



## Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 02:08 AM UTC

PDB ID : 8AP6 / pdb\_00008ap6  
EMDB ID : EMD-15559  
Title : Trypanosoma brucei mitochondrial F1Fo ATP synthase dimer  
Authors : Muehleip, A.; Gahura, O.; Zikova, A.; Amunts, A.  
Deposited on : 2022-08-09  
Resolution : 3.20 Å(reported)

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.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : **NOT EXECUTED**  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

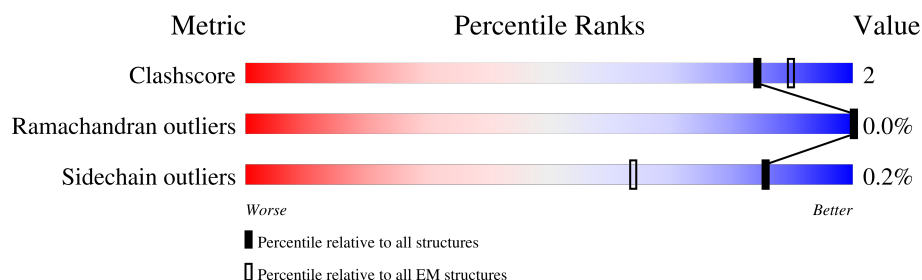
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 Å.

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.



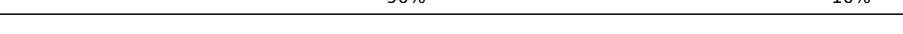
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 229148                      | 23984                       |
| Ramachandran outliers | 224038                      | 23583                       |
| Sidechain outliers    | 223484                      | 23102                       |

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  $\leq 5\%$ .

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 231    | 93% 7%           |
| 1   | a     | 231    | 93% 7%           |
| 2   | A1    | 584    | 86% 5% 9%        |
| 2   | A2    | 584    | 85% 5% 9%        |
| 2   | B1    | 584    | 84% 5% 10%       |
| 2   | B2    | 584    | 84% 5% 10%       |
| 2   | C1    | 584    | 85% • 10%        |
| 2   | C2    | 584    | 85% • 10%        |
| 3   | C     | 114    | 65% 10% • 25%    |

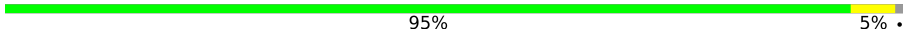
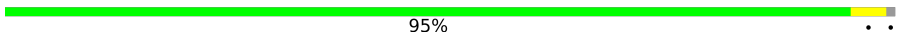
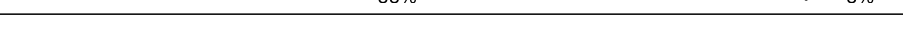
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 3   | c     | 114    |    |
| 4   | D     | 370    |    |
| 4   | d     | 370    |    |
| 5   | D1    | 519    |    |
| 5   | D2    | 519    |    |
| 5   | E1    | 519    |    |
| 5   | E2    | 519    |    |
| 5   | F1    | 519    |    |
| 5   | F2    | 519    |    |
| 6   | E     | 396    |    |
| 6   | e     | 396    |    |
| 7   | F     | 145    |    |
| 7   | f     | 145    |  |
| 8   | G     | 269    |  |
| 8   | g     | 269    |  |
| 9   | G1    | 305    |  |
| 9   | G2    | 305    |  |
| 10  | H     | 157    |  |
| 10  | h     | 157    |  |
| 11  | H1    | 182    |  |
| 11  | H2    | 182    |  |
| 12  | I     | 104    |  |
| 12  | i     | 104    |  |
| 13  | I1    | 75     |  |
| 13  | I2    | 75     |  |

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| Mol | Chain | Length | Quality of chain                                                                                 |
|-----|-------|--------|--------------------------------------------------------------------------------------------------|
| 14  | J     | 169    |  95% 5%        |
| 14  | j     | 169    |  95% . .       |
| 15  | J1    | 188    |  81% 7% 12%    |
| 15  | J2    | 188    |  80% 9% 12%    |
| 15  | K1    | 188    |  82% 6% 12%    |
| 15  | K2    | 188    |  84% . 12%     |
| 15  | L1    | 188    |  85% . 12%     |
| 15  | L2    | 188    |  85% . 12%     |
| 16  | K     | 124    |  82% . 15%     |
| 16  | k     | 124    |  82% . 15%     |
| 17  | L     | 92     |  67% . 29%     |
| 17  | l     | 92     |  65% 5% 29%    |
| 18  | M     | 144    |  84% 6% 10%  |
| 18  | m     | 144    |  84% 6% 10%  |
| 19  | M1    | 255    |  88% . 8%    |
| 19  | M2    | 255    |  88% . 8%    |
| 20  | N     | 156    |  84% . . 11% |
| 20  | n     | 156    |  85% . . 11% |
| 21  | O     | 101    |  91% . 5%    |
| 21  | o     | 101    |  91% . 5%    |
| 22  | O1    | 118    |  54% 12% 34% |
| 22  | O2    | 118    |  54% 12% 34% |
| 22  | P1    | 118    |  58% 8% 34%  |
| 22  | P2    | 118    |  58% 8% 34%  |
| 22  | Q1    | 118    |  60% 6% 34%  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 22  | Q2    | 118    |                  |
| 22  | R1    | 118    |                  |
| 22  | R2    | 118    |                  |
| 22  | S1    | 118    |                  |
| 22  | S2    | 118    |                  |
| 22  | T1    | 118    |                  |
| 22  | T2    | 118    |                  |
| 22  | U1    | 118    |                  |
| 22  | U2    | 118    |                  |
| 22  | V1    | 118    |                  |
| 22  | V2    | 118    |                  |
| 22  | W1    | 118    |                  |
| 22  | W2    | 118    |                  |
| 22  | X1    | 118    |                  |
| 22  | X2    | 118    |                  |
| 23  | P     | 105    |                  |
| 23  | p     | 105    |                  |
| 24  | Q     | 98     |                  |
| 24  | q     | 98     |                  |
| 25  | R     | 62     |                  |
| 25  | r     | 62     |                  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 31  | Q7G  | E     | 402 | X         | -        | -       | -                |
| 31  | Q7G  | N     | 201 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 31  | Q7G  | e     | 407 | X         | -        | -       | -                |
| 31  | Q7G  | n     | 201 | X         | -        | -       | -                |

## 2 Entry composition [i](#)

There are 34 unique types of molecules in this entry. The entry contains 251552 atoms, of which 126980 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 ATP synthase subunit a.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 1   | A     | 231      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4076  | 1459 | 2044 | 261 | 284 | 28 |         |       |
| 1   | a     | 231      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4076  | 1459 | 2044 | 261 | 284 | 28 |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| A     | 23      | TRP      | -      | insertion | UNP P24499 |
| A     | 180     | TRP      | -      | insertion | UNP P24499 |
| a     | 23      | TRP      | -      | insertion | UNP P24499 |
| a     | 180     | TRP      | -      | insertion | UNP P24499 |

- Molecule 2 is a protein called ATP synthase subunit alpha, mitochondrial.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 2   | A1    | 530      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 8280  | 2612 | 4196 | 710 | 742 | 20 |         |       |
| 2   | A2    | 530      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 8280  | 2612 | 4196 | 710 | 742 | 20 |         |       |
| 2   | B1    | 523      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 8198  | 2585 | 4161 | 702 | 730 | 20 |         |       |
| 2   | B2    | 523      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 8198  | 2585 | 4161 | 702 | 730 | 20 |         |       |
| 2   | C1    | 523      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 8193  | 2587 | 4154 | 701 | 731 | 20 |         |       |
| 2   | C2    | 523      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 8193  | 2587 | 4154 | 701 | 731 | 20 |         |       |

- Molecule 3 is a protein called subunit-8.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 3   | C     | 86       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1460  | 494 | 715 | 116 | 130 | 5 |         |       |
| 3   | c     | 86       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1460  | 494 | 715 | 116 | 130 | 5 |         |       |

- Molecule 4 is a protein called subunit-d.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 4   | D     | 332      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 5499  | 1710 | 2762 | 505 | 514 | 8 |         |       |
| 4   | d     | 332      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 5499  | 1710 | 2762 | 505 | 514 | 8 |         |       |

- Molecule 5 is a protein called ATP synthase subunit beta, mitochondrial.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 5   | D1    | 487      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 7430  | 2329 | 3741 | 631 | 710 | 19 |         |       |
| 5   | D2    | 487      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 7430  | 2329 | 3741 | 631 | 710 | 19 |         |       |
| 5   | E1    | 486      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 7415  | 2324 | 3733 | 630 | 709 | 19 |         |       |
| 5   | E2    | 486      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 7415  | 2324 | 3733 | 630 | 709 | 19 |         |       |
| 5   | F1    | 489      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 7461  | 2339 | 3758 | 633 | 712 | 19 |         |       |
| 5   | F2    | 489      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 7461  | 2339 | 3758 | 633 | 712 | 19 |         |       |

- Molecule 6 is a protein called ATPTB1.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 6   | E     | 383      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6281  | 2060 | 3061 | 558 | 585 | 17 |         |       |
| 6   | e     | 383      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6281  | 2060 | 3061 | 558 | 585 | 17 |         |       |

- Molecule 7 is a protein called subunit-f.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 7   | F     | 135      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2256  | 744 | 1111 | 201 | 195 | 5 |         |       |

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| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 7   | f     | 135      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2256  | 744 | 1111 | 201 | 195 | 5 |         |       |

- Molecule 8 is a protein called ATPTB3.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 8   | G     | 268      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3953  | 1211 | 2020 | 343 | 378 | 1 |         |       |
| 8   | g     | 268      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3953  | 1211 | 2020 | 343 | 378 | 1 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| G     | 176     | ALA      | VAL    | conflict | UNP A0A3L6KRX7 |
| g     | 176     | ALA      | VAL    | conflict | UNP A0A3L6KRX7 |

- Molecule 9 is a protein called ATP synthase gamma subunit.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 9   | G1    | 300      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 4774  | 1507 | 2387 | 423 | 448 | 9 |         |       |
| 9   | G2    | 300      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 4774  | 1507 | 2387 | 423 | 448 | 9 |         |       |

- Molecule 10 is a protein called ATPTB4.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 10  | H     | 137      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2158  | 680 | 1088 | 184 | 203 | 3 |         |       |
| 10  | h     | 137      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2158  | 680 | 1088 | 184 | 203 | 3 |         |       |

- Molecule 11 is a protein called ATP synthase, epsilon chain, putative.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 11  | H1    | 161      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2483  | 788 | 1232 | 211 | 248 | 4 |         |       |
| 11  | H2    | 161      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2483  | 788 | 1232 | 211 | 248 | 4 |         |       |

- Molecule 12 is a protein called subunit-i/j.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 12  | I     | 103      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1740  | 574 | 857 | 152 | 151 | 6 |         |       |
| 12  | i     | 103      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1740  | 574 | 857 | 152 | 151 | 6 |         |       |

- Molecule 13 is a protein called ATP synthase subunit epsilon, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|-----|---|---------|-------|
| 13  | I1    | 65       | Total | C   | H   | N  | O   | S | 0       | 0     |
|     |       |          | 1046  | 332 | 513 | 97 | 102 | 2 |         |       |
| 13  | I2    | 65       | Total | C   | H   | N  | O   | S | 0       | 0     |
|     |       |          | 1046  | 332 | 513 | 97 | 102 | 2 |         |       |

- Molecule 14 is a protein called ATP6.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 14  | J     | 168      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2835  | 919 | 1411 | 249 | 249 | 7 |         |       |
| 14  | j     | 168      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2835  | 919 | 1411 | 249 | 249 | 7 |         |       |

- Molecule 15 is a protein called ATP synthase subunit p18, mitochondrial.

| Mol | Chain | Residues | Atoms |     |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|----|---------|-------|
| 15  | J1    | 166      | Total | C   | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 2590  | 822 | 1276 | 221 | 257 | 14 |         |       |
| 15  | J2    | 166      | Total | C   | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 2590  | 822 | 1276 | 221 | 257 | 14 |         |       |
| 15  | K1    | 166      | Total | C   | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 2591  | 822 | 1276 | 221 | 258 | 14 |         |       |
| 15  | K2    | 166      | Total | C   | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 2591  | 822 | 1276 | 221 | 258 | 14 |         |       |
| 15  | L1    | 165      | Total | C   | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 2581  | 819 | 1271 | 220 | 257 | 14 |         |       |
| 15  | L2    | 165      | Total | C   | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 2581  | 819 | 1271 | 220 | 257 | 14 |         |       |

- Molecule 16 is a protein called subunit-k.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 16  | K     | 105      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1749  | 577 | 876 | 149 | 141 | 6 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 16  | k     | 105      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1749  | 577 | 876 | 149 | 141 | 6 |         |       |

- Molecule 17 is a protein called subunit-e.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| 17  | L     | 65       | Total | C   | H   | N   | O  | S | 0       | 0     |
|     |       |          | 1082  | 340 | 545 | 104 | 92 | 1 |         |       |
| 17  | l     | 65       | Total | C   | H   | N   | O  | S | 0       | 0     |
|     |       |          | 1082  | 340 | 545 | 104 | 92 | 1 |         |       |

- Molecule 18 is a protein called subunit-g.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 18  | M     | 129      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2069  | 662 | 1042 | 177 | 186 | 2 |         |       |
| 18  | m     | 129      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2069  | 662 | 1042 | 177 | 186 | 2 |         |       |

- Molecule 19 is a protein called oligomycin sensitivity conferring protein.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 19  | M1    | 234      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3750  | 1212 | 1873 | 302 | 360 | 3 |         |       |
| 19  | M2    | 234      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3750  | 1212 | 1873 | 302 | 360 | 3 |         |       |

- Molecule 20 is a protein called ATPTB11.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 20  | N     | 139      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2210  | 730 | 1082 | 183 | 208 | 7 |         |       |
| 20  | n     | 139      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2210  | 730 | 1082 | 183 | 208 | 7 |         |       |

- Molecule 21 is a protein called ATPTB12.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 21  | O     | 96       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1556  | 506 | 767 | 140 | 140 | 3 |         |       |
| 21  | o     | 96       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1556  | 506 | 767 | 140 | 140 | 3 |         |       |

- Molecule 22 is a protein called ATPase subunit 9, putative.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 22  | O1    | 78       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 1165  | 376 | 600 | 89 | 96 | 4 |         |       |
| 22  | O2    | 78       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 1165  | 376 | 600 | 89 | 96 | 4 |         |       |
| 22  | P1    | 78       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 1165  | 376 | 600 | 89 | 96 | 4 |         |       |
| 22  | P2    | 78       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 1165  | 376 | 600 | 89 | 96 | 4 |         |       |
| 22  | Q1    | 78       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 1165  | 376 | 600 | 89 | 96 | 4 |         |       |
| 22  | Q2    | 78       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 1165  | 376 | 600 | 89 | 96 | 4 |         |       |
| 22  | R1    | 78       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 1165  | 376 | 600 | 89 | 96 | 4 |         |       |
| 22  | R2    | 78       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 1165  | 376 | 600 | 89 | 96 | 4 |         |       |
| 22  | S1    | 78       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 1166  | 376 | 601 | 89 | 96 | 4 |         |       |
| 22  | S2    | 78       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 1166  | 376 | 601 | 89 | 96 | 4 |         |       |
| 22  | T1    | 78       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 1166  | 376 | 601 | 89 | 96 | 4 |         |       |
| 22  | T2    | 78       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 1166  | 376 | 601 | 89 | 96 | 4 |         |       |
| 22  | U1    | 78       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 1165  | 376 | 600 | 89 | 96 | 4 |         |       |
| 22  | U2    | 78       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 1165  | 376 | 600 | 89 | 96 | 4 |         |       |
| 22  | V1    | 78       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 1165  | 376 | 600 | 89 | 96 | 4 |         |       |
| 22  | V2    | 78       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 1165  | 376 | 600 | 89 | 96 | 4 |         |       |
| 22  | W1    | 78       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 1165  | 376 | 600 | 89 | 96 | 4 |         |       |
| 22  | W2    | 78       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 1165  | 376 | 600 | 89 | 96 | 4 |         |       |
| 22  | X1    | 78       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 1165  | 376 | 600 | 89 | 96 | 4 |         |       |
| 22  | X2    | 78       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 1165  | 376 | 600 | 89 | 96 | 4 |         |       |

- Molecule 23 is a protein called subunit-b.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 23  | P     | 80       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1335  | 448 | 651 | 108 | 125 | 3 |         |       |
| 23  | p     | 80       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1335  | 448 | 651 | 108 | 125 | 3 |         |       |

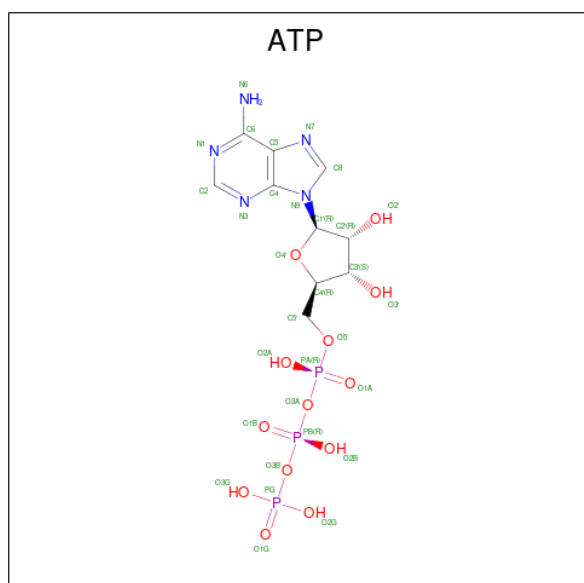
- Molecule 24 is a protein called ATPEG3.

| Mol | Chain | Residues | Atoms |     |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|--|---------|-------|
| 24  | Q     | 85       | Total | C   | H   | N   | O   |  | 0       | 0     |
|     |       |          | 1486  | 499 | 720 | 142 | 125 |  |         |       |
| 24  | q     | 85       | Total | C   | H   | N   | O   |  | 0       | 0     |
|     |       |          | 1486  | 499 | 720 | 142 | 125 |  |         |       |

- Molecule 25 is a protein called ATPEG4.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 25  | R     | 62       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 1040  | 358 | 498 | 94 | 85 | 5 |         |       |
| 25  | r     | 62       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 1040  | 358 | 498 | 94 | 85 | 5 |         |       |

- Molecule 26 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



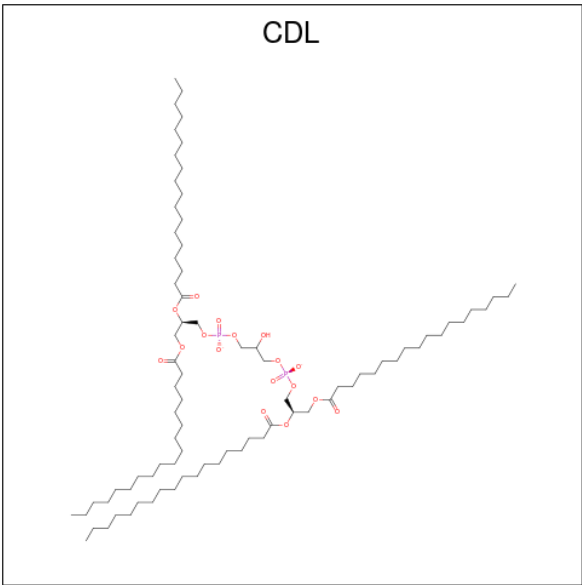
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| Mol | Chain | Residues | Atoms |    |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|----|---|---------|
| 26  | A2    | 1        | Total | C  | H  | N | O  | P | 0       |
|     |       |          | 43    | 10 | 12 | 5 | 13 | 3 |         |
| 26  | B1    | 1        | Total | C  | H  | N | O  | P | 0       |
|     |       |          | 43    | 10 | 12 | 5 | 13 | 3 |         |
| 26  | B2    | 1        | Total | C  | H  | N | O  | P | 0       |
|     |       |          | 43    | 10 | 12 | 5 | 13 | 3 |         |
| 26  | C1    | 1        | Total | C  | H  | N | O  | P | 0       |
|     |       |          | 43    | 10 | 12 | 5 | 13 | 3 |         |
| 26  | C2    | 1        | Total | C  | H  | N | O  | P | 0       |
|     |       |          | 43    | 10 | 12 | 5 | 13 | 3 |         |
| 26  | F1    | 1        | Total | C  | H  | N | O  | P | 0       |
|     |       |          | 43    | 10 | 12 | 5 | 13 | 3 |         |
| 26  | F2    | 1        | Total | C  | H  | N | O  | P | 0       |
|     |       |          | 43    | 10 | 12 | 5 | 13 | 3 |         |

- Molecule 27 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 27  | A1    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 27  | A2    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 27  | B1    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 27  | B2    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 27  | C1    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 27  | C2    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 27  | D1    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 27  | D2    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 27  | F1    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 27  | F2    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 28 is CARDIOLIPIN (CCD ID: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



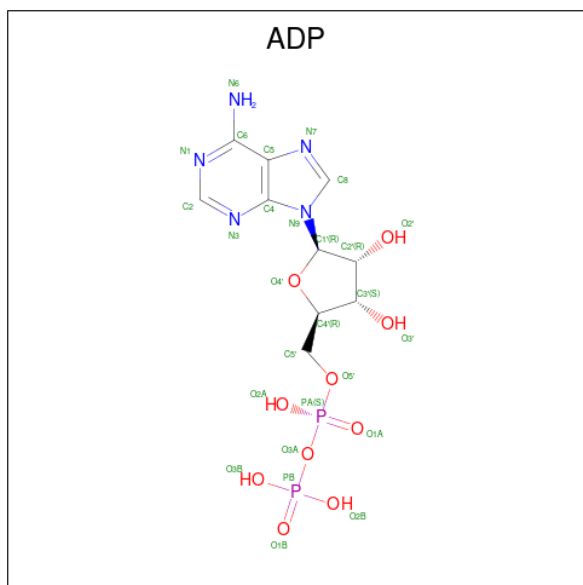
| Mol | Chain | Residues | Atoms |    |     |    |   | AltConf |
|-----|-------|----------|-------|----|-----|----|---|---------|
| 28  | C     | 1        | Total | C  | H   | O  | P | 0       |
|     |       |          | 256   | 81 | 156 | 17 | 2 |         |
| 28  | E     | 1        | Total | C  | H   | O  | P | 0       |
|     |       |          | 256   | 81 | 156 | 17 | 2 |         |
| 28  | E     | 1        | Total | C  | H   | O  | P | 0       |
|     |       |          | 256   | 81 | 156 | 17 | 2 |         |
| 28  | E     | 1        | Total | C  | H   | O  | P | 0       |
|     |       |          | 256   | 81 | 156 | 17 | 2 |         |
| 28  | E     | 1        | Total | C  | H   | O  | P | 0       |
|     |       |          | 256   | 81 | 156 | 17 | 2 |         |
| 28  | E     | 1        | Total | C  | H   | O  | P | 0       |
|     |       |          | 256   | 81 | 156 | 17 | 2 |         |
| 28  | F     | 1        | Total | C  | H   | O  | P | 0       |
|     |       |          | 256   | 81 | 156 | 17 | 2 |         |
| 28  | J     | 1        | Total | C  | H   | O  | P | 0       |
|     |       |          | 256   | 81 | 156 | 17 | 2 |         |
| 28  | J     | 1        | Total | C  | H   | O  | P | 0       |
|     |       |          | 256   | 81 | 156 | 17 | 2 |         |
| 28  | L     | 1        | Total | C  | H   | O  | P | 0       |
|     |       |          | 256   | 81 | 156 | 17 | 2 |         |
| 28  | M     | 1        | Total | C  | H   | O  | P | 0       |
|     |       |          | 256   | 81 | 156 | 17 | 2 |         |
| 28  | Q     | 1        | Total | C  | H   | O  | P | 0       |
|     |       |          | 256   | 81 | 156 | 17 | 2 |         |
| 28  | c     | 1        | Total | C  | H   | O  | P | 0       |
|     |       |          | 256   | 81 | 156 | 17 | 2 |         |
| 28  | e     | 1        | Total | C  | H   | O  | P | 0       |
|     |       |          | 256   | 81 | 156 | 17 | 2 |         |

