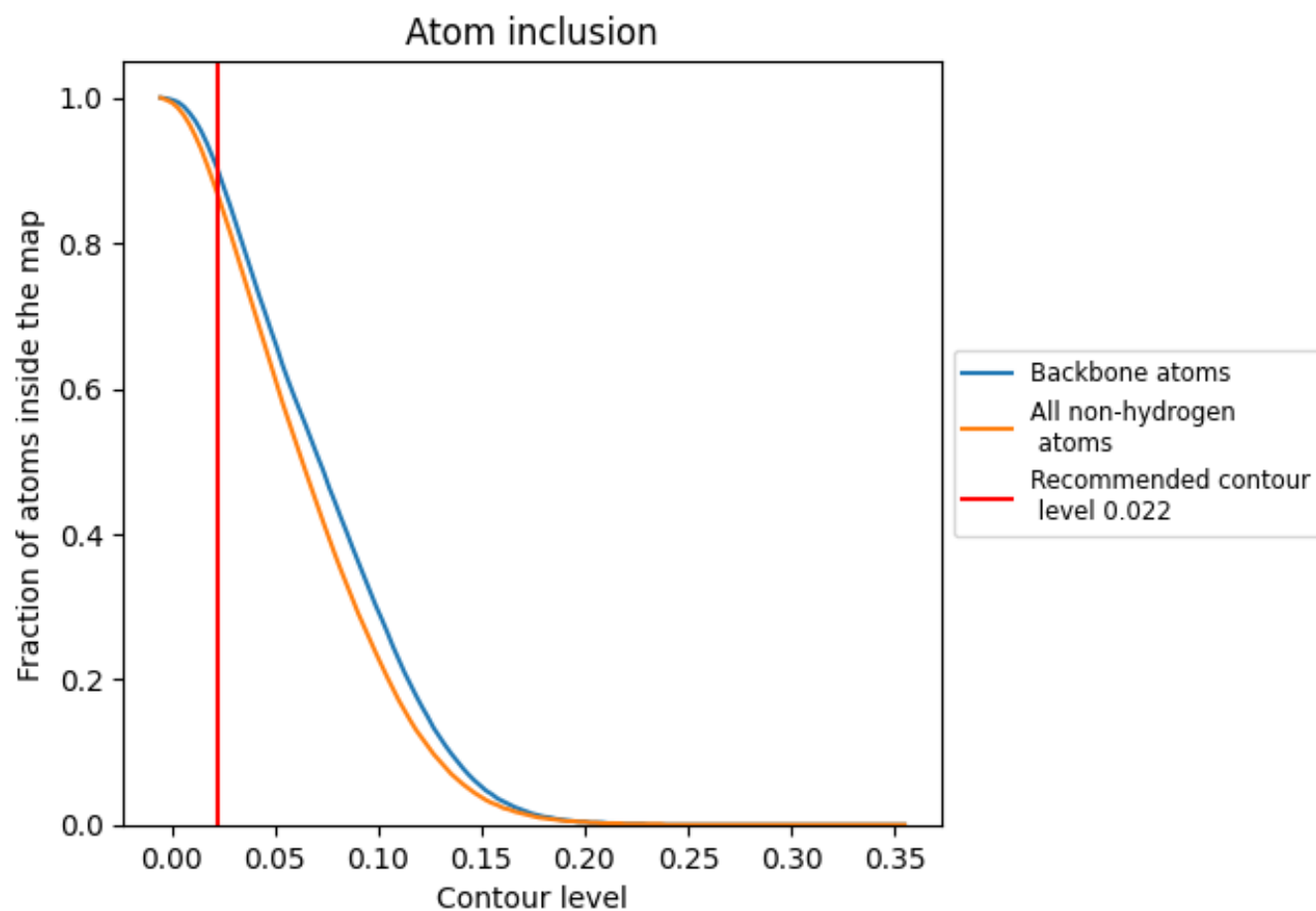
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.022).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 87% 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 (0.022) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.8700   |  0.6140   |
| A     |  0.8780   |  0.6130   |
| B     |  0.9480   |  0.6720   |
| C     |  0.9660   |  0.6810   |
| D     |  0.9650   |  0.6770   |
| E     |  0.8900   |  0.6190   |
| F     |  0.9150   |  0.6310   |
| G     |  0.9230   |  0.6480   |
| H     |  0.9340   |  0.6480   |
| I     |  0.9730   |  0.6840   |
| J     |  0.8890   |  0.6210   |
| K     |  0.9590   |  0.6620   |
| L     |  0.8520   |  0.5900   |
| M     |  0.9430   |  0.6520   |
| N     |  0.9630  |  0.6670  |
| O     |  0.8380 |  0.5960 |
| P     |  0.8750 |  0.6160 |
| Q     |  0.9230 |  0.6570 |
| R     |  0.9160 |  0.6460 |
| S     |  0.7960 |  0.5780 |
| T     |  0.6970 |  0.5290 |
| U     |  0.5960 |  0.4500 |
| V     |  0.9050 |  0.6380 |
| W     |  0.9080 |  0.6390 |
| X     |  0.8930 |  0.6270 |
| Y     |  0.8240 |  0.5950 |
| Z     |  0.8960 |  0.6340 |
| a     |  0.9490 |  0.6540 |
| b     |  0.8680 |  0.6220 |
| c     |  0.8350 |  0.5970 |
| d     |  0.8810 |  0.6220 |
| e     |  0.8690 |  0.6230 |
| f     |  0.6930 |  0.5300 |
| g     |  0.8010 |  0.5790 |
| h     |  0.8950 |  0.6270 |



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| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| i     |  0.6170 |  0.4760 |
| j     |  0.5810 |  0.4600 |
| k     |  0.4870 |  0.4200 |
| l     |  0.7730 |  0.5390 |
| m     |  0.7820 |  0.5620 |
| n     |  0.7260 |  0.5070 |
| o     |  0.5070 |  0.4100 |
| p     |  0.7670 |  0.5590 |
| q     |  0.9280 |  0.6530 |
| r     |  0.9330 |  0.6520 |
| s     |  0.7960 |  0.5740 |