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| Mol | Chain | Residues | Atoms |    |     |    |   | AltConf |
|-----|-------|----------|-------|----|-----|----|---|---------|
| 28  | e     | 1        | Total | C  | H   | O  | P | 0       |
|     |       |          | 256   | 81 | 156 | 17 | 2 |         |
| 28  | e     | 1        | Total | C  | H   | O  | P | 0       |
|     |       |          | 256   | 81 | 156 | 17 | 2 |         |
| 28  | e     | 1        | Total | C  | H   | O  | P | 0       |
|     |       |          | 256   | 81 | 156 | 17 | 2 |         |
| 28  | e     | 1        | Total | C  | H   | O  | P | 0       |
|     |       |          | 256   | 81 | 156 | 17 | 2 |         |
| 28  | f     | 1        | Total | C  | H   | O  | P | 0       |
|     |       |          | 256   | 81 | 156 | 17 | 2 |         |
| 28  | j     | 1        | Total | C  | H   | O  | P | 0       |
|     |       |          | 256   | 81 | 156 | 17 | 2 |         |
| 28  | j     | 1        | Total | C  | H   | O  | P | 0       |
|     |       |          | 256   | 81 | 156 | 17 | 2 |         |
| 28  | l     | 1        | Total | C  | H   | O  | P | 0       |
|     |       |          | 256   | 81 | 156 | 17 | 2 |         |
| 28  | m     | 1        | Total | C  | H   | O  | P | 0       |
|     |       |          | 256   | 81 | 156 | 17 | 2 |         |
| 28  | q     | 1        | Total | C  | H   | O  | P | 0       |
|     |       |          | 256   | 81 | 156 | 17 | 2 |         |

- Molecule 29 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



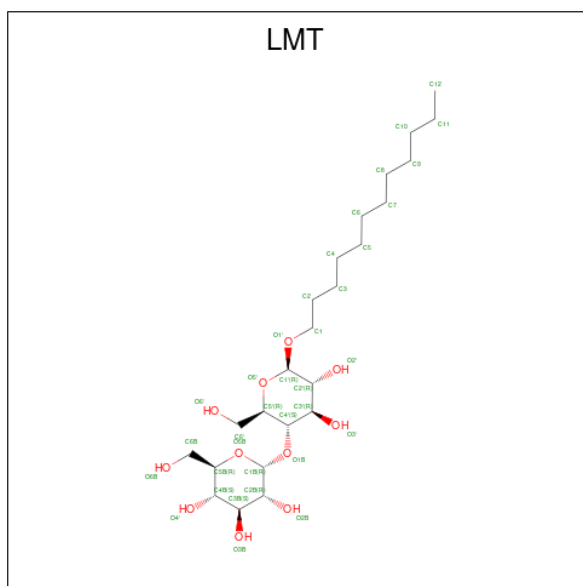
| Mol | Chain | Residues | Atoms |    |    |   |    | AltConf |
|-----|-------|----------|-------|----|----|---|----|---------|
| 29  | D1    | 1        | Total | C  | H  | N | O  | P       |
|     |       |          | 39    | 10 | 12 | 5 | 10 | 2       |
|     |       |          |       |    |    |   |    | 0       |

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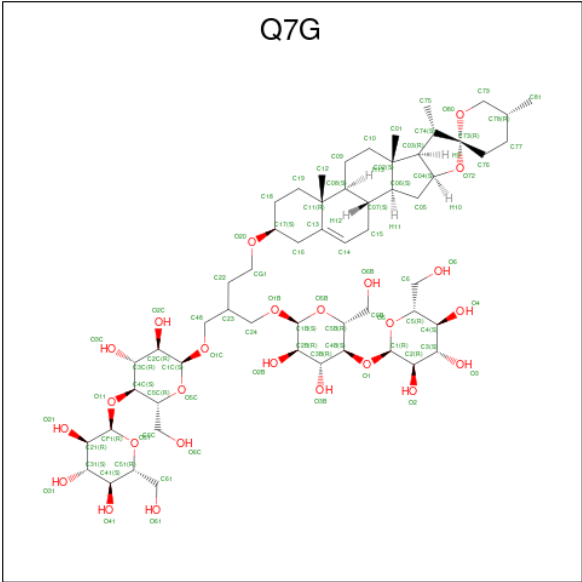
| Mol | Chain | Residues | Atoms |    |    |   |    | AltConf |   |
|-----|-------|----------|-------|----|----|---|----|---------|---|
| 29  | D2    | 1        | Total | C  | H  | N | O  | P       | 0 |
|     |       |          | 39    | 10 | 12 | 5 | 10 | 2       |   |

- Molecule 30 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



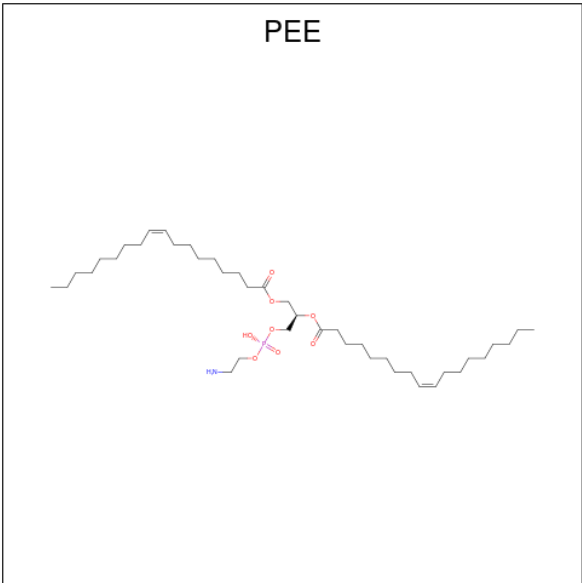
| Mol | Chain | Residues | Atoms |    |    |    | AltConf |
|-----|-------|----------|-------|----|----|----|---------|
| 30  | E     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 74    | 24 | 39 | 11 |         |
| 30  | J     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 74    | 24 | 39 | 11 |         |
| 30  | e     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 74    | 24 | 39 | 11 |         |
| 30  | j     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 74    | 24 | 39 | 11 |         |

- Molecule 31 is 2-[[[(4-O-alpha-D-glucopyranosyl-alpha-D-glucopyranosyl)oxy]methyl]-4-[[[(3 beta,9beta,14beta,17beta,25R)-spirost-5-en-3-yl]oxy]butyl 4-O-alpha-D-glucopyranosyl-alpha-D-glucopyranoside (CCD ID: Q7G) (formula:  $C_{56}H_{92}O_{25}$ ).



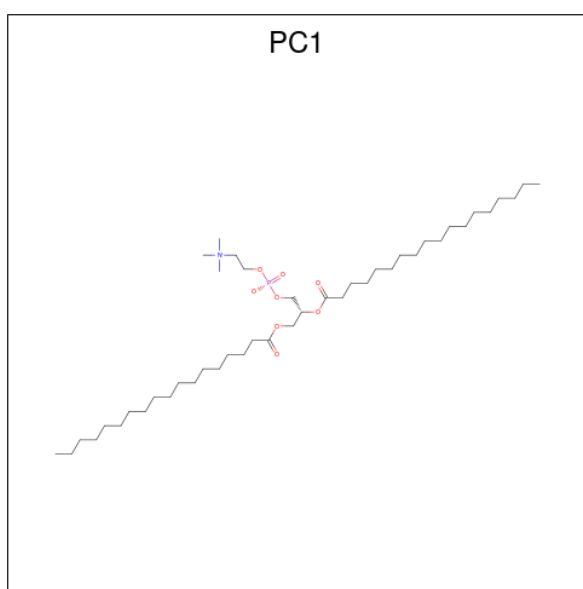
| Mol | Chain | Residues | Atoms |    |    |    | AltConf |
|-----|-------|----------|-------|----|----|----|---------|
| 31  | E     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 108   | 38 | 60 | 10 |         |
| 31  | N     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 129   | 44 | 70 | 15 |         |
| 31  | e     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 108   | 38 | 60 | 10 |         |
| 31  | n     | 1        | Total | C  | H  | O  | 0       |
|     |       |          | 129   | 44 | 70 | 15 |         |

- Molecule 32 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula:  $C_{41}H_{78}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms        |         |         |        |        | AltConf |   |
|-----|-------|----------|--------------|---------|---------|--------|--------|---------|---|
| 32  | F     | 1        | Total<br>133 | C<br>41 | H<br>82 | N<br>1 | O<br>8 | P<br>1  | 0 |
| 32  | R     | 1        | Total<br>133 | C<br>41 | H<br>82 | N<br>1 | O<br>8 | P<br>1  | 0 |
| 32  | f     | 1        | Total<br>133 | C<br>41 | H<br>82 | N<br>1 | O<br>8 | P<br>1  | 0 |
| 32  | r     | 1        | Total<br>133 | C<br>41 | H<br>82 | N<br>1 | O<br>8 | P<br>1  | 0 |

- Molecule 33 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C<sub>44</sub>H<sub>88</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



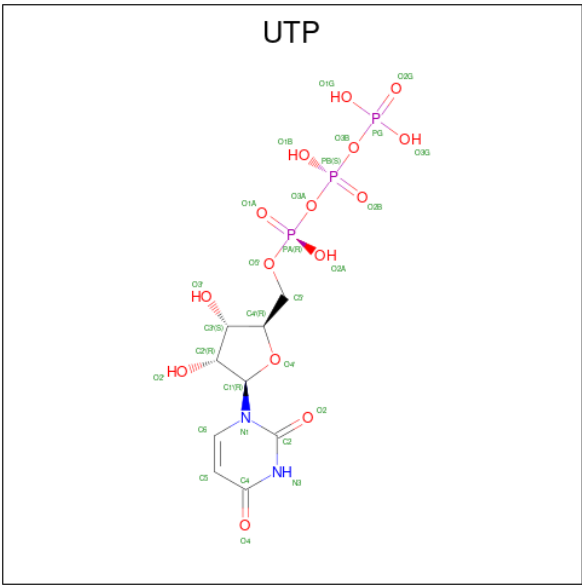
| Mol | Chain | Residues | Atoms        |         |         |        |        |        | AltConf |
|-----|-------|----------|--------------|---------|---------|--------|--------|--------|---------|
| 33  | F     | 1        | Total<br>142 | C<br>44 | H<br>88 | N<br>1 | O<br>8 | P<br>1 | 0       |
| 33  | F     | 1        | Total<br>142 | C<br>44 | H<br>88 | N<br>1 | O<br>8 | P<br>1 | 0       |
| 33  | I     | 1        | Total<br>142 | C<br>44 | H<br>88 | N<br>1 | O<br>8 | P<br>1 | 0       |
| 33  | J     | 1        | Total<br>142 | C<br>44 | H<br>88 | N<br>1 | O<br>8 | P<br>1 | 0       |
| 33  | f     | 1        | Total<br>142 | C<br>44 | H<br>88 | N<br>1 | O<br>8 | P<br>1 | 0       |
| 33  | f     | 1        | Total<br>142 | C<br>44 | H<br>88 | N<br>1 | O<br>8 | P<br>1 | 0       |
| 33  | i     | 1        | Total<br>142 | C<br>44 | H<br>88 | N<br>1 | O<br>8 | P<br>1 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---|---------|
| 33  | j     | 1        | Total | C  | H  | N | O | P | 0       |
|     |       |          | 142   | 44 | 88 | 1 | 8 | 1 |         |

- Molecule 34 is URIDINE 5'-TRIPHOSPHATE (CCD ID: UTP) (formula: C<sub>9</sub>H<sub>15</sub>N<sub>2</sub>O<sub>15</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |   |    |   |    |   | AltConf |
|-----|-------|----------|-------|---|----|---|----|---|---------|
| 34  | H1    | 1        | Total | C | H  | N | O  | P | 0       |
|     |       |          | 40    | 9 | 11 | 2 | 15 | 3 |         |
| 34  | H2    | 1        | Total | C | H  | N | O  | P | 0       |
|     |       |          | 40    | 9 | 11 | 2 | 15 | 3 |         |

### 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. 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. 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: ATP synthase subunit a

Chain A: 



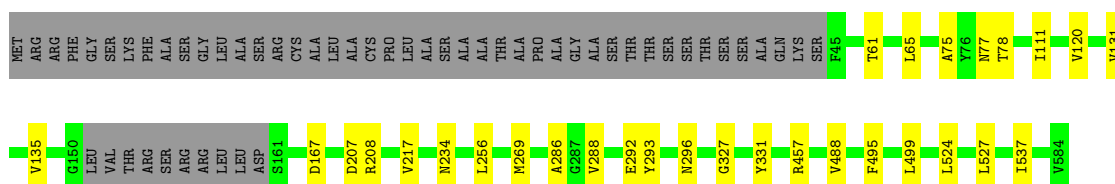
- Molecule 1: ATP synthase subunit a

Chain a: 



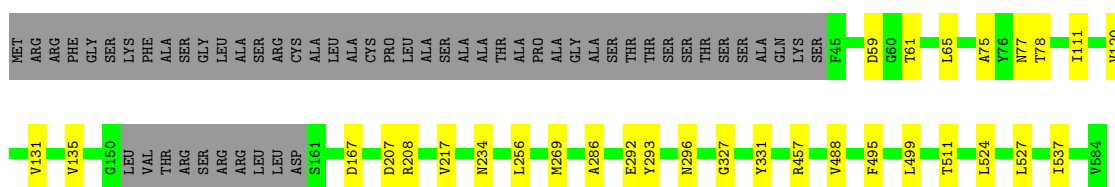
- Molecule 2: ATP synthase subunit alpha, mitochondrial

Chain A1: 



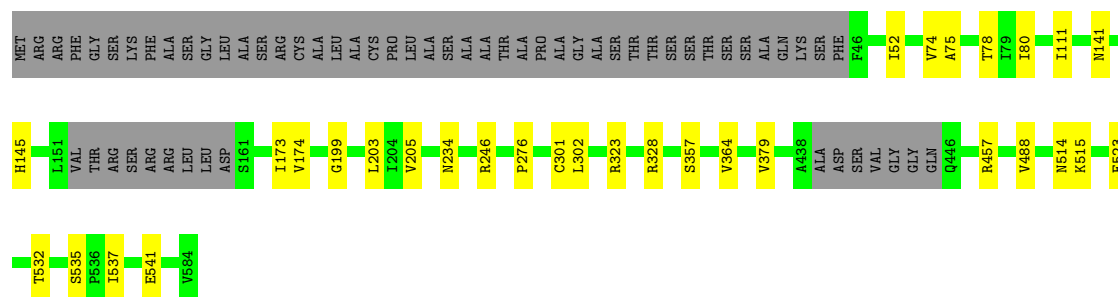
- Molecule 2: ATP synthase subunit alpha, mitochondrial

Chain A2: 



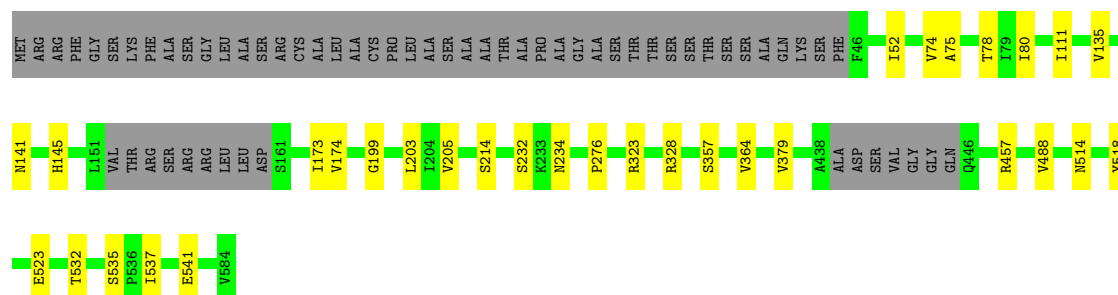
- Molecule 2: ATP synthase subunit alpha, mitochondrial

Chain B1: 



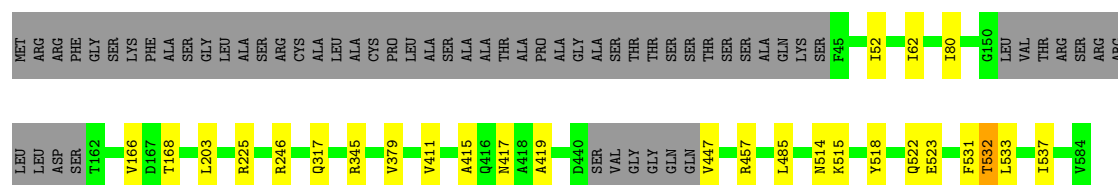
- Molecule 2: ATP synthase subunit alpha, mitochondrial

Chain B2: 84% 5% 10%



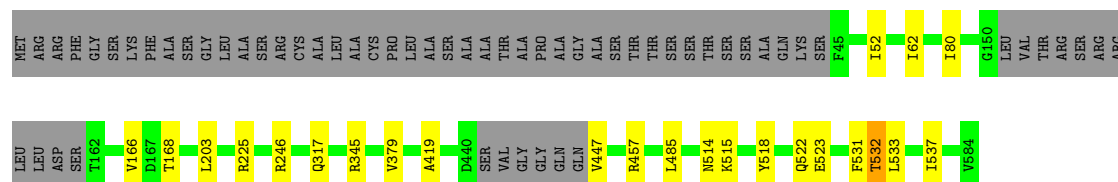
- Molecule 2: ATP synthase subunit alpha, mitochondrial

Chain C1: 85% 10% 5%



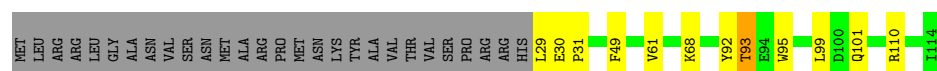
- Molecule 2: ATP synthase subunit alpha, mitochondrial

Chain C2: 85% 10% 5%



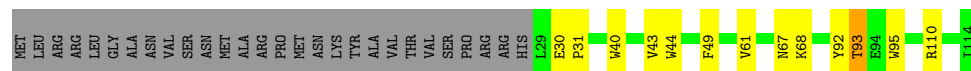
- Molecule 3: subunit-8

Chain C: 65% 10% 25%



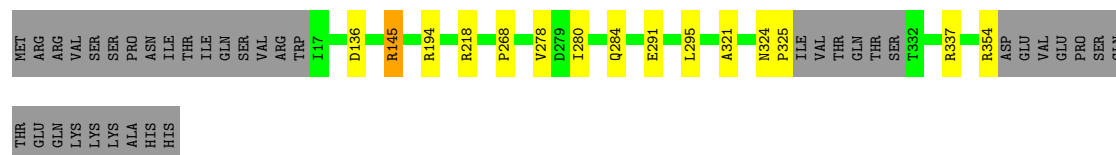
- Molecule 3: subunit-8

Chain c:  64% 11% 25%



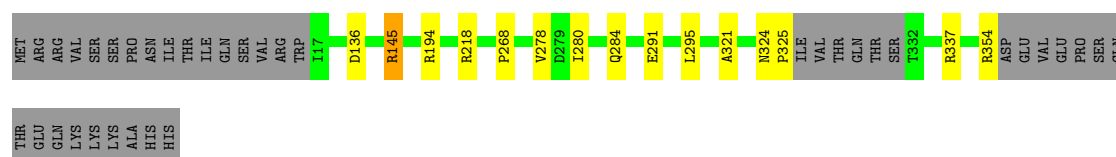
- Molecule 4: subunit-d

Chain D:  86% 10%



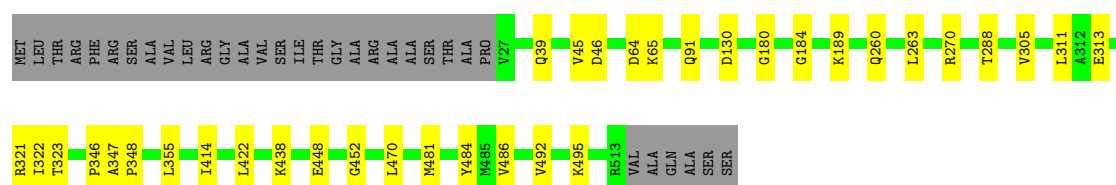
- Molecule 4: subunit-d

Chain d:  86% 10%



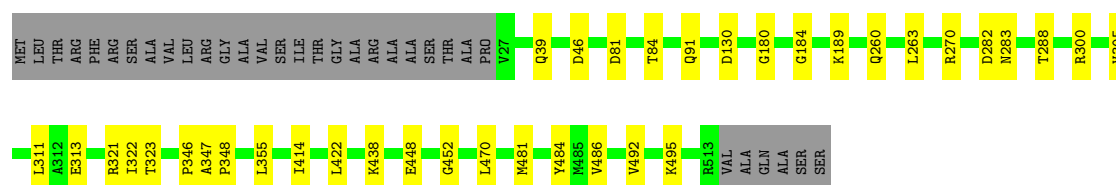
- Molecule 5: ATP synthase subunit beta, mitochondrial

Chain D1:  87% 7% 6%



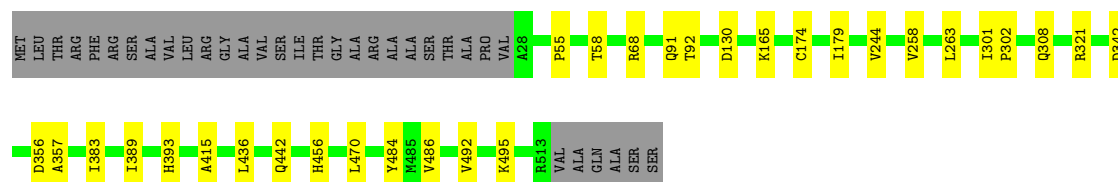
- Molecule 5: ATP synthase subunit beta, mitochondrial

Chain D2:  87% 7% 6%



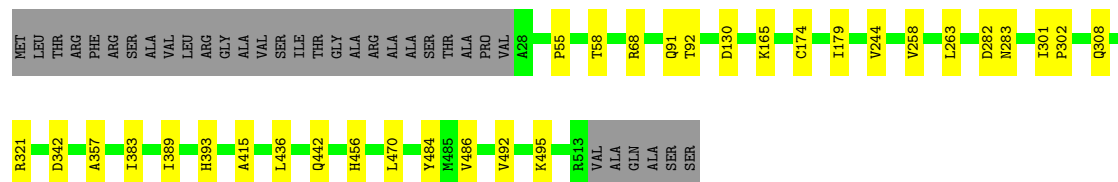
- Molecule 5: ATP synthase subunit beta, mitochondrial

Chain E1:  88% 6% 6%



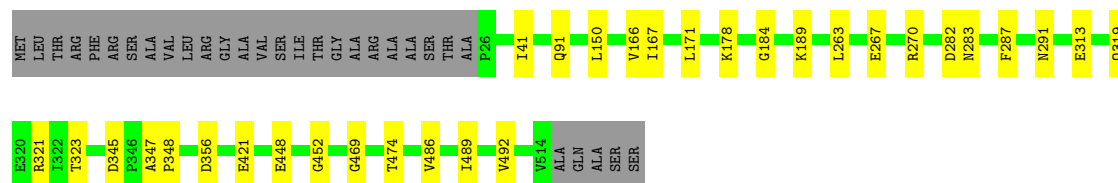
- Molecule 5: ATP synthase subunit beta, mitochondrial

Chain E2: 87% 6% 6%



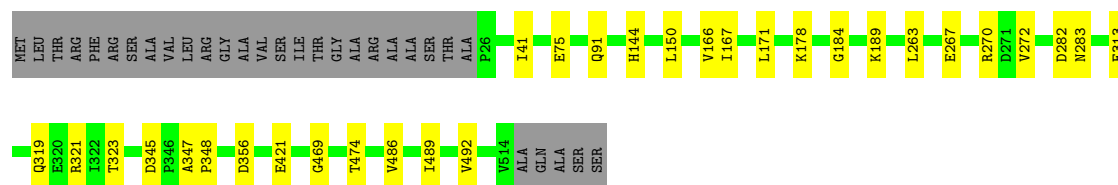
- Molecule 5: ATP synthase subunit beta, mitochondrial

Chain F1: 88% 6% 6%



- Molecule 5: ATP synthase subunit beta, mitochondrial

Chain F2: 88% 6% 6%



- Molecule 6: ATP6B1

Chain E: 93% 6% 6%



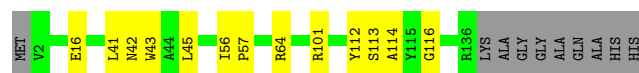
- Molecule 6: ATP6B1

Chain e: 93% 6% 6%



- Molecule 7: subunit-f

Chain F:  84% 9% 7%



- Molecule 7: subunit-f

Chain f:  84% 9% 7%



- Molecule 8: ATPTB3

Chain G:  90% 9%



- Molecule 8: ATPTB3

Chain g:  90% 10%



- Molecule 9: ATP synthase gamma subunit

Chain G1:  90% 8%



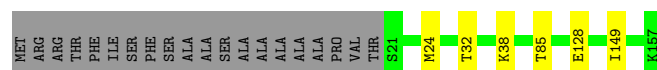
- Molecule 9: ATP synthase gamma subunit

Chain G2:  90% 9%



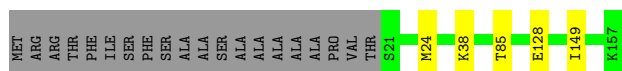
- Molecule 10: ATPTB4

Chain H:  83% 13%



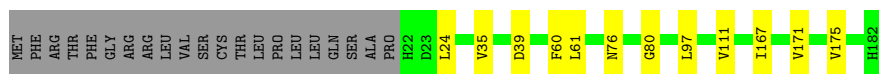
- Molecule 10: ATPTB4

Chain h:  84% 13%



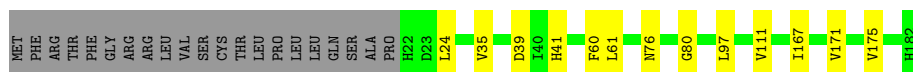
- Molecule 11: ATP synthase, epsilon chain, putative

Chain H1:  82% 7% 12%



- Molecule 11: ATP synthase, epsilon chain, putative

Chain H2:  81% 7% 12%



- Molecule 12: subunit-i/j

Chain I:  91% 8%



- Molecule 12: subunit-i/j

Chain i:  91% 8%



- Molecule 13: ATP synthase subunit epsilon, mitochondrial

Chain I1:  76% 11% 13%

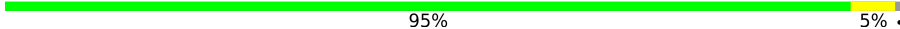


- Molecule 13: ATP synthase subunit epsilon, mitochondrial

Chain I2:  73% 13% 13%

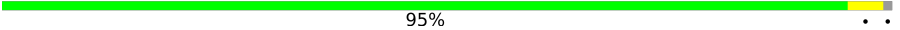


- Molecule 14: ATPTB6

Chain J:  95% 5%



- Molecule 14: ATPTB6

Chain j:  95%



- Molecule 15: ATP synthase subunit p18, mitochondrial

Chain J1:  81% 7% 12%



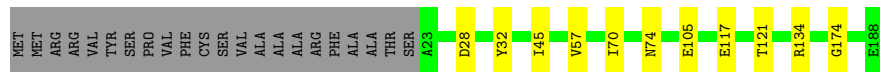
- Molecule 15: ATP synthase subunit p18, mitochondrial

Chain J2:  80% 9% 12%



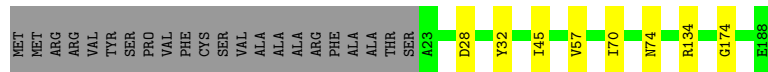
- Molecule 15: ATP synthase subunit p18, mitochondrial

Chain K1:  82% 6% 12%



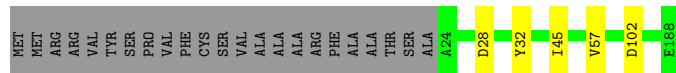
- Molecule 15: ATP synthase subunit p18, mitochondrial

Chain K2:  84% 12%



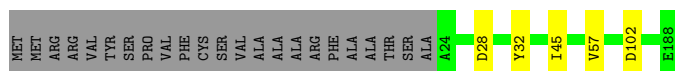
- Molecule 15: ATP synthase subunit p18, mitochondrial

Chain L1:  85% 12%



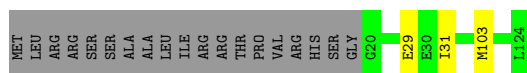
- Molecule 15: ATP synthase subunit p18, mitochondrial

Chain L2:  85% 12%



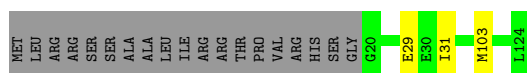
- Molecule 16: subunit-k

Chain K:  82% 15%



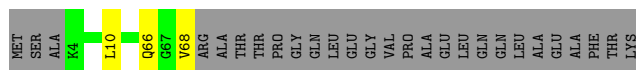
- Molecule 16: subunit-k

Chain k:  82% 15%



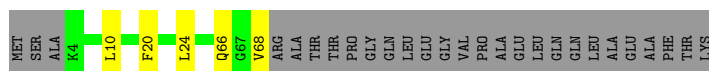
- Molecule 17: subunit-e

Chain L:  67% 29%



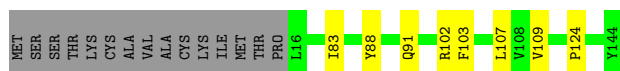
- Molecule 17: subunit-e

Chain l:  65% 5% 29%



- Molecule 18: subunit-g

Chain M:  84% 6% 10%



- Molecule 18: subunit-g

Chain m:  84% 6% 10%



- Molecule 19: oligomycin sensitivity conferring protein

Chain M1:  88% 8%



- Molecule 19: oligomycin sensitivity conferring protein

Chain M2: 88% 8%



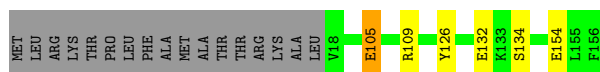
- Molecule 20: ATPTB11

Chain N: 84% 11%



- Molecule 20: ATPTB11

Chain n: 85% 11%



- Molecule 21: ATPTB12

Chain O: 91% 5%



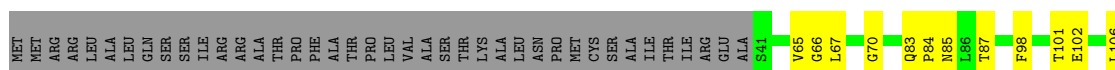
- Molecule 21: ATPTB12

Chain o: 91% 5%

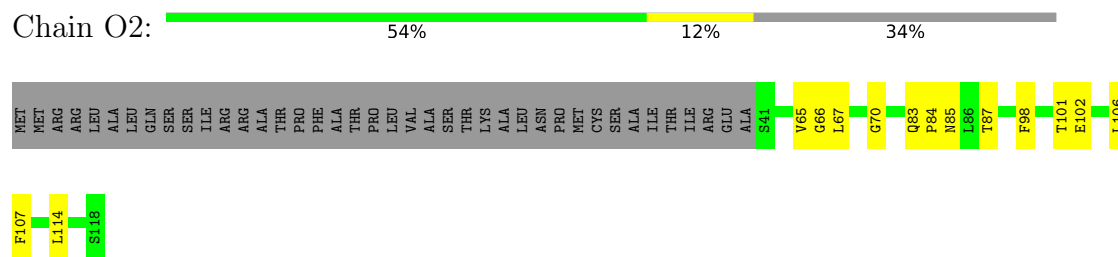


- Molecule 22: ATPase subunit 9, putative

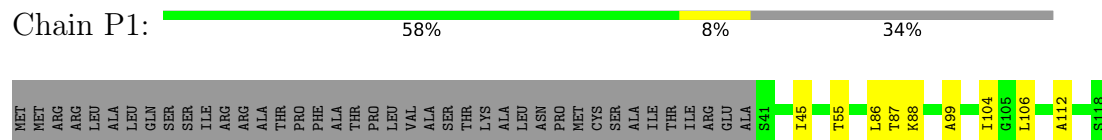
Chain O1: 54% 12% 34%



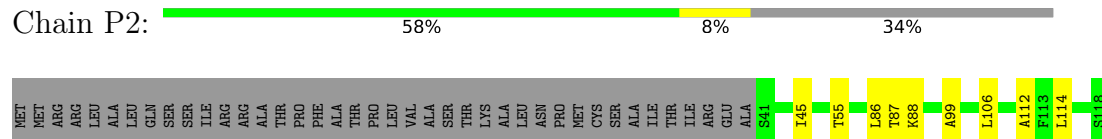
- Molecule 22: ATPase subunit 9, putative



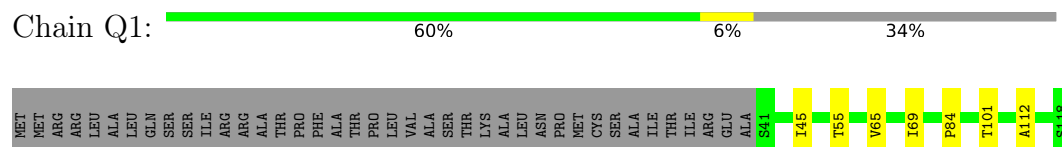
- Molecule 22: ATPase subunit 9, putative



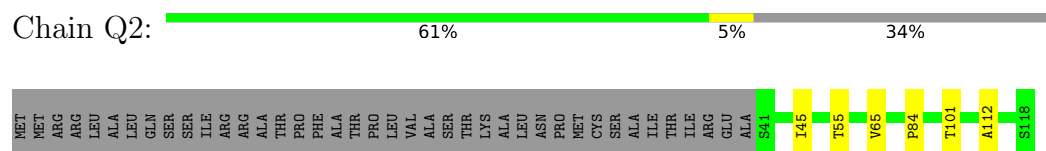
- Molecule 22: ATPase subunit 9, putative



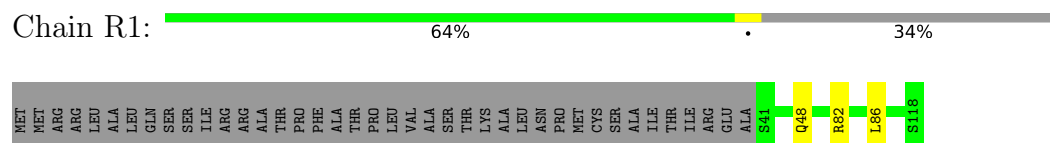
- Molecule 22: ATPase subunit 9, putative



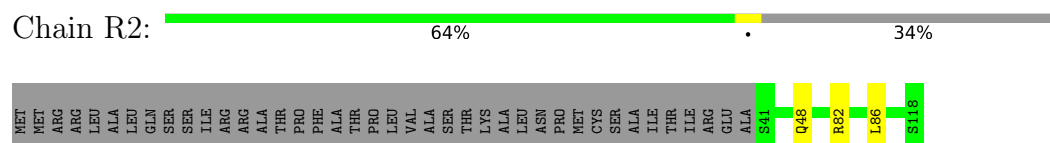
- Molecule 22: ATPase subunit 9, putative



- Molecule 22: ATPase subunit 9, putative

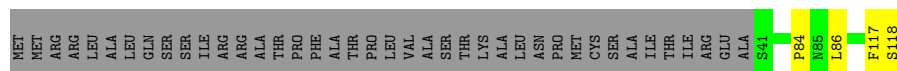


- Molecule 22: ATPase subunit 9, putative



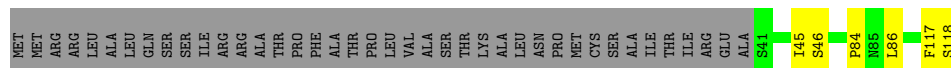
- Molecule 22: ATPase subunit 9, putative

Chain S1:  63% 34%



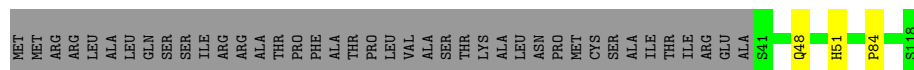
- Molecule 22: ATPase subunit 9, putative

Chain S2:  61% 5% 34%



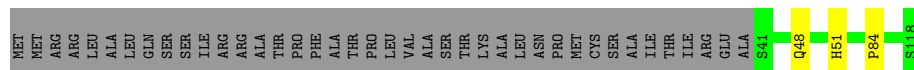
- Molecule 22: ATPase subunit 9, putative

Chain T1:  64% 34%



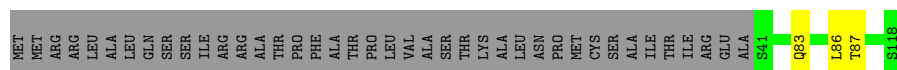
- Molecule 22: ATPase subunit 9, putative

Chain T2:  64% 34%



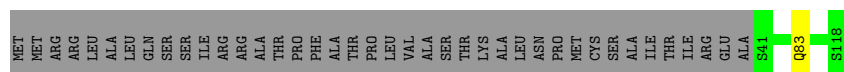
- Molecule 22: ATPase subunit 9, putative

Chain U1:  64% 34%



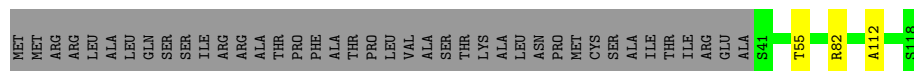
- Molecule 22: ATPase subunit 9, putative

Chain U2:  65% 34%

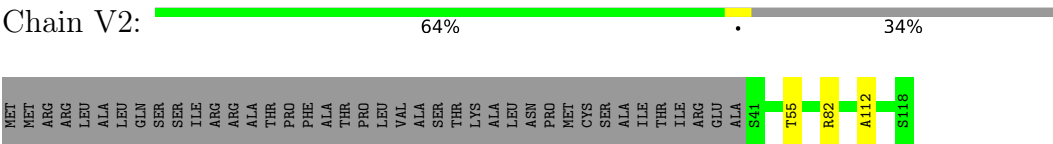


- Molecule 22: ATPase subunit 9, putative

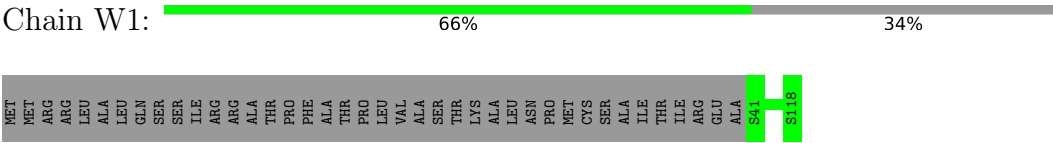
Chain V1:  64% 34%



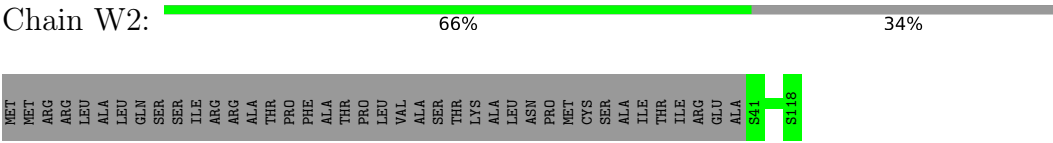
- Molecule 22: ATPase subunit 9, putative



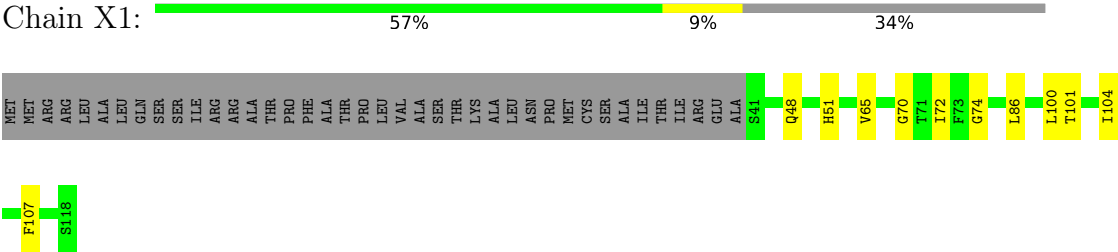
• Molecule 22: ATPase subunit 9, putative



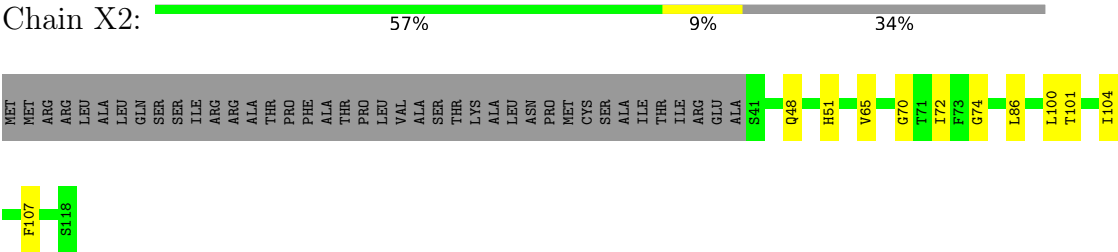
• Molecule 22: ATPase subunit 9, putative



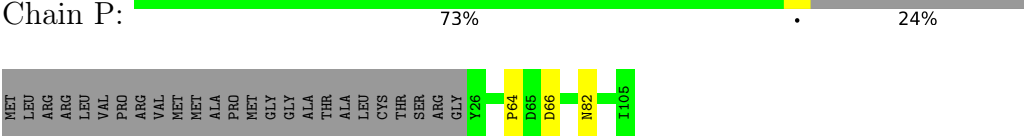
• Molecule 22: ATPase subunit 9, putative



• Molecule 22: ATPase subunit 9, putative



• Molecule 23: subunit-b



• Molecule 23: subunit-b





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 36925                                   | 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 ( $e^-/\text{\AA}^2$ ) | 33                                      | Depositor |
| Minimum defocus (nm)                 | 1600                                    | Depositor |
| Maximum defocus (nm)                 | 3200                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 QUANTUM (4k x 4k)              | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, CDL, ATP, Q7G, PC1, LMT, UTP, PEE, AME

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     | 0.20         | 0/2111      | 0.26        | 0/2861      |
| 1   | a     | 0.20         | 0/2111      | 0.26        | 0/2861      |
| 2   | A1    | 0.07         | 0/4159      | 0.22        | 0/5632      |
| 2   | A2    | 0.07         | 0/4159      | 0.22        | 0/5632      |
| 2   | B1    | 0.07         | 0/4110      | 0.22        | 0/5566      |
| 2   | B2    | 0.07         | 0/4110      | 0.22        | 0/5566      |
| 2   | C1    | 0.07         | 0/4113      | 0.22        | 0/5569      |
| 2   | C2    | 0.07         | 0/4113      | 0.22        | 0/5569      |
| 3   | C     | 0.18         | 0/772       | 0.28        | 0/1054      |
| 3   | c     | 0.18         | 0/772       | 0.32        | 0/1054      |
| 4   | D     | 0.12         | 0/2786      | 0.25        | 0/3760      |
| 4   | d     | 0.12         | 0/2786      | 0.25        | 0/3760      |
| 5   | D1    | 0.08         | 0/3745      | 0.23        | 0/5077      |
| 5   | D2    | 0.08         | 0/3745      | 0.23        | 0/5077      |
| 5   | E1    | 0.07         | 0/3738      | 0.22        | 0/5067      |
| 5   | E2    | 0.07         | 0/3738      | 0.22        | 0/5067      |
| 5   | F1    | 0.08         | 0/3760      | 0.24        | 0/5098      |
| 5   | F2    | 0.08         | 0/3760      | 0.24        | 0/5098      |
| 6   | E     | 0.16         | 0/3305      | 0.21        | 0/4482      |
| 6   | e     | 0.16         | 0/3305      | 0.21        | 0/4482      |
| 7   | F     | 0.18         | 0/1183      | 0.28        | 0/1601      |
| 7   | f     | 0.18         | 0/1183      | 0.28        | 0/1601      |
| 8   | G     | 0.07         | 0/1953      | 0.20        | 0/2650      |
| 8   | g     | 0.07         | 0/1953      | 0.20        | 0/2650      |
| 9   | G1    | 0.07         | 0/2427      | 0.20        | 0/3268      |
| 9   | G2    | 0.07         | 0/2427      | 0.20        | 0/3268      |
| 10  | H     | 0.05         | 0/1088      | 0.16        | 0/1466      |
| 10  | h     | 0.05         | 0/1088      | 0.16        | 0/1466      |
| 11  | H1    | 0.13         | 0/1274      | 0.22        | 0/1728      |
| 11  | H2    | 0.13         | 0/1274      | 0.22        | 0/1728      |
| 12  | I     | 0.17         | 0/913       | 0.22        | 0/1240      |
| 12  | i     | 0.17         | 0/913       | 0.22        | 0/1240      |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 13  | I1    | 0.06         | 0/547   | 0.18        | 0/738   |
| 13  | I2    | 0.06         | 0/547   | 0.18        | 0/738   |
| 14  | J     | 0.14         | 0/1462  | 0.20        | 0/1973  |
| 14  | j     | 0.14         | 0/1462  | 0.20        | 0/1973  |
| 15  | J1    | 0.05         | 0/1341  | 0.16        | 0/1810  |
| 15  | J2    | 0.05         | 0/1341  | 0.17        | 0/1810  |
| 15  | K1    | 0.05         | 0/1342  | 0.18        | 0/1810  |
| 15  | K2    | 0.05         | 0/1342  | 0.18        | 0/1810  |
| 15  | L1    | 0.05         | 0/1337  | 0.17        | 0/1803  |
| 15  | L2    | 0.05         | 0/1337  | 0.17        | 0/1803  |
| 16  | K     | 0.13         | 0/904   | 0.22        | 0/1228  |
| 16  | k     | 0.13         | 0/904   | 0.22        | 0/1228  |
| 17  | L     | 0.14         | 0/547   | 0.18        | 0/735   |
| 17  | l     | 0.14         | 0/547   | 0.18        | 0/735   |
| 18  | M     | 0.15         | 0/1049  | 0.21        | 0/1423  |
| 18  | m     | 0.15         | 0/1049  | 0.21        | 0/1423  |
| 19  | M1    | 0.08         | 0/1916  | 0.21        | 0/2591  |
| 19  | M2    | 0.08         | 0/1916  | 0.21        | 0/2591  |
| 20  | N     | 0.17         | 0/1166  | 0.23        | 0/1581  |
| 20  | n     | 0.17         | 0/1166  | 0.23        | 0/1581  |
| 21  | O     | 0.13         | 0/814   | 0.20        | 0/1100  |
| 21  | o     | 0.13         | 0/814   | 0.19        | 0/1100  |
| 22  | O1    | 0.10         | 0/574   | 0.28        | 0/777   |
| 22  | O2    | 0.10         | 0/574   | 0.28        | 0/777   |
| 22  | P1    | 0.15         | 0/574   | 0.29        | 0/777   |
| 22  | P2    | 0.15         | 0/574   | 0.29        | 0/777   |
| 22  | Q1    | 0.09         | 0/574   | 0.19        | 0/777   |
| 22  | Q2    | 0.09         | 0/574   | 0.19        | 0/777   |
| 22  | R1    | 0.09         | 0/574   | 0.20        | 0/777   |
| 22  | R2    | 0.09         | 0/574   | 0.20        | 0/777   |
| 22  | S1    | 0.08         | 0/574   | 0.19        | 0/777   |
| 22  | S2    | 0.08         | 0/574   | 0.19        | 0/777   |
| 22  | T1    | 0.07         | 0/574   | 0.20        | 0/777   |
| 22  | T2    | 0.08         | 0/574   | 0.20        | 0/777   |
| 22  | U1    | 0.08         | 0/574   | 0.20        | 0/777   |
| 22  | U2    | 0.08         | 0/574   | 0.20        | 0/777   |
| 22  | V1    | 0.08         | 0/574   | 0.19        | 0/777   |
| 22  | V2    | 0.08         | 0/574   | 0.19        | 0/777   |
| 22  | W1    | 0.07         | 0/574   | 0.18        | 0/777   |
| 22  | W2    | 0.07         | 0/574   | 0.18        | 0/777   |
| 22  | X1    | 0.08         | 0/574   | 0.25        | 0/777   |
| 22  | X2    | 0.08         | 0/574   | 0.25        | 0/777   |
| 23  | P     | 0.15         | 0/707   | 0.23        | 0/957   |

| Mol | Chain | Bond lengths |             | Bond angles |             |
|-----|-------|--------------|-------------|-------------|-------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$ |
| 23  | p     | 0.15         | 0/707       | 0.23        | 0/957       |
| 24  | Q     | 0.17         | 0/799       | 0.24        | 0/1091      |
| 24  | q     | 0.17         | 0/799       | 0.24        | 0/1091      |
| 25  | R     | 0.18         | 0/567       | 0.23        | 0/767       |
| 25  | r     | 0.18         | 0/567       | 0.23        | 0/767       |
| All | All   | 0.11         | 0/123350    | 0.22        | 0/166992    |

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](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2032  | 2044     | 2044     | 17      | 0            |
| 1   | a     | 2032  | 2044     | 2044     | 17      | 0            |
| 2   | A1    | 4084  | 4196     | 4196     | 19      | 0            |
| 2   | A2    | 4084  | 4196     | 4196     | 20      | 0            |
| 2   | B1    | 4037  | 4161     | 4160     | 22      | 0            |
| 2   | B2    | 4037  | 4161     | 4160     | 23      | 0            |
| 2   | C1    | 4039  | 4154     | 4154     | 21      | 0            |
| 2   | C2    | 4039  | 4154     | 4154     | 19      | 0            |
| 3   | C     | 745   | 715      | 715      | 10      | 0            |
| 3   | c     | 745   | 715      | 715      | 11      | 0            |
| 4   | D     | 2737  | 2762     | 2763     | 15      | 0            |
| 4   | d     | 2737  | 2762     | 2763     | 15      | 0            |
| 5   | D1    | 3689  | 3741     | 3741     | 21      | 0            |
| 5   | D2    | 3689  | 3741     | 3741     | 23      | 0            |
| 5   | E1    | 3682  | 3733     | 3733     | 23      | 0            |
| 5   | E2    | 3682  | 3733     | 3733     | 22      | 0            |
| 5   | F1    | 3703  | 3758     | 3758     | 21      | 0            |
| 5   | F2    | 3703  | 3758     | 3758     | 22      | 0            |
| 6   | E     | 3220  | 3061     | 3061     | 10      | 0            |
| 6   | e     | 3220  | 3061     | 3061     | 9       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 7   | F     | 1145  | 1111     | 1111     | 11      | 0            |
| 7   | f     | 1145  | 1111     | 1111     | 10      | 0            |
| 8   | G     | 1933  | 2020     | 2020     | 14      | 0            |
| 8   | g     | 1933  | 2020     | 2020     | 15      | 0            |
| 9   | G1    | 2387  | 2387     | 2387     | 19      | 0            |
| 9   | G2    | 2387  | 2387     | 2387     | 23      | 0            |
| 10  | H     | 1070  | 1088     | 1088     | 5       | 0            |
| 10  | h     | 1070  | 1088     | 1088     | 4       | 0            |
| 11  | H1    | 1251  | 1232     | 1231     | 10      | 0            |
| 11  | H2    | 1251  | 1232     | 1231     | 10      | 0            |
| 12  | I     | 883   | 857      | 857      | 6       | 0            |
| 12  | i     | 883   | 857      | 857      | 6       | 0            |
| 13  | I1    | 533   | 513      | 513      | 6       | 0            |
| 13  | I2    | 533   | 513      | 513      | 8       | 0            |
| 14  | J     | 1424  | 1411     | 1411     | 6       | 0            |
| 14  | j     | 1424  | 1411     | 1411     | 5       | 0            |
| 15  | J1    | 1314  | 1276     | 1276     | 10      | 0            |
| 15  | J2    | 1314  | 1276     | 1276     | 11      | 0            |
| 15  | K1    | 1315  | 1276     | 1276     | 8       | 0            |
| 15  | K2    | 1315  | 1276     | 1276     | 6       | 0            |
| 15  | L1    | 1310  | 1271     | 1271     | 4       | 0            |
| 15  | L2    | 1310  | 1271     | 1271     | 4       | 0            |
| 16  | K     | 873   | 876      | 876      | 3       | 0            |
| 16  | k     | 873   | 876      | 876      | 3       | 0            |
| 17  | L     | 537   | 545      | 545      | 2       | 0            |
| 17  | l     | 537   | 545      | 545      | 3       | 0            |
| 18  | M     | 1027  | 1042     | 1042     | 5       | 0            |
| 18  | m     | 1027  | 1042     | 1042     | 5       | 0            |
| 19  | M1    | 1877  | 1873     | 1873     | 7       | 0            |
| 19  | M2    | 1877  | 1873     | 1873     | 6       | 0            |
| 20  | N     | 1128  | 1082     | 1082     | 5       | 0            |
| 20  | n     | 1128  | 1082     | 1082     | 4       | 0            |
| 21  | O     | 789   | 767      | 767      | 3       | 0            |
| 21  | o     | 789   | 767      | 767      | 3       | 0            |
| 22  | O1    | 565   | 600      | 599      | 12      | 0            |
| 22  | O2    | 565   | 600      | 599      | 12      | 0            |
| 22  | P1    | 565   | 600      | 599      | 10      | 0            |
| 22  | P2    | 565   | 600      | 599      | 10      | 0            |
| 22  | Q1    | 565   | 600      | 599      | 5       | 0            |
| 22  | Q2    | 565   | 600      | 599      | 4       | 0            |
| 22  | R1    | 565   | 600      | 599      | 3       | 0            |
| 22  | R2    | 565   | 600      | 599      | 3       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 22  | S1    | 565   | 601      | 599      | 3       | 0            |
| 22  | S2    | 565   | 601      | 599      | 4       | 0            |
| 22  | T1    | 565   | 601      | 599      | 2       | 0            |
| 22  | T2    | 565   | 601      | 599      | 2       | 0            |
| 22  | U1    | 565   | 600      | 599      | 2       | 0            |
| 22  | U2    | 565   | 600      | 599      | 1       | 0            |
| 22  | V1    | 565   | 600      | 599      | 2       | 0            |
| 22  | V2    | 565   | 600      | 599      | 2       | 0            |
| 22  | W1    | 565   | 600      | 599      | 0       | 0            |
| 22  | W2    | 565   | 600      | 599      | 0       | 0            |
| 22  | X1    | 565   | 600      | 599      | 6       | 0            |
| 22  | X2    | 565   | 600      | 599      | 6       | 0            |
| 23  | P     | 684   | 651      | 651      | 4       | 0            |
| 23  | p     | 684   | 651      | 651      | 4       | 0            |
| 24  | Q     | 766   | 720      | 720      | 7       | 0            |
| 24  | q     | 766   | 720      | 720      | 6       | 0            |
| 25  | R     | 542   | 498      | 498      | 4       | 0            |
| 25  | r     | 542   | 498      | 498      | 3       | 0            |
| 26  | A1    | 31    | 12       | 12       | 0       | 0            |
| 26  | A2    | 31    | 12       | 12       | 0       | 0            |
| 26  | B1    | 31    | 12       | 12       | 0       | 0            |
| 26  | B2    | 31    | 12       | 12       | 1       | 0            |
| 26  | C1    | 31    | 12       | 12       | 0       | 0            |
| 26  | C2    | 31    | 12       | 12       | 0       | 0            |
| 26  | F1    | 31    | 12       | 12       | 0       | 0            |
| 26  | F2    | 31    | 12       | 12       | 0       | 0            |
| 27  | A1    | 1     | 0        | 0        | 0       | 0            |
| 27  | A2    | 1     | 0        | 0        | 0       | 0            |
| 27  | B1    | 1     | 0        | 0        | 0       | 0            |
| 27  | B2    | 1     | 0        | 0        | 0       | 0            |
| 27  | C1    | 1     | 0        | 0        | 0       | 0            |
| 27  | C2    | 1     | 0        | 0        | 0       | 0            |
| 27  | D1    | 1     | 0        | 0        | 0       | 0            |
| 27  | D2    | 1     | 0        | 0        | 0       | 0            |
| 27  | F1    | 1     | 0        | 0        | 0       | 0            |
| 27  | F2    | 1     | 0        | 0        | 0       | 0            |
| 28  | C     | 100   | 156      | 156      | 1       | 0            |
| 28  | E     | 500   | 780      | 780      | 4       | 0            |
| 28  | F     | 100   | 156      | 156      | 0       | 0            |
| 28  | J     | 200   | 312      | 312      | 1       | 0            |
| 28  | L     | 100   | 156      | 156      | 0       | 0            |
| 28  | M     | 100   | 156      | 156      | 1       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 28  | Q     | 100    | 156      | 156      | 1       | 0            |
| 28  | c     | 100    | 156      | 156      | 1       | 0            |
| 28  | e     | 500    | 780      | 780      | 4       | 0            |
| 28  | f     | 100    | 156      | 156      | 0       | 0            |
| 28  | j     | 200    | 312      | 312      | 1       | 0            |
| 28  | l     | 100    | 156      | 156      | 0       | 0            |
| 28  | m     | 100    | 156      | 156      | 0       | 0            |
| 28  | q     | 100    | 156      | 156      | 0       | 0            |
| 29  | D1    | 27     | 12       | 12       | 0       | 0            |
| 29  | D2    | 27     | 12       | 12       | 0       | 0            |
| 30  | E     | 35     | 39       | 46       | 0       | 0            |
| 30  | J     | 35     | 39       | 46       | 0       | 0            |
| 30  | e     | 35     | 39       | 46       | 0       | 0            |
| 30  | j     | 35     | 39       | 46       | 0       | 0            |
| 31  | E     | 48     | 60       | 0        | 0       | 0            |
| 31  | N     | 59     | 70       | 0        | 0       | 0            |
| 31  | e     | 48     | 60       | 0        | 0       | 0            |
| 31  | n     | 59     | 70       | 0        | 0       | 0            |
| 32  | F     | 51     | 82       | 82       | 0       | 0            |
| 32  | R     | 51     | 82       | 82       | 0       | 0            |
| 32  | f     | 51     | 82       | 82       | 0       | 0            |
| 32  | r     | 51     | 82       | 82       | 1       | 0            |
| 33  | F     | 108    | 176      | 176      | 1       | 0            |
| 33  | I     | 54     | 88       | 88       | 0       | 0            |
| 33  | J     | 54     | 88       | 88       | 0       | 0            |
| 33  | f     | 108    | 176      | 176      | 1       | 0            |
| 33  | i     | 54     | 88       | 88       | 0       | 0            |
| 33  | j     | 54     | 88       | 88       | 0       | 0            |
| 34  | H1    | 29     | 11       | 11       | 2       | 0            |
| 34  | H2    | 29     | 11       | 11       | 2       | 0            |
| All | All   | 124572 | 126980   | 126722   | 585     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (585) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 3:C:93:THR:HG21  | 4:D:136:ASP:OD2 | 1.72                     | 0.89              |
| 5:F2:421:GLU:OE2 | 9:G2:82:SER:N   | 2.16                     | 0.79              |
| 5:F1:421:GLU:OE2 | 9:G1:82:SER:N   | 2.16                     | 0.78              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:H1:80:GLY:O     | 22:U1:83:GLN:NE2   | 2.19                     | 0.76              |
| 11:H2:80:GLY:O     | 22:U2:83:GLN:NE2   | 2.19                     | 0.75              |
| 14:j:19:ARG:NH2    | 24:q:77:GLU:O      | 2.21                     | 0.74              |
| 14:J:19:ARG:NH2    | 24:Q:77:GLU:O      | 2.21                     | 0.73              |
| 11:H1:76:ASN:ND2   | 34:H1:201:UTP:O1G  | 2.23                     | 0.71              |
| 11:H2:76:ASN:ND2   | 34:H2:201:UTP:O1G  | 2.23                     | 0.71              |
| 2:C2:447:VAL:N     | 13:I2:59:ALA:O     | 2.23                     | 0.70              |
| 2:C1:447:VAL:N     | 13:I1:59:ALA:O     | 2.23                     | 0.70              |
| 5:E2:165:LYS:NZ    | 5:E2:486:VAL:O     | 2.21                     | 0.69              |
| 15:K1:28:ASP:OD1   | 15:K1:32:TYR:N     | 2.26                     | 0.68              |
| 15:K2:28:ASP:OD1   | 15:K2:32:TYR:N     | 2.26                     | 0.68              |
| 5:E2:415:ALA:O     | 9:G2:34:ARG:NH2    | 2.28                     | 0.67              |
| 5:D1:184:GLY:O     | 5:D1:189:LYS:NZ    | 2.27                     | 0.67              |
| 5:E1:415:ALA:O     | 9:G1:34:ARG:NH2    | 2.28                     | 0.67              |
| 5:D2:184:GLY:O     | 5:D2:189:LYS:NZ    | 2.27                     | 0.67              |
| 1:A:8:ASP:OD1      | 20:N:126:TYR:OH    | 2.13                     | 0.67              |
| 22:X2:70:GLY:O     | 22:X2:74:GLY:N     | 2.28                     | 0.67              |
| 5:E1:263:LEU:HD21  | 5:E1:321:ARG:HB2   | 1.78                     | 0.66              |
| 5:E1:165:LYS:NZ    | 5:E1:486:VAL:O     | 2.21                     | 0.66              |
| 1:a:8:ASP:OD1      | 20:n:126:TYR:OH    | 2.13                     | 0.66              |
| 3:c:93:THR:HG21    | 4:d:136:ASP:OD2    | 1.96                     | 0.66              |
| 6:e:250:ASP:OD1    | 6:e:270:TYR:OH     | 2.12                     | 0.65              |
| 5:E2:263:LEU:HD21  | 5:E2:321:ARG:HB2   | 1.78                     | 0.65              |
| 22:X1:70:GLY:O     | 22:X1:74:GLY:N     | 2.28                     | 0.65              |
| 6:e:62:ARG:NH2     | 28:e:402:CDL:OB4   | 2.30                     | 0.65              |
| 7:f:101:ARG:NH1    | 25:r:45:ASP:O      | 2.30                     | 0.65              |
| 7:f:101:ARG:NH2    | 18:m:124:PRO:O     | 2.30                     | 0.64              |
| 2:C1:419:ALA:HA    | 2:C1:532:THR:HG23  | 1.79                     | 0.64              |
| 1:A:150:ASN:HA     | 22:P2:106:LEU:HD13 | 1.78                     | 0.64              |
| 3:C:68:LYS:NZ      | 4:D:284:GLN:O      | 2.30                     | 0.64              |
| 22:P1:106:LEU:HD13 | 1:a:150:ASN:HA     | 1.80                     | 0.63              |
| 6:E:250:ASP:OD1    | 6:E:270:TYR:OH     | 2.11                     | 0.63              |
| 2:C2:419:ALA:HA    | 2:C2:532:THR:HG23  | 1.79                     | 0.63              |
| 6:E:62:ARG:NH2     | 28:E:404:CDL:OB4   | 2.31                     | 0.63              |
| 5:D2:260:GLN:N     | 5:D2:260:GLN:OE1   | 2.32                     | 0.63              |
| 5:D1:260:GLN:OE1   | 5:D1:260:GLN:N     | 2.32                     | 0.62              |
| 5:F2:486:VAL:HG21  | 5:F2:492:VAL:HG22  | 1.81                     | 0.62              |
| 2:B2:537:ILE:HD13  | 15:J2:142:VAL:HG22 | 1.81                     | 0.62              |
| 7:f:112:TYR:HB3    | 7:f:116:GLY:HA3    | 1.82                     | 0.62              |
| 7:F:101:ARG:NH1    | 25:R:45:ASP:O      | 2.31                     | 0.62              |
| 7:F:101:ARG:NH2    | 18:M:124:PRO:O     | 2.30                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:F1:486:VAL:HG21  | 5:F1:492:VAL:HG22  | 1.81                     | 0.62              |
| 14:J:128:LEU:HD21  | 14:J:142:LEU:HD12  | 1.82                     | 0.62              |
| 7:F:112:TYR:HB3    | 7:F:116:GLY:HA3    | 1.82                     | 0.61              |
| 1:A:194:PHE:CE1    | 22:O2:106:LEU:HD13 | 2.36                     | 0.61              |
| 22:O1:106:LEU:HD13 | 1:a:194:PHE:CE1    | 2.36                     | 0.61              |
| 2:B1:537:ILE:HD13  | 15:J1:142:VAL:HG22 | 1.81                     | 0.61              |
| 22:O2:84:PRO:O     | 22:O2:87:THR:HG23  | 2.01                     | 0.61              |
| 14:j:128:LEU:HD21  | 14:j:142:LEU:HD12  | 1.82                     | 0.60              |
| 7:F:64:ARG:NH2     | 25:R:33:GLU:OE2    | 2.33                     | 0.60              |
| 9:G1:134:SER:OG    | 13:I1:45:ARG:NH1   | 2.34                     | 0.60              |
| 1:A:208:LEU:HD21   | 22:P2:99:ALA:HB2   | 1.83                     | 0.60              |
| 22:O1:84:PRO:O     | 22:O1:87:THR:HG23  | 2.01                     | 0.60              |
| 3:c:61:VAL:HG13    | 4:d:278:VAL:HG11   | 1.84                     | 0.60              |
| 9:G2:134:SER:OG    | 13:I2:45:ARG:NH1   | 2.34                     | 0.59              |
| 22:T1:48:GLN:O     | 22:T1:51:HIS:ND1   | 2.36                     | 0.59              |
| 7:f:64:ARG:NH2     | 25:r:33:GLU:OE2    | 2.32                     | 0.59              |
| 5:D1:486:VAL:HG21  | 5:D1:492:VAL:HG22  | 1.85                     | 0.59              |
| 7:F:113:SER:OG     | 7:F:114:ALA:N      | 2.36                     | 0.59              |
| 8:G:44:ALA:N       | 8:G:241:GLU:OE2    | 2.36                     | 0.59              |
| 8:g:44:ALA:N       | 8:g:241:GLU:OE2    | 2.36                     | 0.59              |
| 22:T2:48:GLN:O     | 22:T2:51:HIS:ND1   | 2.36                     | 0.59              |
| 5:E2:68:ARG:NH1    | 5:E2:92:THR:O      | 2.36                     | 0.59              |
| 9:G1:97:VAL:HG12   | 9:G1:97:VAL:O      | 2.03                     | 0.59              |
| 3:c:68:LYS:NZ      | 4:d:284:GLN:O      | 2.31                     | 0.59              |
| 5:D2:486:VAL:HG21  | 5:D2:492:VAL:HG22  | 1.85                     | 0.58              |
| 9:G2:97:VAL:HG12   | 9:G2:97:VAL:O      | 2.03                     | 0.58              |
| 2:A1:457:ARG:NH2   | 2:A1:488:VAL:O     | 2.36                     | 0.58              |
| 6:E:185:ASN:ND2    | 6:E:325:ASP:OD1    | 2.35                     | 0.58              |
| 5:D2:347:ALA:HB3   | 5:D2:348:PRO:HD3   | 1.86                     | 0.58              |
| 3:C:61:VAL:HG13    | 4:D:278:VAL:HG11   | 1.86                     | 0.58              |
| 5:E1:68:ARG:NH1    | 5:E1:92:THR:O      | 2.36                     | 0.58              |
| 9:G2:195:ASN:OD1   | 9:G2:196:GLN:N     | 2.37                     | 0.58              |
| 9:G2:90:ILE:HD11   | 9:G2:162:ASN:HD21  | 1.69                     | 0.58              |
| 2:A2:457:ARG:NH2   | 2:A2:488:VAL:O     | 2.36                     | 0.57              |
| 5:D1:347:ALA:HB3   | 5:D1:348:PRO:HD3   | 1.85                     | 0.57              |
| 19:M1:250:GLU:OE1  | 4:d:194:ARG:NH1    | 2.38                     | 0.57              |
| 6:e:185:ASN:ND2    | 6:e:325:ASP:OD1    | 2.35                     | 0.57              |
| 5:F1:184:GLY:O     | 5:F1:189:LYS:NZ    | 2.38                     | 0.57              |
| 9:G1:195:ASN:OD1   | 9:G1:196:GLN:N     | 2.37                     | 0.56              |
| 2:A2:75:ALA:HB3    | 2:A2:78:THR:HG21   | 1.87                     | 0.56              |
| 4:D:194:ARG:NH1    | 19:M2:250:GLU:OE1  | 2.38                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:G1:90:ILE:HD11  | 9:G1:162:ASN:HD21  | 1.69                     | 0.56              |
| 22:P1:99:ALA:HB2  | 1:a:208:LEU:HD21   | 1.86                     | 0.56              |
| 10:h:128:GLU:HG2  | 10:h:149:ILE:HD11  | 1.87                     | 0.56              |
| 21:O:100:PHE:CE1  | 22:R2:48:GLN:HB2   | 2.41                     | 0.56              |
| 2:A1:75:ALA:HB3   | 2:A1:78:THR:HG21   | 1.87                     | 0.56              |
| 2:C1:246:ARG:NH1  | 5:F1:356:ASP:OD1   | 2.39                     | 0.56              |
| 5:F2:184:GLY:O    | 5:F2:189:LYS:NZ    | 2.38                     | 0.56              |
| 22:O1:98:PHE:CD1  | 22:X1:100:LEU:HD13 | 2.41                     | 0.56              |
| 22:S2:117:PHE:O   | 22:S2:118:SER:OG   | 2.20                     | 0.56              |
| 1:a:68:LEU:HD13   | 7:f:45:LEU:HD11    | 1.89                     | 0.55              |
| 5:D2:484:TYR:O    | 5:D2:495:LYS:NZ    | 2.40                     | 0.55              |
| 22:O2:98:PHE:CD1  | 22:X2:100:LEU:HD13 | 2.41                     | 0.55              |
| 1:A:68:LEU:HD13   | 7:F:45:LEU:HD11    | 1.88                     | 0.55              |
| 8:G:155:LYS:O     | 8:G:159:THR:HG22   | 2.07                     | 0.55              |
| 5:D1:484:TYR:O    | 5:D1:495:LYS:NZ    | 2.39                     | 0.55              |
| 10:H:128:GLU:HG2  | 10:H:149:ILE:HD11  | 1.87                     | 0.55              |
| 17:l:66:GLN:HG3   | 17:l:68:VAL:HG23   | 1.89                     | 0.55              |
| 17:L:66:GLN:HG3   | 17:L:68:VAL:HG23   | 1.89                     | 0.55              |
| 13:I1:57:ASP:OD1  | 13:I1:61:GLY:N     | 2.40                     | 0.54              |
| 7:f:113:SER:OG    | 7:f:114:ALA:N      | 2.36                     | 0.54              |
| 2:C2:246:ARG:NH1  | 5:F2:356:ASP:OD1   | 2.39                     | 0.54              |
| 9:G1:156:ARG:NH2  | 9:G1:158:GLN:OE1   | 2.41                     | 0.54              |
| 13:I2:57:ASP:OD1  | 13:I2:61:GLY:N     | 2.40                     | 0.54              |
| 15:J2:58:LEU:O    | 15:J2:62:ASN:ND2   | 2.40                     | 0.54              |
| 22:R1:48:GLN:HB2  | 21:o:100:PHE:CE1   | 2.43                     | 0.54              |
| 8:g:155:LYS:O     | 8:g:159:THR:HG22   | 2.07                     | 0.54              |
| 5:E2:130:ASP:O    | 15:L2:32:TYR:OH    | 2.26                     | 0.54              |
| 15:J1:58:LEU:O    | 15:J1:62:ASN:ND2   | 2.40                     | 0.54              |
| 8:g:58:ALA:HB3    | 8:g:80:ARG:HB3     | 1.90                     | 0.54              |
| 5:E1:130:ASP:O    | 15:L1:32:TYR:OH    | 2.26                     | 0.53              |
| 5:E2:302:PRO:HD2  | 9:G2:279:LEU:HD11  | 1.91                     | 0.53              |
| 3:c:40:TRP:O      | 3:c:43:VAL:HG12    | 2.09                     | 0.53              |
| 8:G:58:ALA:HB3    | 8:G:80:ARG:HB3     | 1.90                     | 0.53              |
| 1:A:26:LEU:HD22   | 7:F:43:TRP:CZ2     | 2.45                     | 0.52              |
| 14:j:54:TYR:O     | 14:j:92:ARG:NH1    | 2.40                     | 0.52              |
| 2:B2:328:ARG:NH2  | 5:F2:345:ASP:OD1   | 2.42                     | 0.52              |
| 5:E2:174:CYS:HB3  | 5:E2:383:ILE:HG21  | 1.91                     | 0.52              |
| 8:G:59:VAL:HG13   | 8:G:216:VAL:HB     | 1.92                     | 0.52              |
| 1:a:26:LEU:HD22   | 7:f:43:TRP:CZ2     | 2.45                     | 0.52              |
| 2:B1:328:ARG:NH2  | 5:F1:345:ASP:OD1   | 2.42                     | 0.52              |
| 2:B2:532:THR:HG23 | 2:B2:535:SER:N     | 2.25                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:D:291:GLU:O     | 4:D:295:LEU:N      | 2.43                     | 0.52              |
| 8:g:59:VAL:HG13   | 8:g:216:VAL:HB     | 1.92                     | 0.52              |
| 5:E2:442:GLN:NE2  | 5:E2:456:HIS:O     | 2.42                     | 0.52              |
| 9:G2:156:ARG:NH2  | 9:G2:158:GLN:OE1   | 2.41                     | 0.52              |
| 1:A:93:TYR:CE2    | 1:A:220:LEU:HD22   | 2.45                     | 0.52              |
| 9:G1:16:ASN:OD1   | 9:G1:256:GLN:NE2   | 2.43                     | 0.52              |
| 9:G2:16:ASN:OD1   | 9:G2:256:GLN:NE2   | 2.43                     | 0.52              |
| 2:B2:203:LEU:HD13 | 2:B2:379:VAL:HG11  | 1.92                     | 0.52              |
| 5:F1:178:LYS:NZ   | 5:F1:319:GLN:O     | 2.43                     | 0.52              |
| 22:O2:83:GLN:OE1  | 22:O2:85:ASN:ND2   | 2.42                     | 0.52              |
| 2:B1:532:THR:HG23 | 2:B1:535:SER:N     | 2.25                     | 0.51              |
| 1:A:231:VAL:O     | 6:E:170:TRP:NE1    | 2.43                     | 0.51              |
| 2:B2:457:ARG:NH2  | 2:B2:488:VAL:O     | 2.41                     | 0.51              |
| 5:F2:178:LYS:NZ   | 5:F2:319:GLN:O     | 2.43                     | 0.51              |
| 5:E1:302:PRO:HD2  | 9:G1:279:LEU:HD11  | 1.90                     | 0.51              |
| 22:X2:65:VAL:HG13 | 22:X2:101:THR:HG22 | 1.93                     | 0.51              |
| 5:E1:174:CYS:HB3  | 5:E1:383:ILE:HG21  | 1.91                     | 0.51              |
| 5:E1:389:ILE:HD12 | 5:E1:393:HIS:ND1   | 2.26                     | 0.51              |
| 5:E1:442:GLN:NE2  | 5:E1:456:HIS:O     | 2.42                     | 0.51              |
| 2:B1:203:LEU:HD13 | 2:B1:379:VAL:HG11  | 1.92                     | 0.51              |
| 4:D:145:ARG:HD2   | 4:D:145:ARG:O      | 2.11                     | 0.51              |
| 22:P1:86:LEU:HD11 | 22:Q1:84:PRO:HB3   | 1.93                     | 0.51              |
| 22:X1:65:VAL:HG13 | 22:X1:101:THR:HG22 | 1.93                     | 0.51              |
| 34:H2:201:UTP:O2G | 22:V2:82:ARG:NH1   | 2.43                     | 0.51              |
| 22:P1:99:ALA:CB   | 1:a:212:ILE:HD11   | 2.41                     | 0.51              |
| 24:q:77:GLU:OE2   | 24:q:79:HIS:NE2    | 2.44                     | 0.51              |
| 5:D2:448:GLU:O    | 5:D2:452:GLY:N     | 2.38                     | 0.51              |
| 24:Q:77:GLU:OE2   | 24:Q:79:HIS:NE2    | 2.44                     | 0.51              |
| 1:a:231:VAL:O     | 6:e:170:TRP:NE1    | 2.42                     | 0.51              |
| 2:B1:52:ILE:C     | 2:B1:52:ILE:HD12   | 2.37                     | 0.50              |
| 11:H1:61:LEU:N    | 11:H1:61:LEU:HD12  | 2.26                     | 0.50              |
| 10:H:85:THR:HG22  | 10:H:85:THR:O      | 2.11                     | 0.50              |
| 22:Q1:55:THR:HG23 | 22:Q1:112:ALA:HB1  | 1.93                     | 0.50              |
| 15:K2:45:ILE:HG13 | 15:K2:57:VAL:HG11  | 1.94                     | 0.50              |
| 4:d:145:ARG:HD2   | 4:d:145:ARG:O      | 2.11                     | 0.50              |
| 1:A:157:LEU:HD22  | 22:O2:107:PHE:CD1  | 2.46                     | 0.50              |
| 2:B1:199:GLY:N    | 2:B1:357:SER:OG    | 2.45                     | 0.50              |
| 2:B2:199:GLY:N    | 2:B2:357:SER:OG    | 2.45                     | 0.50              |
| 2:C2:515:LYS:O    | 15:K2:134:ARG:NH1  | 2.43                     | 0.50              |
| 10:h:85:THR:O     | 10:h:85:THR:HG22   | 2.11                     | 0.50              |
| 2:A2:292:GLU:O    | 2:A2:296:ASN:ND2   | 2.42                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:C:99:LEU:O      | 3:C:101:GLN:NE2    | 2.45                     | 0.50              |
| 5:E2:389:ILE:HD12 | 5:E2:393:HIS:ND1   | 2.26                     | 0.50              |
| 14:J:54:TYR:O     | 14:J:92:ARG:NH1    | 2.40                     | 0.50              |
| 2:B2:523:GLU:CB   | 15:J2:135:LEU:HD11 | 2.42                     | 0.50              |
| 5:D1:91:GLN:OE1   | 5:D1:91:GLN:N      | 2.45                     | 0.50              |
| 15:K1:45:ILE:HG13 | 15:K1:57:VAL:HG11  | 1.94                     | 0.50              |
| 5:E1:342:ASP:OD2  | 9:G1:268:GLN:NE2   | 2.43                     | 0.50              |
| 1:a:93:TYR:CE2    | 1:a:220:LEU:HD22   | 2.45                     | 0.50              |
| 2:B1:203:LEU:HD13 | 2:B1:379:VAL:CG1   | 2.42                     | 0.50              |
| 11:H2:61:LEU:N    | 11:H2:61:LEU:HD12  | 2.26                     | 0.50              |
| 2:A1:327:GLY:N    | 2:A1:331:TYR:O     | 2.43                     | 0.49              |
| 2:C1:225:ARG:NH2  | 2:C1:522:GLN:OE1   | 2.45                     | 0.49              |
| 6:E:229:MET:SD    | 6:E:235:ASN:ND2    | 2.84                     | 0.49              |
| 2:B2:203:LEU:HD13 | 2:B2:379:VAL:CG1   | 2.42                     | 0.49              |
| 19:M1:162:HIS:NE2 | 19:M1:168:LEU:O    | 2.39                     | 0.49              |
| 22:X1:48:GLN:O    | 22:X1:51:HIS:ND1   | 2.43                     | 0.49              |
| 5:D2:91:GLN:N     | 5:D2:91:GLN:OE1    | 2.45                     | 0.49              |
| 22:Q2:55:THR:HG23 | 22:Q2:112:ALA:HB1  | 1.93                     | 0.49              |
| 22:Q2:65:VAL:HG13 | 22:Q2:101:THR:HG22 | 1.93                     | 0.49              |
| 2:B2:52:ILE:HD12  | 2:B2:52:ILE:C      | 2.37                     | 0.49              |
| 5:F1:270:ARG:NH1  | 5:F1:323:THR:O     | 2.42                     | 0.49              |
| 22:O1:107:PHE:CD1 | 1:a:157:LEU:HD22   | 2.47                     | 0.49              |
| 22:X2:48:GLN:O    | 22:X2:51:HIS:ND1   | 2.44                     | 0.49              |
| 8:g:5:LEU:HD21    | 8:g:245:LEU:HD11   | 1.94                     | 0.49              |
| 23:p:66:ASP:OD2   | 25:r:10:ARG:NH1    | 2.46                     | 0.49              |
| 2:B1:523:GLU:CB   | 15:J1:135:LEU:HD11 | 2.42                     | 0.49              |
| 2:B2:514:ASN:O    | 2:B2:518:TYR:OH    | 2.17                     | 0.49              |
| 4:d:291:GLU:O     | 4:d:295:LEU:N      | 2.43                     | 0.49              |
| 2:B1:173:ILE:HG23 | 2:B1:174:VAL:HG13  | 1.95                     | 0.49              |
| 22:Q1:65:VAL:HG13 | 22:Q1:101:THR:HG22 | 1.93                     | 0.49              |
| 9:G1:95:ASP:O     | 9:G1:98:VAL:HG23   | 2.12                     | 0.49              |
| 4:D:280:ILE:HD12  | 4:D:280:ILE:O      | 2.13                     | 0.49              |
| 5:E2:342:ASP:OD2  | 9:G2:268:GLN:NE2   | 2.43                     | 0.49              |
| 8:G:5:LEU:HD21    | 8:G:245:LEU:HD11   | 1.94                     | 0.49              |
| 11:H1:39:ASP:OD1  | 11:H1:39:ASP:N     | 2.45                     | 0.49              |
| 15:K2:174:GLY:N   | 19:M2:229:ASP:OD2  | 2.44                     | 0.49              |
| 4:d:280:ILE:O     | 4:d:280:ILE:HD12   | 2.13                     | 0.49              |
| 13:I1:70:ILE:N    | 13:I1:70:ILE:HD12  | 2.28                     | 0.48              |
| 2:B2:173:ILE:HG23 | 2:B2:174:VAL:HG13  | 1.95                     | 0.48              |
| 9:G2:95:ASP:O     | 9:G2:98:VAL:HG23   | 2.13                     | 0.48              |
| 22:P2:86:LEU:HD11 | 22:Q2:84:PRO:HB3   | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:S1:117:PHE:O   | 22:S1:118:SER:OG  | 2.20                     | 0.48              |
| 3:C:110:ARG:NH2   | 8:G:98:ASP:OD2    | 2.46                     | 0.48              |
| 4:D:324:ASN:HB2   | 4:D:325:PRO:HD3   | 1.96                     | 0.48              |
| 34:H1:201:UTP:O2G | 22:V1:82:ARG:NH1  | 2.43                     | 0.48              |
| 3:c:110:ARG:NH2   | 8:g:98:ASP:OD2    | 2.46                     | 0.48              |
| 4:d:324:ASN:HB2   | 4:d:325:PRO:HD3   | 1.96                     | 0.48              |
| 1:A:212:ILE:HD11  | 22:P2:99:ALA:CB   | 2.44                     | 0.48              |
| 2:B2:232:SER:OG   | 15:J2:52:ASP:OD1  | 2.26                     | 0.48              |
| 5:D2:263:LEU:HD21 | 5:D2:321:ARG:HB2  | 1.96                     | 0.48              |
| 5:E2:301:ILE:HG23 | 9:G2:279:LEU:HD13 | 1.96                     | 0.48              |
| 13:I2:70:ILE:N    | 13:I2:70:ILE:HD12 | 2.28                     | 0.48              |
| 1:a:93:TYR:CD2    | 1:a:220:LEU:HD22  | 2.48                     | 0.48              |
| 1:A:166:TYR:OH    | 33:F:204:PC1:O12  | 2.25                     | 0.48              |
| 17:l:10:LEU:HD13  | 18:m:83:ILE:HD11  | 1.95                     | 0.48              |
| 5:E1:301:ILE:HG23 | 9:G1:279:LEU:HD13 | 1.96                     | 0.48              |
| 23:P:66:ASP:OD2   | 25:R:10:ARG:NH1   | 2.44                     | 0.48              |
| 17:L:10:LEU:HD13  | 18:M:83:ILE:HD11  | 1.96                     | 0.48              |
| 2:B1:141:ASN:OD1  | 2:B1:145:HIS:N    | 2.47                     | 0.48              |
| 24:q:49:ALA:N     | 24:q:50:PRO:CD    | 2.77                     | 0.48              |
| 1:A:93:TYR:CD2    | 1:A:220:LEU:HD22  | 2.48                     | 0.48              |
| 2:A1:292:GLU:O    | 2:A1:296:ASN:ND2  | 2.42                     | 0.48              |
| 2:C2:514:ASN:O    | 2:C2:518:TYR:OH   | 2.30                     | 0.48              |
| 2:B2:141:ASN:OD1  | 2:B2:145:HIS:N    | 2.47                     | 0.47              |
| 5:E1:55:PRO:O     | 5:E1:58:THR:OG1   | 2.30                     | 0.47              |
| 22:O2:102:GLU:O   | 22:O2:106:LEU:HG  | 2.14                     | 0.47              |
| 12:i:62:ARG:NH2   | 20:n:134:SER:O    | 2.46                     | 0.47              |
| 6:E:26:THR:HG23   | 6:E:91:TYR:OH     | 2.15                     | 0.47              |
| 12:I:87:PRO:O     | 12:I:91:GLY:N     | 2.40                     | 0.47              |
| 2:B1:457:ARG:NH2  | 2:B1:488:VAL:O    | 2.41                     | 0.47              |
| 5:D1:263:LEU:HD21 | 5:D1:321:ARG:HB2  | 1.96                     | 0.47              |
| 12:I:88:LYS:O     | 21:O:32:GLN:NE2   | 2.46                     | 0.47              |
| 22:P2:87:THR:HG23 | 22:P2:88:LYS:N    | 2.29                     | 0.47              |
| 22:O1:102:GLU:O   | 22:O1:106:LEU:HG  | 2.14                     | 0.47              |
| 6:e:229:MET:SD    | 6:e:235:ASN:ND2   | 2.84                     | 0.47              |
| 10:H:38:LYS:N     | 19:M2:215:THR:O   | 2.47                     | 0.47              |
| 19:M1:215:THR:O   | 10:h:38:LYS:N     | 2.47                     | 0.47              |
| 2:A2:327:GLY:N    | 2:A2:331:TYR:O    | 2.43                     | 0.47              |
| 2:C2:225:ARG:NH2  | 2:C2:522:GLN:OE1  | 2.45                     | 0.47              |
| 5:F1:41:ILE:HG23  | 5:F1:41:ILE:O     | 2.15                     | 0.47              |
| 11:H2:39:ASP:N    | 11:H2:39:ASP:OD1  | 2.45                     | 0.47              |
| 12:I:16:LEU:O     | 12:I:20:THR:HG22  | 2.15                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:P1:99:ALA:HB1  | 1:a:212:ILE:CD1   | 2.45                     | 0.47              |
| 6:e:26:THR:HG23   | 6:e:91:TYR:OH     | 2.15                     | 0.47              |
| 12:i:88:LYS:O     | 21:o:32:GLN:NE2   | 2.46                     | 0.47              |
| 5:E2:308:GLN:OE1  | 5:E2:308:GLN:N    | 2.40                     | 0.47              |
| 22:P1:87:THR:HG23 | 22:P1:88:LYS:N    | 2.30                     | 0.47              |
| 24:Q:49:ALA:N     | 24:Q:50:PRO:CD    | 2.77                     | 0.47              |
| 5:F2:41:ILE:HG23  | 5:F2:41:ILE:O     | 2.15                     | 0.47              |
| 2:A2:167:ASP:OD1  | 2:A2:167:ASP:N    | 2.48                     | 0.47              |
| 2:B2:514:ASN:ND2  | 2:B2:541:GLU:O    | 2.47                     | 0.47              |
| 15:J2:86:LYS:HD2  | 15:J2:91:VAL:HG21 | 1.97                     | 0.47              |
| 2:C1:515:LYS:O    | 15:K1:134:ARG:NH1 | 2.43                     | 0.46              |
| 15:J1:45:ILE:HG13 | 15:J1:57:VAL:HG11 | 1.97                     | 0.46              |
| 12:i:16:LEU:O     | 12:i:20:THR:HG22  | 2.15                     | 0.46              |
| 2:C1:203:LEU:HD13 | 2:C1:379:VAL:CG1  | 2.45                     | 0.46              |
| 20:N:154:GLU:OE1  | 20:N:154:GLU:N    | 2.44                     | 0.46              |
| 3:C:30:GLU:N      | 3:C:31:PRO:CD     | 2.79                     | 0.46              |
| 2:C1:62:ILE:HD12  | 2:C1:62:ILE:C     | 2.41                     | 0.46              |
| 2:C2:523:GLU:OE1  | 2:C2:523:GLU:N    | 2.48                     | 0.46              |
| 2:A1:167:ASP:OD1  | 2:A1:167:ASP:N    | 2.48                     | 0.46              |
| 9:G2:208:ASN:OD1  | 22:R2:82:ARG:NH2  | 2.44                     | 0.46              |
| 16:k:29:GLU:N     | 16:k:29:GLU:OE1   | 2.49                     | 0.46              |
| 2:A2:524:LEU:HD23 | 2:A2:527:LEU:HD12 | 1.97                     | 0.46              |
| 2:C2:203:LEU:HD13 | 2:C2:379:VAL:CG1  | 2.45                     | 0.46              |
| 3:c:30:GLU:N      | 3:c:31:PRO:CD     | 2.79                     | 0.46              |
| 20:n:154:GLU:OE1  | 20:n:154:GLU:N    | 2.44                     | 0.46              |
| 5:E1:179:ILE:N    | 5:E1:179:ILE:HD12 | 2.31                     | 0.46              |
| 16:K:29:GLU:OE1   | 16:K:29:GLU:N     | 2.49                     | 0.46              |
| 15:K1:174:GLY:N   | 19:M1:229:ASP:OD2 | 2.44                     | 0.46              |
| 22:O1:83:GLN:OE1  | 22:O1:85:ASN:ND2  | 2.42                     | 0.46              |
| 2:A1:524:LEU:HD23 | 2:A1:527:LEU:HD12 | 1.97                     | 0.46              |
| 9:G1:208:ASN:OD1  | 22:R1:82:ARG:NH2  | 2.44                     | 0.46              |
| 12:I:62:ARG:NH2   | 20:N:134:SER:O    | 2.46                     | 0.46              |
| 2:C1:531:PHE:O    | 2:C1:532:THR:CB   | 2.64                     | 0.46              |
| 5:F2:270:ARG:NH1  | 5:F2:323:THR:O    | 2.42                     | 0.46              |
| 15:J1:86:LYS:HD2  | 15:J1:91:VAL:HG21 | 1.97                     | 0.46              |
| 15:J2:45:ILE:HG13 | 15:J2:57:VAL:HG11 | 1.97                     | 0.46              |
| 2:C1:523:GLU:OE1  | 2:C1:523:GLU:N    | 2.48                     | 0.46              |
| 5:F1:282:ASP:HA   | 5:F1:283:ASN:HA   | 1.82                     | 0.46              |
| 4:D:354:ARG:HG3   | 9:G2:61:ARG:HH22  | 1.81                     | 0.45              |
| 5:D2:270:ARG:NH1  | 5:D2:323:THR:O    | 2.44                     | 0.45              |
| 5:D2:282:ASP:HA   | 5:D2:283:ASN:HA   | 1.82                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 5:F2:263:LEU:HD21  | 5:F2:321:ARG:HB2  | 1.98                     | 0.45              |
| 8:G:55:VAL:HG12    | 8:G:219:THR:HG22  | 1.99                     | 0.45              |
| 2:A2:61:THR:HG22   | 2:A2:111:ILE:CD1  | 2.47                     | 0.45              |
| 2:B2:234:ASN:ND2   | 15:J2:102:ASP:OD2 | 2.48                     | 0.45              |
| 2:C2:62:ILE:HD12   | 2:C2:62:ILE:C     | 2.41                     | 0.45              |
| 2:C2:168:THR:OG1   | 2:C2:345:ARG:NH2  | 2.50                     | 0.45              |
| 22:P1:55:THR:HG23  | 22:P1:112:ALA:HB1 | 1.99                     | 0.45              |
| 3:c:43:VAL:HG13    | 3:c:44:TRP:N      | 2.31                     | 0.45              |
| 1:A:9:LEU:HD11     | 1:A:66:PHE:CE2    | 2.52                     | 0.45              |
| 2:C2:531:PHE:O     | 2:C2:532:THR:CB   | 2.64                     | 0.45              |
| 9:G1:61:ARG:HH22   | 4:d:354:ARG:HG3   | 1.82                     | 0.45              |
| 2:A2:77:ASN:O      | 2:A2:77:ASN:ND2   | 2.50                     | 0.45              |
| 5:E1:436:LEU:HD23  | 5:E1:470:LEU:HD23 | 1.98                     | 0.45              |
| 15:K2:70:ILE:O     | 15:K2:74:ASN:ND2  | 2.48                     | 0.45              |
| 2:A1:234:ASN:ND2   | 15:L1:102:ASP:OD2 | 2.44                     | 0.45              |
| 2:B1:514:ASN:ND2   | 2:B1:541:GLU:O    | 2.47                     | 0.45              |
| 2:C1:168:THR:OG1   | 2:C1:345:ARG:NH2  | 2.50                     | 0.45              |
| 5:D2:305:VAL:HG21  | 5:D2:346:PRO:CD   | 2.47                     | 0.45              |
| 5:F1:263:LEU:HD21  | 5:F1:321:ARG:HB2  | 1.98                     | 0.45              |
| 22:P2:87:THR:HG23  | 22:P2:88:LYS:H    | 1.82                     | 0.45              |
| 22:S2:86:LEU:HD22  | 22:T2:84:PRO:HB3  | 1.99                     | 0.45              |
| 5:D1:288:THR:HG23  | 5:D1:311:LEU:HD13 | 1.99                     | 0.45              |
| 5:D2:470:LEU:HD23  | 5:D2:470:LEU:O    | 2.17                     | 0.45              |
| 5:E2:179:ILE:HD12  | 5:E2:179:ILE:N    | 2.31                     | 0.45              |
| 3:c:92:TYR:O       | 3:c:92:TYR:CD1    | 2.70                     | 0.45              |
| 2:B1:80:ILE:HD12   | 2:B1:80:ILE:C     | 2.42                     | 0.44              |
| 18:M:88:TYR:O      | 18:M:91:GLN:NE2   | 2.50                     | 0.44              |
| 22:O1:106:LEU:HD22 | 1:a:194:PHE:CE1   | 2.53                     | 0.44              |
| 3:c:95:TRP:HZ2     | 4:d:136:ASP:OD1   | 2.00                     | 0.44              |
| 4:D:218:ARG:HG3    | 4:D:218:ARG:O     | 2.18                     | 0.44              |
| 5:E2:244:VAL:HG12  | 5:E2:258:VAL:HG23 | 1.99                     | 0.44              |
| 22:R1:86:LEU:HD11  | 22:S1:84:PRO:HB3  | 2.00                     | 0.44              |
| 5:D2:130:ASP:O     | 15:K2:32:TYR:OH   | 2.30                     | 0.44              |
| 2:A1:61:THR:HG22   | 2:A1:111:ILE:CD1  | 2.47                     | 0.44              |
| 3:C:95:TRP:HZ2     | 4:D:136:ASP:OD1   | 2.00                     | 0.44              |
| 5:D1:470:LEU:HD23  | 5:D1:470:LEU:O    | 2.17                     | 0.44              |
| 9:G2:186:ASP:OD1   | 9:G2:196:GLN:NE2  | 2.40                     | 0.44              |
| 22:P2:55:THR:HG23  | 22:P2:112:ALA:HB1 | 1.99                     | 0.44              |
| 22:S1:86:LEU:HD22  | 22:T1:84:PRO:HB3  | 1.99                     | 0.44              |
| 4:d:268:PRO:HB2    | 6:e:327:ALA:HB3   | 2.00                     | 0.44              |
| 2:A1:77:ASN:O      | 2:A1:77:ASN:ND2   | 2.50                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:B2:111:ILE:HD12 | 2:B2:276:PRO:HB3   | 1.99                     | 0.44              |
| 2:C1:457:ARG:NE   | 2:C1:485:LEU:O     | 2.50                     | 0.44              |
| 5:E2:436:LEU:HD23 | 5:E2:470:LEU:HD23  | 1.98                     | 0.44              |
| 8:G:196:VAL:HG12  | 8:G:197:ALA:N      | 2.33                     | 0.44              |
| 4:d:218:ARG:HG3   | 4:d:218:ARG:O      | 2.18                     | 0.44              |
| 5:D1:130:ASP:O    | 15:K1:32:TYR:OH    | 2.30                     | 0.44              |
| 5:D1:305:VAL:HG21 | 5:D1:346:PRO:CD    | 2.47                     | 0.44              |
| 5:D1:448:GLU:O    | 5:D1:452:GLY:N     | 2.38                     | 0.44              |
| 11:H1:97:LEU:C    | 11:H1:97:LEU:HD23  | 2.42                     | 0.44              |
| 11:H2:97:LEU:C    | 11:H2:97:LEU:HD23  | 2.42                     | 0.44              |
| 2:A2:65:LEU:HD22  | 2:A2:120:VAL:HG21  | 2.00                     | 0.44              |
| 2:C2:52:ILE:C     | 2:C2:52:ILE:HD12   | 2.42                     | 0.44              |
| 22:P1:87:THR:HG23 | 22:P1:88:LYS:H     | 1.82                     | 0.44              |
| 1:a:9:LEU:HD11    | 1:a:66:PHE:CE2     | 2.52                     | 0.44              |
| 2:C1:52:ILE:HD12  | 2:C1:52:ILE:C      | 2.42                     | 0.44              |
| 5:D1:270:ARG:NH1  | 5:D1:323:THR:O     | 2.44                     | 0.44              |
| 5:E2:486:VAL:HG21 | 5:E2:492:VAL:HG22  | 2.00                     | 0.44              |
| 2:A1:269:MET:SD   | 2:A1:286:ALA:HB3   | 2.58                     | 0.44              |
| 2:A2:269:MET:SD   | 2:A2:286:ALA:HB3   | 2.58                     | 0.44              |
| 2:B2:80:ILE:C     | 2:B2:80:ILE:HD12   | 2.42                     | 0.44              |
| 2:C2:166:VAL:O    | 2:C2:166:VAL:HG12  | 2.18                     | 0.44              |
| 5:E2:282:ASP:HA   | 5:E2:283:ASN:HA    | 1.85                     | 0.44              |
| 22:R2:86:LEU:HD11 | 22:S2:84:PRO:HB3   | 2.00                     | 0.44              |
| 2:A1:131:VAL:HG11 | 2:A1:293:TYR:HB2   | 2.00                     | 0.43              |
| 5:E2:484:TYR:O    | 5:E2:495:LYS:NZ    | 2.50                     | 0.43              |
| 8:G:96:ALA:HA     | 8:G:99:VAL:HG12    | 2.00                     | 0.43              |
| 8:G:174:THR:HG23  | 8:G:175:ALA:N      | 2.33                     | 0.43              |
| 2:B2:323:ARG:HA   | 5:E2:301:ILE:HD12  | 1.99                     | 0.43              |
| 3:C:49:PHE:O      | 12:I:15:GLN:NE2    | 2.50                     | 0.43              |
| 28:C:201:CDL:H872 | 28:C:201:CDL:H832  | 2.00                     | 0.43              |
| 5:D2:263:LEU:HD21 | 5:D2:321:ARG:CB    | 2.48                     | 0.43              |
| 15:J2:138:CYS:O   | 15:J2:142:VAL:HG23 | 2.18                     | 0.43              |
| 8:g:55:VAL:HG12   | 8:g:219:THR:HG22   | 1.99                     | 0.43              |
| 8:g:96:ALA:HA     | 8:g:99:VAL:HG12    | 2.00                     | 0.43              |
| 8:g:174:THR:HG23  | 8:g:175:ALA:N      | 2.33                     | 0.43              |
| 10:h:24:MET:SD    | 10:h:24:MET:N      | 2.91                     | 0.43              |
| 5:D2:288:THR:HG23 | 5:D2:311:LEU:HD13  | 1.99                     | 0.43              |
| 28:e:402:CDL:H151 | 28:j:202:CDL:H872  | 2.01                     | 0.43              |
| 2:B1:323:ARG:HA   | 5:E1:301:ILE:HD12  | 1.99                     | 0.43              |
| 5:D1:263:LEU:HD21 | 5:D1:321:ARG:CB    | 2.48                     | 0.43              |
| 28:E:404:CDL:H151 | 28:J:203:CDL:H872  | 2.01                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 16:K:103:MET:HE1  | 24:Q:80:LEU:HA     | 2.01                     | 0.43              |
| 22:O1:70:GLY:HA2  | 22:X1:72:ILE:HD11  | 2.01                     | 0.43              |
| 2:A1:217:VAL:HG11 | 2:A1:256:LEU:HD23  | 2.01                     | 0.43              |
| 2:A2:61:THR:HG21  | 5:D2:313:GLU:OE2   | 2.19                     | 0.43              |
| 4:D:268:PRO:HB2   | 6:E:327:ALA:HB3    | 2.00                     | 0.43              |
| 5:E1:244:VAL:HG12 | 5:E1:258:VAL:HG23  | 1.99                     | 0.43              |
| 5:F2:75:GLU:OE2   | 5:F2:144:HIS:NE2   | 2.49                     | 0.43              |
| 15:J1:181:GLY:O   | 15:J1:185:VAL:HG23 | 2.19                     | 0.43              |
| 1:A:212:ILE:CD1   | 22:P2:99:ALA:HB1   | 2.48                     | 0.43              |
| 2:A1:537:ILE:HD12 | 2:A1:537:ILE:N     | 2.34                     | 0.43              |
| 2:A2:131:VAL:HG11 | 2:A2:293:TYR:HB2   | 2.00                     | 0.43              |
| 5:E1:484:TYR:O    | 5:E1:495:LYS:NZ    | 2.49                     | 0.43              |
| 8:G:151:ASN:OD1   | 8:G:152:GLU:N      | 2.52                     | 0.43              |
| 14:J:30:GLU:OE1   | 24:Q:72:ASN:ND2    | 2.50                     | 0.43              |
| 28:e:402:CDL:H861 | 28:e:403:CDL:H673  | 2.01                     | 0.43              |
| 12:i:87:PRO:O     | 12:i:91:GLY:N      | 2.40                     | 0.43              |
| 2:B1:111:ILE:HD12 | 2:B1:276:PRO:HB3   | 1.99                     | 0.43              |
| 2:C2:531:PHE:O    | 2:C2:532:THR:HB    | 2.19                     | 0.43              |
| 6:E:371:THR:HG23  | 23:P:64:PRO:CG     | 2.49                     | 0.43              |
| 10:H:24:MET:SD    | 10:H:24:MET:N      | 2.91                     | 0.43              |
| 15:J1:138:CYS:O   | 15:J1:142:VAL:HG23 | 2.18                     | 0.43              |
| 2:C1:166:VAL:HG12 | 2:C1:166:VAL:O     | 2.18                     | 0.43              |
| 2:C1:531:PHE:O    | 2:C1:532:THR:HB    | 2.19                     | 0.43              |
| 5:F2:91:GLN:N     | 5:F2:91:GLN:OE1    | 2.52                     | 0.43              |
| 5:F2:267:GLU:OE2  | 5:F2:321:ARG:NE    | 2.43                     | 0.43              |
| 19:M2:90:VAL:CG2  | 19:M2:108:VAL:HG22 | 2.49                     | 0.43              |
| 2:A1:61:THR:HG21  | 5:D1:313:GLU:OE2   | 2.19                     | 0.43              |
| 2:A2:217:VAL:HG11 | 2:A2:256:LEU:HD23  | 2.01                     | 0.43              |
| 8:G:56:HIS:NE2    | 8:G:219:THR:O      | 2.52                     | 0.43              |
| 9:G1:186:ASP:OD1  | 9:G1:196:GLN:NE2   | 2.40                     | 0.43              |
| 9:G2:48:ARG:HB3   | 11:H2:35:VAL:HG22  | 2.01                     | 0.43              |
| 15:L2:45:ILE:HG13 | 15:L2:57:VAL:HG11  | 2.01                     | 0.43              |
| 21:o:86:TYR:O     | 21:o:91:ARG:NE     | 2.52                     | 0.43              |
| 2:A1:288:VAL:O    | 2:A1:292:GLU:N     | 2.46                     | 0.42              |
| 5:E1:486:VAL:HG21 | 5:E1:492:VAL:HG22  | 2.00                     | 0.42              |
| 5:E2:55:PRO:O     | 5:E2:58:THR:OG1    | 2.30                     | 0.42              |
| 5:F1:91:GLN:OE1   | 5:F1:91:GLN:N      | 2.52                     | 0.42              |
| 15:L2:28:ASP:OD1  | 15:L2:32:TYR:N     | 2.44                     | 0.42              |
| 28:c:201:CDL:H872 | 28:c:201:CDL:H832  | 2.00                     | 0.42              |
| 6:e:371:THR:HG23  | 23:p:64:PRO:CG     | 2.49                     | 0.42              |
| 8:g:196:VAL:HG12  | 8:g:197:ALA:N      | 2.33                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:160:MET:HE2    | 22:O2:114:LEU:HD13 | 2.02                     | 0.42              |
| 2:A1:65:LEU:HD22   | 2:A1:120:VAL:HG21  | 2.00                     | 0.42              |
| 2:B1:52:ILE:HD13   | 2:B1:74:VAL:HG21   | 2.01                     | 0.42              |
| 2:C2:457:ARG:NE    | 2:C2:485:LEU:O     | 2.50                     | 0.42              |
| 4:D:324:ASN:CB     | 4:D:325:PRO:HD3    | 2.49                     | 0.42              |
| 5:D1:180:GLY:HA3   | 5:D1:355:LEU:HD13  | 2.01                     | 0.42              |
| 5:D2:438:LYS:NZ    | 5:D2:481:MET:SD    | 2.85                     | 0.42              |
| 7:F:56:ILE:HB      | 7:F:57:PRO:HD3     | 2.01                     | 0.42              |
| 5:F1:150:LEU:HD23  | 5:F1:150:LEU:O     | 2.19                     | 0.42              |
| 15:J2:36:THR:HG22  | 15:J2:36:THR:O     | 2.20                     | 0.42              |
| 8:g:151:ASN:OD1    | 8:g:152:GLU:N      | 2.52                     | 0.42              |
| 5:E1:308:GLN:OE1   | 5:E1:308:GLN:N     | 2.40                     | 0.42              |
| 12:i:17:LYS:HA     | 12:i:20:THR:HG22   | 2.01                     | 0.42              |
| 2:A2:234:ASN:ND2   | 15:L2:102:ASP:OD2  | 2.44                     | 0.42              |
| 2:A2:537:ILE:HD12  | 2:A2:537:ILE:N     | 2.34                     | 0.42              |
| 2:B2:52:ILE:HD13   | 2:B2:74:VAL:HG21   | 2.01                     | 0.42              |
| 2:B2:75:ALA:HB3    | 2:B2:78:THR:HG21   | 2.01                     | 0.42              |
| 5:D2:180:GLY:HA3   | 5:D2:355:LEU:HD13  | 2.01                     | 0.42              |
| 4:d:324:ASN:CB     | 4:d:325:PRO:HD3    | 2.49                     | 0.42              |
| 1:A:194:PHE:CE1    | 22:O2:106:LEU:HD22 | 2.54                     | 0.42              |
| 5:E1:263:LEU:HD21  | 5:E1:321:ARG:CB    | 2.49                     | 0.42              |
| 5:F2:166:VAL:HG23  | 5:F2:167:ILE:N     | 2.34                     | 0.42              |
| 12:I:17:LYS:HA     | 12:I:20:THR:HG22   | 2.01                     | 0.42              |
| 13:I2:31:LEU:O     | 13:I2:34:THR:OG1   | 2.35                     | 0.42              |
| 18:M:102:ARG:NH2   | 23:P:82:ASN:OD1    | 2.48                     | 0.42              |
| 7:f:16:GLU:OE1     | 7:f:16:GLU:N       | 2.52                     | 0.42              |
| 18:m:88:TYR:O      | 18:m:91:GLN:NE2    | 2.50                     | 0.42              |
| 2:C1:80:ILE:C      | 2:C1:80:ILE:HD12   | 2.45                     | 0.42              |
| 8:G:57:THR:HB      | 8:G:218:HIS:HB2    | 2.02                     | 0.42              |
| 15:L1:45:ILE:HG13  | 15:L1:57:VAL:HG11  | 2.01                     | 0.42              |
| 22:O2:70:GLY:HA2   | 22:X2:72:ILE:HD11  | 2.01                     | 0.42              |
| 8:g:269:LEU:HD12   | 8:g:269:LEU:C      | 2.44                     | 0.42              |
| 24:q:76:VAL:O      | 24:q:76:VAL:HG12   | 2.19                     | 0.42              |
| 2:A2:59:ASP:OD1    | 5:D2:300:ARG:NH2   | 2.53                     | 0.42              |
| 7:F:16:GLU:OE1     | 7:F:16:GLU:N       | 2.52                     | 0.42              |
| 5:F2:150:LEU:HD23  | 5:F2:150:LEU:O     | 2.19                     | 0.42              |
| 9:G1:48:ARG:HB3    | 11:H1:35:VAL:HG22  | 2.01                     | 0.42              |
| 19:M2:66:ILE:HD12  | 19:M2:66:ILE:N     | 2.34                     | 0.42              |
| 22:O1:114:LEU:HD13 | 1:a:160:MET:HE2    | 2.00                     | 0.42              |
| 22:V1:55:THR:HG23  | 22:V1:112:ALA:O    | 2.19                     | 0.42              |
| 5:E1:91:GLN:N      | 5:E1:91:GLN:OE1    | 2.53                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:F1:166:VAL:HG23  | 5:F1:167:ILE:N     | 2.34                     | 0.42              |
| 8:G:269:LEU:HD12   | 8:G:269:LEU:C      | 2.44                     | 0.42              |
| 19:M1:66:ILE:HD12  | 19:M1:66:ILE:N     | 2.34                     | 0.42              |
| 8:g:56:HIS:NE2     | 8:g:219:THR:O      | 2.52                     | 0.42              |
| 2:A2:207:ASP:OD1   | 2:A2:208:ARG:N     | 2.45                     | 0.42              |
| 5:F2:469:GLY:O     | 5:F2:474:THR:HG22  | 2.20                     | 0.42              |
| 9:G1:127:ILE:N     | 9:G1:127:ILE:HD12  | 2.35                     | 0.42              |
| 11:H1:60:PHE:CD1   | 11:H1:60:PHE:C     | 2.98                     | 0.42              |
| 22:O1:65:VAL:HG13  | 22:O1:101:THR:HG22 | 2.02                     | 0.42              |
| 22:P2:45:ILE:HD12  | 22:Q2:45:ILE:HG23  | 2.01                     | 0.42              |
| 7:f:56:ILE:HB      | 7:f:57:PRO:HD3     | 2.01                     | 0.42              |
| 2:C1:514:ASN:O     | 2:C1:518:TYR:OH    | 2.30                     | 0.41              |
| 5:F1:448:GLU:O     | 5:F1:452:GLY:N     | 2.49                     | 0.41              |
| 15:J1:36:THR:O     | 15:J1:36:THR:HG22  | 2.19                     | 0.41              |
| 19:M1:90:VAL:CG2   | 19:M1:108:VAL:HG22 | 2.49                     | 0.41              |
| 22:V2:55:THR:HG23  | 22:V2:112:ALA:O    | 2.19                     | 0.41              |
| 8:g:80:ARG:NE      | 8:g:203:GLU:OE1    | 2.44                     | 0.41              |
| 16:k:103:MET:HE1   | 24:q:80:LEU:HA     | 2.01                     | 0.41              |
| 2:A1:207:ASP:OD1   | 2:A1:208:ARG:N     | 2.45                     | 0.41              |
| 5:D2:39:GLN:NE2    | 5:D2:46:ASP:OD2    | 2.53                     | 0.41              |
| 28:E:404:CDL:H861  | 28:E:405:CDL:H673  | 2.01                     | 0.41              |
| 11:H2:60:PHE:CD1   | 11:H2:60:PHE:C     | 2.98                     | 0.41              |
| 11:H2:167:ILE:HD13 | 13:I2:23:TYR:HD1   | 1.86                     | 0.41              |
| 22:P1:104:ILE:HD12 | 22:Q1:69:ILE:HD12  | 2.01                     | 0.41              |
| 18:m:102:ARG:NH2   | 23:p:82:ASN:OD1    | 2.48                     | 0.41              |
| 2:C1:317:GLN:NE2   | 5:F1:313:GLU:OE1   | 2.46                     | 0.41              |
| 4:D:337:ARG:HD2    | 5:F2:489:ILE:HG21  | 2.02                     | 0.41              |
| 5:F2:421:GLU:OE2   | 9:G2:82:SER:CA     | 2.69                     | 0.41              |
| 15:J2:181:GLY:O    | 15:J2:185:VAL:HG23 | 2.19                     | 0.41              |
| 19:M2:162:HIS:NE2  | 19:M2:168:LEU:O    | 2.39                     | 0.41              |
| 3:c:49:PHE:O       | 12:i:15:GLN:NE2    | 2.53                     | 0.41              |
| 2:C2:537:ILE:N     | 2:C2:537:ILE:HD12  | 2.35                     | 0.41              |
| 4:D:321:ALA:O      | 4:D:325:PRO:CD     | 2.69                     | 0.41              |
| 22:S2:45:ILE:HG22  | 22:S2:46:SER:N     | 2.36                     | 0.41              |
| 2:A1:135:VAL:O     | 2:A1:135:VAL:HG12  | 2.21                     | 0.41              |
| 5:D2:263:LEU:HD13  | 5:D2:322:ILE:HG12  | 2.02                     | 0.41              |
| 5:F1:171:LEU:N     | 5:F1:171:LEU:HD23  | 2.36                     | 0.41              |
| 20:N:105:GLU:OE2   | 20:N:109:ARG:NH2   | 2.49                     | 0.41              |
| 24:Q:76:VAL:O      | 24:Q:76:VAL:HG12   | 2.19                     | 0.41              |
| 2:B1:205:VAL:HG12  | 2:B1:364:VAL:HB    | 2.03                     | 0.41              |
| 2:C2:80:ILE:HD12   | 2:C2:80:ILE:C      | 2.45                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:G2:174:VAL:CG2  | 11:H2:24:LEU:HD13  | 2.50                     | 0.41              |
| 19:M1:90:VAL:HG21 | 19:M1:108:VAL:HG22 | 2.03                     | 0.41              |
| 22:P1:45:ILE:HD12 | 22:Q1:45:ILE:HG23  | 2.02                     | 0.41              |
| 2:A2:135:VAL:O    | 2:A2:135:VAL:HG12  | 2.21                     | 0.41              |
| 2:C1:537:ILE:N    | 2:C1:537:ILE:HD12  | 2.35                     | 0.41              |
| 9:G1:174:VAL:CG2  | 11:H1:24:LEU:HD13  | 2.50                     | 0.41              |
| 9:G2:127:ILE:HD12 | 9:G2:127:ILE:N     | 2.35                     | 0.41              |
| 22:O2:66:GLY:O    | 22:O2:67:LEU:C     | 2.64                     | 0.41              |
| 1:a:166:TYR:OH    | 33:f:204:PC1:O12   | 2.26                     | 0.41              |
| 8:g:57:THR:HB     | 8:g:218:HIS:HB2    | 2.02                     | 0.41              |
| 2:B1:75:ALA:HB3   | 2:B1:78:THR:HG21   | 2.01                     | 0.41              |
| 3:C:29:LEU:HD12   | 22:P2:114:LEU:HD23 | 2.01                     | 0.41              |
| 7:F:64:ARG:NH1    | 25:R:33:GLU:OE1    | 2.48                     | 0.41              |
| 5:F1:287:PHE:O    | 5:F1:291:ASN:ND2   | 2.47                     | 0.41              |
| 20:N:63:SER:O     | 20:N:64:TYR:C      | 2.64                     | 0.41              |
| 2:A2:511:THR:O    | 2:A2:511:THR:HG22  | 2.21                     | 0.41              |
| 2:C1:532:THR:HG22 | 2:C1:533:LEU:N     | 2.36                     | 0.41              |
| 2:C2:317:GLN:NE2  | 5:F2:313:GLU:OE1   | 2.46                     | 0.41              |
| 5:D1:438:LYS:NZ   | 5:D1:481:MET:SD    | 2.85                     | 0.41              |
| 6:E:111:TYR:OH    | 24:Q:47:TRP:O      | 2.30                     | 0.41              |
| 28:E:405:CDL:H651 | 28:E:405:CDL:H612  | 2.03                     | 0.41              |
| 5:E1:179:ILE:HG13 | 5:E1:357:ALA:HB3   | 2.03                     | 0.41              |
| 5:E2:91:GLN:OE1   | 5:E2:91:GLN:N      | 2.53                     | 0.41              |
| 5:F1:347:ALA:HB3  | 5:F1:348:PRO:CD    | 2.51                     | 0.41              |
| 5:F2:282:ASP:HA   | 5:F2:283:ASN:HA    | 1.81                     | 0.41              |
| 5:F2:347:ALA:HB3  | 5:F2:348:PRO:CD    | 2.51                     | 0.41              |
| 11:H1:171:VAL:O   | 11:H1:175:VAL:HG23 | 2.21                     | 0.41              |
| 13:I1:35:VAL:HG12 | 13:I1:36:LYS:N     | 2.36                     | 0.41              |
| 13:I2:35:VAL:HG12 | 13:I2:36:LYS:N     | 2.36                     | 0.41              |
| 18:M:103:PHE:CZ   | 18:M:107:LEU:HD11  | 2.56                     | 0.41              |
| 28:M:201:CDL:H261 | 32:r:101:PEE:H44   | 2.02                     | 0.41              |
| 22:O1:66:GLY:O    | 22:O1:67:LEU:C     | 2.64                     | 0.41              |
| 22:O1:84:PRO:HB3  | 22:X1:86:LEU:HD11  | 2.03                     | 0.41              |
| 22:O2:65:VAL:HG13 | 22:O2:101:THR:HG22 | 2.02                     | 0.41              |
| 7:f:41:LEU:HD23   | 7:f:45:LEU:HD12    | 2.03                     | 0.41              |
| 14:j:30:GLU:OE1   | 24:q:72:ASN:ND2    | 2.50                     | 0.41              |
| 17:l:20:PHE:CE2   | 17:l:24:LEU:HD11   | 2.55                     | 0.41              |
| 2:B1:234:ASN:ND2  | 15:J1:102:ASP:OD2  | 2.48                     | 0.41              |
| 2:C2:532:THR:HG22 | 2:C2:533:LEU:N     | 2.36                     | 0.41              |
| 5:E2:179:ILE:HG13 | 5:E2:357:ALA:HB3   | 2.03                     | 0.41              |
| 5:F1:267:GLU:OE2  | 5:F1:321:ARG:NE    | 2.43                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:G2:134:SER:HG    | 13:I2:45:ARG:HH12  | 1.66                     | 0.41              |
| 15:K1:117:GLU:O    | 15:K1:121:THR:HG23 | 2.21                     | 0.41              |
| 1:a:26:LEU:O       | 3:c:67:ASN:ND2     | 2.53                     | 0.41              |
| 4:d:321:ALA:O      | 4:d:325:PRO:CD     | 2.69                     | 0.41              |
| 14:j:68:PRO:HG3    | 16:k:31:ILE:HD13   | 2.03                     | 0.41              |
| 20:n:105:GLU:OE2   | 20:n:109:ARG:NH2   | 2.49                     | 0.41              |
| 1:A:49:LEU:HD23    | 1:A:49:LEU:H       | 1.86                     | 0.40              |
| 2:B2:205:VAL:HG12  | 2:B2:364:VAL:HB    | 2.03                     | 0.40              |
| 5:D1:414:ILE:CG1   | 5:D1:422:LEU:HD11  | 2.51                     | 0.40              |
| 5:F1:469:GLY:O     | 5:F1:474:THR:HG22  | 2.20                     | 0.40              |
| 5:F1:489:ILE:HG21  | 4:d:337:ARG:HD2    | 2.02                     | 0.40              |
| 9:G2:33:TYR:O      | 9:G2:37:GLN:HB2    | 2.21                     | 0.40              |
| 11:H2:171:VAL:O    | 11:H2:175:VAL:HG23 | 2.21                     | 0.40              |
| 22:O2:84:PRO:HB3   | 22:X2:86:LEU:HD11  | 2.03                     | 0.40              |
| 2:B1:515:LYS:O     | 15:J1:134:ARG:NH1  | 2.55                     | 0.40              |
| 2:B2:214:SER:OG    | 26:B2:601:ATP:O2A  | 2.30                     | 0.40              |
| 3:C:92:TYR:CD2     | 3:C:92:TYR:O       | 2.75                     | 0.40              |
| 6:E:371:THR:HG23   | 23:P:64:PRO:HG3    | 2.03                     | 0.40              |
| 5:F2:171:LEU:HD23  | 5:F2:171:LEU:N     | 2.36                     | 0.40              |
| 5:F2:272:VAL:O     | 5:F2:272:VAL:HG12  | 2.22                     | 0.40              |
| 11:H1:167:ILE:HD13 | 13:I1:23:TYR:HD1   | 1.86                     | 0.40              |
| 14:J:147:ILE:O     | 14:J:147:ILE:HG23  | 2.22                     | 0.40              |
| 21:O:86:TYR:O      | 21:O:91:ARG:NE     | 2.52                     | 0.40              |
| 28:e:403:CDL:H651  | 28:e:403:CDL:H612  | 2.03                     | 0.40              |
| 2:A1:495:PHE:CE2   | 2:A1:499:LEU:HD11  | 2.56                     | 0.40              |
| 2:B1:246:ARG:NH2   | 5:E1:356:ASP:OD1   | 2.51                     | 0.40              |
| 2:C1:417:ASN:ND2   | 15:K1:105:GLU:OE2  | 2.55                     | 0.40              |
| 5:D1:64:ASP:OD1    | 5:D1:65:LYS:N      | 2.54                     | 0.40              |
| 9:G1:33:TYR:O      | 9:G1:37:GLN:HB2    | 2.21                     | 0.40              |
| 9:G2:130:ASP:OD1   | 9:G2:130:ASP:N     | 2.54                     | 0.40              |
| 14:J:68:PRO:HG3    | 16:K:31:ILE:HD13   | 2.03                     | 0.40              |
| 15:J2:143:MET:O    | 15:J2:147:CYS:N    | 2.54                     | 0.40              |
| 15:K1:70:ILE:O     | 15:K1:74:ASN:ND2   | 2.48                     | 0.40              |
| 22:U1:86:LEU:O     | 22:U1:87:THR:C     | 2.64                     | 0.40              |
| 2:B2:135:VAL:HG12  | 2:B2:135:VAL:O     | 2.22                     | 0.40              |
| 5:D1:263:LEU:HD13  | 5:D1:322:ILE:HG12  | 2.02                     | 0.40              |
| 5:D2:81:ASP:OD1    | 5:D2:84:THR:N      | 2.41                     | 0.40              |
| 7:F:41:LEU:HD23    | 7:F:45:LEU:HD12    | 2.03                     | 0.40              |
| 9:G2:82:SER:O      | 9:G2:244:ALA:HB3   | 2.22                     | 0.40              |
| 15:L1:28:ASP:OD1   | 15:L1:32:TYR:N     | 2.44                     | 0.40              |
| 28:Q:101:CDL:OB7   | 28:Q:101:CDL:CB3   | 2.69                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:m:103:PHE:CZ   | 18:m:107:LEU:HD11 | 2.56                     | 0.40              |
| 2:A2:495:PHE:CE2  | 2:A2:499:LEU:HD11 | 2.56                     | 0.40              |
| 2:B1:301:CYS:SG   | 2:B1:302:LEU:N    | 2.94                     | 0.40              |
| 2:C1:411:VAL:HG11 | 2:C1:415:ALA:HB2  | 2.03                     | 0.40              |
| 5:D1:39:GLN:NE2   | 5:D1:46:ASP:OD2   | 2.53                     | 0.40              |
| 5:D2:414:ILE:CG1  | 5:D2:422:LEU:HD11 | 2.51                     | 0.40              |
| 10:H:32:THR:O     | 10:H:32:THR:HG22  | 2.21                     | 0.40              |
| 6:e:371:THR:HG23  | 23:p:64:PRO:HG3   | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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     | 229/231 (99%) | 227 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | a     | 229/231 (99%) | 227 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 2   | A1    | 526/584 (90%) | 523 (99%) | 3 (1%)  | 0        | 100         | 100 |
| 2   | A2    | 526/584 (90%) | 523 (99%) | 3 (1%)  | 0        | 100         | 100 |
| 2   | B1    | 517/584 (88%) | 510 (99%) | 7 (1%)  | 0        | 100         | 100 |
| 2   | B2    | 517/584 (88%) | 510 (99%) | 7 (1%)  | 0        | 100         | 100 |
| 2   | C1    | 517/584 (88%) | 512 (99%) | 4 (1%)  | 1 (0%)   | 43          | 73  |
| 2   | C2    | 517/584 (88%) | 512 (99%) | 4 (1%)  | 1 (0%)   | 43          | 73  |
| 3   | C     | 84/114 (74%)  | 83 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 3   | c     | 84/114 (74%)  | 84 (100%) | 0       | 0        | 100         | 100 |
| 4   | D     | 328/370 (89%) | 321 (98%) | 7 (2%)  | 0        | 100         | 100 |
| 4   | d     | 328/370 (89%) | 321 (98%) | 7 (2%)  | 0        | 100         | 100 |
| 5   | D1    | 485/519 (93%) | 478 (99%) | 7 (1%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 5   | D2    | 485/519 (93%) | 478 (99%)  | 7 (1%)  | 0        | 100         | 100 |
| 5   | E1    | 484/519 (93%) | 471 (97%)  | 13 (3%) | 0        | 100         | 100 |
| 5   | E2    | 484/519 (93%) | 471 (97%)  | 13 (3%) | 0        | 100         | 100 |
| 5   | F1    | 487/519 (94%) | 479 (98%)  | 8 (2%)  | 0        | 100         | 100 |
| 5   | F2    | 487/519 (94%) | 479 (98%)  | 8 (2%)  | 0        | 100         | 100 |
| 6   | E     | 381/396 (96%) | 375 (98%)  | 6 (2%)  | 0        | 100         | 100 |
| 6   | e     | 381/396 (96%) | 376 (99%)  | 5 (1%)  | 0        | 100         | 100 |
| 7   | F     | 133/145 (92%) | 131 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 7   | f     | 133/145 (92%) | 131 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 8   | G     | 266/269 (99%) | 263 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 8   | g     | 266/269 (99%) | 263 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 9   | G1    | 298/305 (98%) | 296 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 9   | G2    | 298/305 (98%) | 296 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 10  | H     | 135/157 (86%) | 133 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 10  | h     | 135/157 (86%) | 133 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 11  | H1    | 159/182 (87%) | 158 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 11  | H2    | 159/182 (87%) | 158 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 12  | I     | 101/104 (97%) | 100 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 12  | i     | 101/104 (97%) | 100 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 13  | I1    | 63/75 (84%)   | 63 (100%)  | 0       | 0        | 100         | 100 |
| 13  | I2    | 63/75 (84%)   | 63 (100%)  | 0       | 0        | 100         | 100 |
| 14  | J     | 166/169 (98%) | 163 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 14  | j     | 166/169 (98%) | 163 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 15  | J1    | 164/188 (87%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 15  | J2    | 164/188 (87%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 15  | K1    | 164/188 (87%) | 159 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 15  | K2    | 164/188 (87%) | 159 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 15  | L1    | 163/188 (87%) | 163 (100%) | 0       | 0        | 100         | 100 |
| 15  | L2    | 163/188 (87%) | 162 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 16  | K     | 103/124 (83%) | 99 (96%)   | 4 (4%)  | 0        | 100         | 100 |
| 16  | k     | 103/124 (83%) | 99 (96%)   | 4 (4%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 17  | L     | 63/92 (68%)   | 63 (100%)  | 0       | 0        | 100         | 100 |
| 17  | l     | 63/92 (68%)   | 63 (100%)  | 0       | 0        | 100         | 100 |
| 18  | M     | 127/144 (88%) | 127 (100%) | 0       | 0        | 100         | 100 |
| 18  | m     | 127/144 (88%) | 127 (100%) | 0       | 0        | 100         | 100 |
| 19  | M1    | 230/255 (90%) | 226 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 19  | M2    | 230/255 (90%) | 226 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 20  | N     | 137/156 (88%) | 131 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 20  | n     | 137/156 (88%) | 131 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 21  | O     | 94/101 (93%)  | 94 (100%)  | 0       | 0        | 100         | 100 |
| 21  | o     | 94/101 (93%)  | 94 (100%)  | 0       | 0        | 100         | 100 |
| 22  | O1    | 76/118 (64%)  | 71 (93%)   | 5 (7%)  | 0        | 100         | 100 |
| 22  | O2    | 76/118 (64%)  | 71 (93%)   | 5 (7%)  | 0        | 100         | 100 |
| 22  | P1    | 76/118 (64%)  | 73 (96%)   | 3 (4%)  | 0        | 100         | 100 |
| 22  | P2    | 76/118 (64%)  | 73 (96%)   | 3 (4%)  | 0        | 100         | 100 |
| 22  | Q1    | 76/118 (64%)  | 76 (100%)  | 0       | 0        | 100         | 100 |
| 22  | Q2    | 76/118 (64%)  | 76 (100%)  | 0       | 0        | 100         | 100 |
| 22  | R1    | 76/118 (64%)  | 76 (100%)  | 0       | 0        | 100         | 100 |
| 22  | R2    | 76/118 (64%)  | 76 (100%)  | 0       | 0        | 100         | 100 |
| 22  | S1    | 76/118 (64%)  | 74 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 22  | S2    | 76/118 (64%)  | 74 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 22  | T1    | 76/118 (64%)  | 75 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 22  | T2    | 76/118 (64%)  | 75 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 22  | U1    | 76/118 (64%)  | 72 (95%)   | 4 (5%)  | 0        | 100         | 100 |
| 22  | U2    | 76/118 (64%)  | 72 (95%)   | 4 (5%)  | 0        | 100         | 100 |
| 22  | V1    | 76/118 (64%)  | 74 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 22  | V2    | 76/118 (64%)  | 74 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 22  | W1    | 76/118 (64%)  | 74 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 22  | W2    | 76/118 (64%)  | 74 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 22  | X1    | 76/118 (64%)  | 75 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 22  | X2    | 76/118 (64%)  | 75 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 23  | P     | 78/105 (74%)  | 77 (99%)   | 1 (1%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 23  | p     | 78/105 (74%)      | 77 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 24  | Q     | 83/98 (85%)       | 80 (96%)    | 3 (4%)   | 0        | 100         | 100 |
| 24  | q     | 83/98 (85%)       | 80 (96%)    | 3 (4%)   | 0        | 100         | 100 |
| 25  | R     | 60/62 (97%)       | 59 (98%)    | 1 (2%)   | 0        | 100         | 100 |
| 25  | r     | 60/62 (97%)       | 59 (98%)    | 1 (2%)   | 0        | 100         | 100 |
| All | All   | 15170/17414 (87%) | 14931 (98%) | 237 (2%) | 2 (0%)   | 100         | 100 |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C2    | 532 | THR  |
| 2   | C1    | 532 | THR  |

### 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     | 225/225 (100%) | 224 (100%) | 1 (0%)   | 84          | 86  |
| 1   | a     | 225/225 (100%) | 224 (100%) | 1 (0%)   | 84          | 86  |
| 2   | A1    | 439/479 (92%)  | 439 (100%) | 0        | 100         | 100 |
| 2   | A2    | 439/479 (92%)  | 439 (100%) | 0        | 100         | 100 |
| 2   | B1    | 435/479 (91%)  | 435 (100%) | 0        | 100         | 100 |
| 2   | B2    | 435/479 (91%)  | 435 (100%) | 0        | 100         | 100 |
| 2   | C1    | 434/479 (91%)  | 434 (100%) | 0        | 100         | 100 |
| 2   | C2    | 434/479 (91%)  | 434 (100%) | 0        | 100         | 100 |
| 3   | C     | 80/104 (77%)   | 79 (99%)   | 1 (1%)   | 61          | 78  |
| 3   | c     | 80/104 (77%)   | 79 (99%)   | 1 (1%)   | 61          | 78  |
| 4   | D     | 297/334 (89%)  | 296 (100%) | 1 (0%)   | 86          | 88  |
| 4   | d     | 297/334 (89%)  | 296 (100%) | 1 (0%)   | 86          | 88  |
| 5   | D1    | 398/420 (95%)  | 397 (100%) | 1 (0%)   | 86          | 88  |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 5   | D2    | 398/420 (95%)  | 398 (100%) | 0        | 100         | 100 |
| 5   | E1    | 397/420 (94%)  | 397 (100%) | 0        | 100         | 100 |
| 5   | E2    | 397/420 (94%)  | 397 (100%) | 0        | 100         | 100 |
| 5   | F1    | 400/420 (95%)  | 400 (100%) | 0        | 100         | 100 |
| 5   | F2    | 400/420 (95%)  | 400 (100%) | 0        | 100         | 100 |
| 6   | E     | 334/341 (98%)  | 333 (100%) | 1 (0%)   | 86          | 88  |
| 6   | e     | 334/341 (98%)  | 333 (100%) | 1 (0%)   | 86          | 88  |
| 7   | F     | 119/124 (96%)  | 118 (99%)  | 1 (1%)   | 73          | 82  |
| 7   | f     | 119/124 (96%)  | 118 (99%)  | 1 (1%)   | 73          | 82  |
| 8   | G     | 205/206 (100%) | 205 (100%) | 0        | 100         | 100 |
| 8   | g     | 205/206 (100%) | 205 (100%) | 0        | 100         | 100 |
| 9   | G1    | 253/257 (98%)  | 252 (100%) | 1 (0%)   | 84          | 86  |
| 9   | G2    | 253/257 (98%)  | 252 (100%) | 1 (0%)   | 84          | 86  |
| 10  | H     | 110/123 (89%)  | 110 (100%) | 0        | 100         | 100 |
| 10  | h     | 110/123 (89%)  | 110 (100%) | 0        | 100         | 100 |
| 11  | H1    | 137/156 (88%)  | 136 (99%)  | 1 (1%)   | 76          | 83  |
| 11  | H2    | 137/156 (88%)  | 135 (98%)  | 2 (2%)   | 57          | 76  |
| 12  | I     | 95/96 (99%)    | 95 (100%)  | 0        | 100         | 100 |
| 12  | i     | 95/96 (99%)    | 95 (100%)  | 0        | 100         | 100 |
| 13  | I1    | 58/67 (87%)    | 58 (100%)  | 0        | 100         | 100 |
| 13  | I2    | 58/67 (87%)    | 58 (100%)  | 0        | 100         | 100 |
| 14  | J     | 149/150 (99%)  | 149 (100%) | 0        | 100         | 100 |
| 14  | j     | 149/150 (99%)  | 149 (100%) | 0        | 100         | 100 |
| 15  | J1    | 145/162 (90%)  | 145 (100%) | 0        | 100         | 100 |
| 15  | J2    | 145/162 (90%)  | 145 (100%) | 0        | 100         | 100 |
| 15  | K1    | 145/162 (90%)  | 145 (100%) | 0        | 100         | 100 |
| 15  | K2    | 145/162 (90%)  | 145 (100%) | 0        | 100         | 100 |
| 15  | L1    | 145/162 (90%)  | 145 (100%) | 0        | 100         | 100 |
| 15  | L2    | 145/162 (90%)  | 145 (100%) | 0        | 100         | 100 |
| 16  | K     | 91/107 (85%)   | 91 (100%)  | 0        | 100         | 100 |
| 16  | k     | 91/107 (85%)   | 91 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 17  | L     | 55/75 (73%)   | 55 (100%)  | 0        | 100         | 100 |
| 17  | l     | 55/75 (73%)   | 55 (100%)  | 0        | 100         | 100 |
| 18  | M     | 111/124 (90%) | 110 (99%)  | 1 (1%)   | 70          | 81  |
| 18  | m     | 111/124 (90%) | 110 (99%)  | 1 (1%)   | 70          | 81  |
| 19  | M1    | 200/215 (93%) | 199 (100%) | 1 (0%)   | 81          | 85  |
| 19  | M2    | 200/215 (93%) | 199 (100%) | 1 (0%)   | 81          | 85  |
| 20  | N     | 123/137 (90%) | 121 (98%)  | 2 (2%)   | 55          | 75  |
| 20  | n     | 123/137 (90%) | 121 (98%)  | 2 (2%)   | 55          | 75  |
| 21  | O     | 82/86 (95%)   | 82 (100%)  | 0        | 100         | 100 |
| 21  | o     | 82/86 (95%)   | 82 (100%)  | 0        | 100         | 100 |
| 22  | O1    | 56/89 (63%)   | 56 (100%)  | 0        | 100         | 100 |
| 22  | O2    | 56/89 (63%)   | 56 (100%)  | 0        | 100         | 100 |
| 22  | P1    | 56/89 (63%)   | 56 (100%)  | 0        | 100         | 100 |
| 22  | P2    | 56/89 (63%)   | 56 (100%)  | 0        | 100         | 100 |
| 22  | Q1    | 56/89 (63%)   | 56 (100%)  | 0        | 100         | 100 |
| 22  | Q2    | 56/89 (63%)   | 56 (100%)  | 0        | 100         | 100 |
| 22  | R1    | 56/89 (63%)   | 56 (100%)  | 0        | 100         | 100 |
| 22  | R2    | 56/89 (63%)   | 56 (100%)  | 0        | 100         | 100 |
| 22  | S1    | 56/89 (63%)   | 56 (100%)  | 0        | 100         | 100 |
| 22  | S2    | 56/89 (63%)   | 56 (100%)  | 0        | 100         | 100 |
| 22  | T1    | 56/89 (63%)   | 56 (100%)  | 0        | 100         | 100 |
| 22  | T2    | 56/89 (63%)   | 56 (100%)  | 0        | 100         | 100 |
| 22  | U1    | 56/89 (63%)   | 56 (100%)  | 0        | 100         | 100 |
| 22  | U2    | 56/89 (63%)   | 56 (100%)  | 0        | 100         | 100 |
| 22  | V1    | 56/89 (63%)   | 56 (100%)  | 0        | 100         | 100 |
| 22  | V2    | 56/89 (63%)   | 56 (100%)  | 0        | 100         | 100 |
| 22  | W1    | 56/89 (63%)   | 56 (100%)  | 0        | 100         | 100 |
| 22  | W2    | 56/89 (63%)   | 56 (100%)  | 0        | 100         | 100 |
| 22  | X1    | 56/89 (63%)   | 54 (96%)   | 2 (4%)   | 31          | 63  |
| 22  | X2    | 56/89 (63%)   | 54 (96%)   | 2 (4%)   | 31          | 63  |
| 23  | P     | 75/94 (80%)   | 75 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Rotameric    | Outliers | Percentiles |     |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 23  | p     | 75/94 (80%)       | 75 (100%)    | 0        | 100         | 100 |
| 24  | Q     | 80/92 (87%)       | 80 (100%)    | 0        | 100         | 100 |
| 24  | q     | 80/92 (87%)       | 80 (100%)    | 0        | 100         | 100 |
| 25  | R     | 56/56 (100%)      | 56 (100%)    | 0        | 100         | 100 |
| 25  | r     | 56/56 (100%)      | 56 (100%)    | 0        | 100         | 100 |
| All | All   | 12866/14484 (89%) | 12838 (100%) | 28 (0%)  | 85          | 89  |

All (28) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 144 | PHE  |
| 3   | C     | 93  | THR  |
| 4   | D     | 145 | ARG  |
| 5   | D1    | 45  | VAL  |
| 6   | E     | 226 | THR  |
| 7   | F     | 42  | ASN  |
| 9   | G1    | 237 | GLU  |
| 9   | G2    | 237 | GLU  |
| 11  | H1    | 111 | VAL  |
| 11  | H2    | 41  | HIS  |
| 11  | H2    | 111 | VAL  |
| 18  | M     | 109 | VAL  |
| 19  | M1    | 247 | ASP  |
| 19  | M2    | 247 | ASP  |
| 20  | N     | 105 | GLU  |
| 20  | N     | 132 | GLU  |
| 22  | X1    | 104 | ILE  |
| 22  | X1    | 107 | PHE  |
| 22  | X2    | 104 | ILE  |
| 22  | X2    | 107 | PHE  |
| 1   | a     | 144 | PHE  |
| 3   | c     | 93  | THR  |
| 4   | d     | 145 | ARG  |
| 6   | e     | 226 | THR  |
| 7   | f     | 42  | ASN  |
| 18  | m     | 109 | VAL  |
| 20  | n     | 105 | GLU  |
| 20  | n     | 132 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 150 | ASN  |
| 2   | A1    | 317 | GLN  |
| 2   | A1    | 339 | HIS  |
| 2   | A1    | 386 | GLN  |
| 2   | A1    | 472 | ASN  |
| 2   | A1    | 551 | HIS  |
| 2   | A1    | 556 | HIS  |
| 2   | A2    | 317 | GLN  |
| 2   | A2    | 339 | HIS  |
| 2   | A2    | 386 | GLN  |
| 2   | A2    | 472 | ASN  |
| 2   | A2    | 551 | HIS  |
| 2   | A2    | 556 | HIS  |
| 2   | B1    | 245 | GLN  |
| 2   | B1    | 463 | ASN  |
| 2   | B1    | 472 | ASN  |
| 2   | B2    | 245 | GLN  |
| 2   | B2    | 463 | ASN  |
| 2   | B2    | 472 | ASN  |
| 2   | C1    | 254 | HIS  |
| 2   | C1    | 296 | ASN  |
| 2   | C1    | 339 | HIS  |
| 2   | C2    | 296 | ASN  |
| 2   | C2    | 339 | HIS  |
| 2   | C2    | 472 | ASN  |
| 5   | D1    | 39  | GLN  |
| 5   | D1    | 48  | HIS  |
| 5   | D1    | 354 | HIS  |
| 5   | D2    | 39  | GLN  |
| 5   | D2    | 48  | HIS  |
| 5   | E1    | 36  | HIS  |
| 5   | E1    | 48  | HIS  |
| 5   | E1    | 398 | GLN  |
| 5   | E2    | 36  | HIS  |
| 5   | E2    | 48  | HIS  |
| 5   | E2    | 398 | GLN  |
| 7   | F     | 19  | HIS  |
| 7   | F     | 34  | GLN  |
| 7   | F     | 75  | HIS  |
| 5   | F1    | 36  | HIS  |
| 5   | F1    | 108 | ASN  |
| 5   | F2    | 36  | HIS  |
| 5   | F2    | 108 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | F2    | 411 | GLN  |
| 8   | G     | 143 | GLN  |
| 9   | G1    | 162 | ASN  |
| 9   | G1    | 233 | ASN  |
| 9   | G2    | 162 | ASN  |
| 13  | I1    | 71  | HIS  |
| 13  | I2    | 71  | HIS  |
| 15  | J1    | 82  | GLN  |
| 15  | J1    | 93  | ASN  |
| 15  | J1    | 175 | HIS  |
| 15  | J2    | 82  | GLN  |
| 15  | J2    | 93  | ASN  |
| 15  | J2    | 175 | HIS  |
| 15  | K1    | 82  | GLN  |
| 15  | K2    | 82  | GLN  |
| 15  | L1    | 175 | HIS  |
| 19  | M1    | 112 | ASN  |
| 19  | M1    | 197 | ASN  |
| 19  | M2    | 112 | ASN  |
| 19  | M2    | 197 | ASN  |
| 20  | N     | 144 | HIS  |
| 23  | P     | 39  | GLN  |
| 23  | P     | 95  | GLN  |
| 22  | V1    | 75  | ASN  |
| 22  | V2    | 75  | ASN  |
| 1   | a     | 150 | ASN  |
| 3   | c     | 101 | GLN  |
| 7   | f     | 19  | HIS  |
| 7   | f     | 34  | GLN  |
| 7   | f     | 75  | HIS  |
| 20  | n     | 89  | GLN  |
| 20  | n     | 91  | HIS  |
| 20  | n     | 144 | HIS  |
| 23  | p     | 39  | GLN  |
| 23  | p     | 95  | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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 | $\# Z  > 2$ |
| 6   | AME  | e     | 1   | 6    | 9,10,11      | 0.29 | 0           | 9,11,13     | 0.43 | 0           |
| 6   | AME  | E     | 1   | 6    | 9,10,11      | 0.28 | 0           | 9,11,13     | 0.44 | 0           |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings |
|-----|------|-------|-----|------|---------|-----------|-------|
| 6   | AME  | e     | 1   | 6    | -       | 3/9/10/12 | -     |
| 6   | AME  | E     | 1   | 6    | -       | 3/9/10/12 | -     |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 6   | E     | 1   | AME  | N-CA-CB-CG  |
| 6   | e     | 1   | AME  | N-CA-CB-CG  |
| 6   | E     | 1   | AME  | C-CA-CB-CG  |
| 6   | e     | 1   | AME  | C-CA-CB-CG  |
| 6   | E     | 1   | AME  | CB-CA-N-CT1 |
| 6   | e     | 1   | AME  | CB-CA-N-CT1 |

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 66 ligands modelled in this entry, 10 are monoatomic - leaving 56 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 | $\# Z  > 2$ |
| 28  | CDL  | E     | 403 | -    | 99,99,99     | 0.29 | 0           | 105,111,111 | 0.26 | 0           |
| 28  | CDL  | M     | 201 | -    | 99,99,99     | 0.30 | 0           | 105,111,111 | 0.29 | 0           |
| 32  | PEE  | r     | 101 | -    | 50,50,50     | 0.75 | 2 (4%)      | 53,55,55    | 0.53 | 0           |
| 28  | CDL  | e     | 405 | -    | 99,99,99     | 0.29 | 0           | 105,111,111 | 0.26 | 0           |
| 28  | CDL  | C     | 201 | -    | 99,99,99     | 0.29 | 0           | 105,111,111 | 0.26 | 0           |
| 28  | CDL  | j     | 202 | -    | 99,99,99     | 0.29 | 0           | 105,111,111 | 0.26 | 0           |
| 28  | CDL  | l     | 101 | -    | 99,99,99     | 0.29 | 0           | 105,111,111 | 0.26 | 0           |
| 33  | PC1  | I     | 201 | -    | 53,53,53     | 0.28 | 0           | 59,61,61    | 0.29 | 0           |
| 28  | CDL  | f     | 201 | -    | 99,99,99     | 0.29 | 0           | 105,111,111 | 0.27 | 0           |
| 29  | ADP  | D1    | 601 | 27   | 28,29,29     | 0.40 | 0           | 43,45,45    | 0.48 | 0           |
| 28  | CDL  | e     | 401 | -    | 99,99,99     | 0.29 | 0           | 105,111,111 | 0.26 | 0           |
| 30  | LMT  | E     | 401 | -    | 36,36,36     | 0.15 | 0           | 47,47,47    | 0.47 | 1 (2%)      |
| 33  | PC1  | J     | 204 | -    | 53,53,53     | 0.28 | 0           | 59,61,61    | 0.28 | 0           |
| 34  | UTP  | H2    | 201 | -    | 29,30,30     | 0.29 | 0           | 43,47,47    | 0.32 | 0           |
| 28  | CDL  | Q     | 101 | -    | 99,99,99     | 0.29 | 0           | 105,111,111 | 0.29 | 0           |
| 28  | CDL  | e     | 402 | -    | 99,99,99     | 0.29 | 0           | 105,111,111 | 0.28 | 0           |
| 28  | CDL  | q     | 101 | -    | 99,99,99     | 0.29 | 0           | 105,111,111 | 0.29 | 0           |
| 28  | CDL  | e     | 403 | -    | 99,99,99     | 0.28 | 0           | 105,111,111 | 0.26 | 0           |
| 30  | LMT  | j     | 204 | -    | 36,36,36     | 0.16 | 0           | 47,47,47    | 0.55 | 0           |
| 28  | CDL  | E     | 406 | -    | 99,99,99     | 0.29 | 0           | 105,111,111 | 0.25 | 0           |
| 28  | CDL  | e     | 404 | -    | 99,99,99     | 0.29 | 0           | 105,111,111 | 0.25 | 0           |
| 33  | PC1  | j     | 203 | -    | 53,53,53     | 0.28 | 0           | 59,61,61    | 0.28 | 0           |
| 28  | CDL  | j     | 201 | -    | 99,99,99     | 0.29 | 0           | 105,111,111 | 0.26 | 0           |
| 26  | ATP  | B2    | 601 | 27   | 32,33,33     | 0.27 | 0           | 48,52,52    | 0.28 | 0           |
| 32  | PEE  | f     | 202 | -    | 50,50,50     | 0.78 | 2 (4%)      | 53,55,55    | 0.46 | 0           |
| 34  | UTP  | H1    | 201 | -    | 29,30,30     | 0.29 | 0           | 43,47,47    | 0.32 | 0           |
| 31  | Q7G  | e     | 407 | -    | 54,54,90     | 0.13 | 0           | 80,84,138   | 0.26 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 33  | PC1  | F     | 203 | -    | 53,53,53     | 0.28 | 0        | 59,61,61    | 0.28 | 0        |
| 32  | PEE  | R     | 101 | -    | 50,50,50     | 0.75 | 2 (4%)   | 53,55,55    | 0.52 | 0        |
| 28  | CDL  | J     | 203 | -    | 99,99,99     | 0.29 | 0        | 105,111,111 | 0.26 | 0        |
| 33  | PC1  | i     | 201 | -    | 53,53,53     | 0.28 | 0        | 59,61,61    | 0.29 | 0        |
| 32  | PEE  | F     | 202 | -    | 50,50,50     | 0.78 | 2 (4%)   | 53,55,55    | 0.46 | 0        |
| 26  | ATP  | A1    | 601 | 27   | 32,33,33     | 0.27 | 0        | 48,52,52    | 0.28 | 0        |
| 28  | CDL  | F     | 201 | -    | 99,99,99     | 0.29 | 0        | 105,111,111 | 0.27 | 0        |
| 33  | PC1  | f     | 203 | -    | 53,53,53     | 0.28 | 0        | 59,61,61    | 0.28 | 0        |
| 28  | CDL  | m     | 201 | -    | 99,99,99     | 0.30 | 0        | 105,111,111 | 0.29 | 0        |
| 28  | CDL  | E     | 404 | -    | 99,99,99     | 0.29 | 0        | 105,111,111 | 0.28 | 0        |
| 28  | CDL  | E     | 407 | -    | 99,99,99     | 0.29 | 0        | 105,111,111 | 0.26 | 0        |
| 28  | CDL  | L     | 101 | -    | 99,99,99     | 0.29 | 0        | 105,111,111 | 0.25 | 0        |
| 30  | LMT  | e     | 406 | -    | 36,36,36     | 0.14 | 0        | 47,47,47    | 0.47 | 1 (2%)   |
| 31  | Q7G  | E     | 402 | -    | 54,54,90     | 0.13 | 0        | 80,84,138   | 0.26 | 0        |
| 30  | LMT  | J     | 201 | -    | 36,36,36     | 0.16 | 0        | 47,47,47    | 0.55 | 0        |
| 31  | Q7G  | n     | 201 | -    | 66,66,90     | 0.14 | 0        | 98,102,138  | 0.31 | 0        |
| 26  | ATP  | C2    | 601 | 27   | 32,33,33     | 0.27 | 0        | 48,52,52    | 0.28 | 0        |
| 33  | PC1  | F     | 204 | -    | 53,53,53     | 0.27 | 0        | 59,61,61    | 0.28 | 0        |
| 26  | ATP  | F1    | 601 | 27   | 32,33,33     | 0.27 | 0        | 48,52,52    | 0.27 | 0        |
| 28  | CDL  | J     | 202 | -    | 99,99,99     | 0.29 | 0        | 105,111,111 | 0.26 | 0        |
| 31  | Q7G  | N     | 201 | -    | 66,66,90     | 0.13 | 0        | 98,102,138  | 0.31 | 0        |
| 26  | ATP  | C1    | 601 | 27   | 32,33,33     | 0.27 | 0        | 48,52,52    | 0.28 | 0        |
| 33  | PC1  | f     | 204 | -    | 53,53,53     | 0.27 | 0        | 59,61,61    | 0.28 | 0        |
| 26  | ATP  | A2    | 601 | 27   | 32,33,33     | 0.27 | 0        | 48,52,52    | 0.28 | 0        |
| 26  | ATP  | B1    | 601 | 27   | 32,33,33     | 0.27 | 0        | 48,52,52    | 0.28 | 0        |
| 26  | ATP  | F2    | 601 | 27   | 32,33,33     | 0.28 | 0        | 48,52,52    | 0.27 | 0        |
| 28  | CDL  | E     | 405 | -    | 99,99,99     | 0.29 | 0        | 105,111,111 | 0.27 | 0        |
| 28  | CDL  | c     | 201 | -    | 99,99,99     | 0.29 | 0        | 105,111,111 | 0.26 | 0        |
| 29  | ADP  | D2    | 601 | 27   | 28,29,29     | 0.40 | 0        | 43,45,45    | 0.48 | 0        |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions       | Rings |
|-----|------|-------|-----|------|---------|----------------|-------|
| 28  | CDL  | E     | 403 | -    | -       | 23/110/110/110 | -     |
| 28  | CDL  | M     | 201 | -    | -       | 41/110/110/110 | -     |
| 32  | PEE  | r     | 101 | -    | -       | 28/54/54/54    | -     |
| 28  | CDL  | e     | 405 | -    | -       | 34/110/110/110 | -     |
| 28  | CDL  | C     | 201 | -    | -       | 24/110/110/110 | -     |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions       | Rings    |
|-----|------|-------|-----|------|-----------|----------------|----------|
| 28  | CDL  | j     | 202 | -    | -         | 29/110/110/110 | -        |
| 28  | CDL  | l     | 101 | -    | -         | 24/110/110/110 | -        |
| 33  | PC1  | I     | 201 | -    | -         | 10/57/57/57    | -        |
| 28  | CDL  | f     | 201 | -    | -         | 21/110/110/110 | -        |
| 29  | ADP  | D1    | 601 | 27   | -         | 1/16/32/32     | 0/3/3/3  |
| 28  | CDL  | e     | 401 | -    | -         | 23/110/110/110 | -        |
| 30  | LMT  | E     | 401 | -    | -         | 1/21/61/61     | 0/2/2/2  |
| 33  | PC1  | J     | 204 | -    | -         | 12/57/57/57    | -        |
| 34  | UTP  | H2    | 201 | -    | -         | 4/22/38/38     | 0/2/2/2  |
| 28  | CDL  | Q     | 101 | -    | -         | 26/110/110/110 | -        |
| 28  | CDL  | e     | 402 | -    | -         | 30/110/110/110 | -        |
| 28  | CDL  | q     | 101 | -    | -         | 26/110/110/110 | -        |
| 28  | CDL  | e     | 403 | -    | -         | 29/110/110/110 | -        |
| 30  | LMT  | j     | 204 | -    | -         | 5/21/61/61     | 0/2/2/2  |
| 28  | CDL  | E     | 406 | -    | -         | 19/110/110/110 | -        |
| 28  | CDL  | e     | 404 | -    | -         | 19/110/110/110 | -        |
| 33  | PC1  | j     | 203 | -    | -         | 12/57/57/57    | -        |
| 28  | CDL  | j     | 201 | -    | -         | 24/110/110/110 | -        |
| 26  | ATP  | B2    | 601 | 27   | -         | 4/22/38/38     | 0/3/3/3  |
| 32  | PEE  | f     | 202 | -    | -         | 16/54/54/54    | -        |
| 34  | UTP  | H1    | 201 | -    | -         | 4/22/38/38     | 0/2/2/2  |
| 31  | Q7G  | e     | 407 | -    | 1/1/19/34 | 5/15/123/200   | 0/7/7/10 |
| 33  | PC1  | F     | 203 | -    | -         | 10/57/57/57    | -        |
| 32  | PEE  | R     | 101 | -    | -         | 28/54/54/54    | -        |
| 28  | CDL  | J     | 203 | -    | -         | 29/110/110/110 | -        |
| 33  | PC1  | i     | 201 | -    | -         | 10/57/57/57    | -        |
| 32  | PEE  | F     | 202 | -    | -         | 16/54/54/54    | -        |
| 26  | ATP  | A1    | 601 | 27   | -         | 6/22/38/38     | 0/3/3/3  |
| 28  | CDL  | F     | 201 | -    | -         | 21/110/110/110 | -        |
| 33  | PC1  | f     | 203 | -    | -         | 10/57/57/57    | -        |
| 28  | CDL  | m     | 201 | -    | -         | 41/110/110/110 | -        |
| 31  | Q7G  | E     | 402 | -    | 1/1/19/34 | 5/15/123/200   | 0/7/7/10 |
| 28  | CDL  | E     | 404 | -    | -         | 30/110/110/110 | -        |
| 28  | CDL  | E     | 407 | -    | -         | 35/110/110/110 | -        |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions       | Rings    |
|-----|------|-------|-----|------|-----------|----------------|----------|
| 28  | CDL  | L     | 101 | -    | -         | 24/110/110/110 | -        |
| 30  | LMT  | e     | 406 | -    | -         | 1/21/61/61     | 0/2/2/2  |
| 30  | LMT  | J     | 201 | -    | -         | 5/21/61/61     | 0/2/2/2  |
| 31  | Q7G  | n     | 201 | -    | 2/2/24/34 | 6/20/148/200   | 0/8/8/10 |
| 26  | ATP  | C2    | 601 | 27   | -         | 6/22/38/38     | 0/3/3/3  |
| 33  | PC1  | F     | 204 | -    | -         | 10/57/57/57    | -        |
| 26  | ATP  | F1    | 601 | 27   | -         | 5/22/38/38     | 0/3/3/3  |
| 31  | Q7G  | N     | 201 | -    | 2/2/24/34 | 6/20/148/200   | 0/8/8/10 |
| 28  | CDL  | J     | 202 | -    | -         | 24/110/110/110 | -        |
| 26  | ATP  | C1    | 601 | 27   | -         | 6/22/38/38     | 0/3/3/3  |
| 33  | PC1  | f     | 204 | -    | -         | 10/57/57/57    | -        |
| 26  | ATP  | A2    | 601 | 27   | -         | 6/22/38/38     | 0/3/3/3  |
| 26  | ATP  | B1    | 601 | 27   | -         | 4/22/38/38     | 0/3/3/3  |
| 26  | ATP  | F2    | 601 | 27   | -         | 5/22/38/38     | 0/3/3/3  |
| 28  | CDL  | E     | 405 | -    | -         | 29/110/110/110 | -        |
| 28  | CDL  | c     | 201 | -    | -         | 24/110/110/110 | -        |
| 29  | ADP  | D2    | 601 | 27   | -         | 1/16/32/32     | 0/3/3/3  |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 32  | f     | 202 | PEE  | C39-C38 | 3.66 | 1.52        | 1.31     |
| 32  | F     | 202 | PEE  | C39-C38 | 3.64 | 1.52        | 1.31     |
| 32  | f     | 202 | PEE  | C18-C19 | 3.60 | 1.52        | 1.31     |
| 32  | F     | 202 | PEE  | C18-C19 | 3.60 | 1.52        | 1.31     |
| 32  | r     | 101 | PEE  | C18-C19 | 3.55 | 1.51        | 1.31     |
| 32  | R     | 101 | PEE  | C18-C19 | 3.54 | 1.51        | 1.31     |
| 32  | r     | 101 | PEE  | C39-C38 | 3.43 | 1.51        | 1.31     |
| 32  | R     | 101 | PEE  | C39-C38 | 3.43 | 1.51        | 1.31     |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | e     | 406 | LMT  | C1'-O5'-C5' | -2.12 | 109.58      | 113.72   |
| 30  | E     | 401 | LMT  | C1'-O5'-C5' | -2.10 | 109.61      | 113.72   |

All (6) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 31  | E     | 402 | Q7G  | C1B  |
| 31  | N     | 201 | Q7G  | C1B  |
| 31  | N     | 201 | Q7G  | C1C  |
| 31  | e     | 407 | Q7G  | C1B  |
| 31  | n     | 201 | Q7G  | C1B  |
| 31  | n     | 201 | Q7G  | C1C  |

All (907) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | A1    | 601 | ATP  | PB-O3B-PG-O2G   |
| 26  | A2    | 601 | ATP  | PB-O3B-PG-O2G   |
| 26  | B1    | 601 | ATP  | PB-O3B-PG-O3G   |
| 26  | B2    | 601 | ATP  | PB-O3B-PG-O3G   |
| 26  | C1    | 601 | ATP  | PB-O3B-PG-O2G   |
| 26  | C2    | 601 | ATP  | PB-O3B-PG-O2G   |
| 26  | F1    | 601 | ATP  | PB-O3B-PG-O2G   |
| 26  | F2    | 601 | ATP  | PB-O3B-PG-O2G   |
| 28  | C     | 201 | CDL  | CB3-OB5-PB2-OB2 |
| 28  | C     | 201 | CDL  | CB3-OB5-PB2-OB4 |
| 28  | E     | 403 | CDL  | CB2-OB2-PB2-OB3 |
| 28  | E     | 403 | CDL  | CB2-OB2-PB2-OB4 |
| 28  | E     | 403 | CDL  | CB2-OB2-PB2-OB5 |
| 28  | E     | 403 | CDL  | CB3-OB5-PB2-OB2 |
| 28  | E     | 403 | CDL  | CB3-OB5-PB2-OB3 |
| 28  | E     | 404 | CDL  | CA3-OA5-PA1-OA2 |
| 28  | E     | 404 | CDL  | CA3-OA5-PA1-OA3 |
| 28  | E     | 404 | CDL  | CA3-OA5-PA1-OA4 |
| 28  | E     | 406 | CDL  | CA3-OA5-PA1-OA2 |
| 28  | E     | 406 | CDL  | CA3-OA5-PA1-OA4 |
| 28  | E     | 406 | CDL  | CB3-OB5-PB2-OB2 |
| 28  | E     | 406 | CDL  | CB3-OB5-PB2-OB3 |
| 28  | E     | 406 | CDL  | CB3-OB5-PB2-OB4 |
| 28  | E     | 407 | CDL  | CA3-OA5-PA1-OA2 |
| 28  | E     | 407 | CDL  | CA3-OA5-PA1-OA3 |
| 28  | E     | 407 | CDL  | CA3-OA5-PA1-OA4 |
| 28  | E     | 407 | CDL  | CB3-OB5-PB2-OB2 |
| 28  | E     | 407 | CDL  | CB3-OB5-PB2-OB4 |
| 28  | E     | 407 | CDL  | OB5-CB3-CB4-OB6 |
| 28  | F     | 201 | CDL  | CA2-OA2-PA1-OA4 |
| 28  | F     | 201 | CDL  | CA2-OA2-PA1-OA5 |
| 28  | F     | 201 | CDL  | CB3-OB5-PB2-OB2 |
| 28  | J     | 202 | CDL  | CB2-C1-CA2-OA2  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 28  | J     | 202 | CDL  | CA2-OA2-PA1-OA3 |
| 28  | J     | 202 | CDL  | CA2-OA2-PA1-OA5 |
| 28  | J     | 202 | CDL  | CA3-OA5-PA1-OA2 |
| 28  | J     | 202 | CDL  | CA3-OA5-PA1-OA3 |
| 28  | J     | 202 | CDL  | CA3-OA5-PA1-OA4 |
| 28  | J     | 203 | CDL  | CA2-OA2-PA1-OA4 |
| 28  | J     | 203 | CDL  | CA2-OA2-PA1-OA5 |
| 28  | J     | 203 | CDL  | CB3-OB5-PB2-OB2 |
| 28  | J     | 203 | CDL  | CB3-OB5-PB2-OB4 |
| 28  | L     | 101 | CDL  | CA2-OA2-PA1-OA3 |
| 28  | L     | 101 | CDL  | CA2-OA2-PA1-OA4 |
| 28  | L     | 101 | CDL  | CA2-OA2-PA1-OA5 |
| 28  | L     | 101 | CDL  | CA3-OA5-PA1-OA2 |
| 28  | L     | 101 | CDL  | CB2-OB2-PB2-OB4 |
| 28  | L     | 101 | CDL  | CB2-OB2-PB2-OB5 |
| 28  | M     | 201 | CDL  | CA3-OA5-PA1-OA2 |
| 28  | M     | 201 | CDL  | CA3-OA5-PA1-OA3 |
| 28  | M     | 201 | CDL  | CA3-OA5-PA1-OA4 |
| 28  | M     | 201 | CDL  | OA6-CA4-CA6-OA8 |
| 28  | M     | 201 | CDL  | CB2-OB2-PB2-OB3 |
| 28  | M     | 201 | CDL  | CB2-OB2-PB2-OB4 |
| 28  | M     | 201 | CDL  | CB2-OB2-PB2-OB5 |
| 28  | M     | 201 | CDL  | CB3-OB5-PB2-OB2 |
| 28  | M     | 201 | CDL  | CB3-OB5-PB2-OB3 |
| 28  | Q     | 101 | CDL  | CA2-OA2-PA1-OA5 |
| 28  | Q     | 101 | CDL  | OA5-CA3-CA4-OA6 |
| 28  | Q     | 101 | CDL  | CB2-OB2-PB2-OB3 |
| 28  | Q     | 101 | CDL  | CB2-OB2-PB2-OB4 |
| 28  | Q     | 101 | CDL  | CB3-OB5-PB2-OB3 |
| 28  | c     | 201 | CDL  | CB3-OB5-PB2-OB2 |
| 28  | c     | 201 | CDL  | CB3-OB5-PB2-OB4 |
| 28  | e     | 401 | CDL  | CB2-OB2-PB2-OB3 |
| 28  | e     | 401 | CDL  | CB2-OB2-PB2-OB4 |
| 28  | e     | 401 | CDL  | CB2-OB2-PB2-OB5 |
| 28  | e     | 401 | CDL  | CB3-OB5-PB2-OB2 |
| 28  | e     | 401 | CDL  | CB3-OB5-PB2-OB3 |
| 28  | e     | 402 | CDL  | CA3-OA5-PA1-OA2 |
| 28  | e     | 402 | CDL  | CA3-OA5-PA1-OA3 |
| 28  | e     | 402 | CDL  | CA3-OA5-PA1-OA4 |
| 28  | e     | 404 | CDL  | CA3-OA5-PA1-OA2 |
| 28  | e     | 404 | CDL  | CA3-OA5-PA1-OA4 |
| 28  | e     | 404 | CDL  | CB3-OB5-PB2-OB2 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 28  | e     | 404 | CDL  | CB3-OB5-PB2-OB3 |
| 28  | e     | 404 | CDL  | CB3-OB5-PB2-OB4 |
| 28  | e     | 405 | CDL  | CA3-OA5-PA1-OA2 |
| 28  | e     | 405 | CDL  | CA3-OA5-PA1-OA3 |
| 28  | e     | 405 | CDL  | CA3-OA5-PA1-OA4 |
| 28  | e     | 405 | CDL  | CB3-OB5-PB2-OB2 |
| 28  | e     | 405 | CDL  | CB3-OB5-PB2-OB4 |
| 28  | e     | 405 | CDL  | OB5-CB3-CB4-OB6 |
| 28  | f     | 201 | CDL  | CA2-OA2-PA1-OA4 |
| 28  | f     | 201 | CDL  | CA2-OA2-PA1-OA5 |
| 28  | f     | 201 | CDL  | CB3-OB5-PB2-OB2 |
| 28  | j     | 201 | CDL  | CB2-C1-CA2-OA2  |
| 28  | j     | 201 | CDL  | CA2-OA2-PA1-OA3 |
| 28  | j     | 201 | CDL  | CA2-OA2-PA1-OA5 |
| 28  | j     | 201 | CDL  | CA3-OA5-PA1-OA2 |
| 28  | j     | 201 | CDL  | CA3-OA5-PA1-OA3 |
| 28  | j     | 201 | CDL  | CA3-OA5-PA1-OA4 |
| 28  | j     | 202 | CDL  | CA2-OA2-PA1-OA4 |
| 28  | j     | 202 | CDL  | CA2-OA2-PA1-OA5 |
| 28  | j     | 202 | CDL  | CB3-OB5-PB2-OB2 |
| 28  | j     | 202 | CDL  | CB3-OB5-PB2-OB4 |
| 28  | l     | 101 | CDL  | CA2-OA2-PA1-OA3 |
| 28  | l     | 101 | CDL  | CA2-OA2-PA1-OA4 |
| 28  | l     | 101 | CDL  | CA2-OA2-PA1-OA5 |
| 28  | l     | 101 | CDL  | CA3-OA5-PA1-OA2 |
| 28  | l     | 101 | CDL  | CB2-OB2-PB2-OB5 |
| 28  | m     | 201 | CDL  | CA3-OA5-PA1-OA2 |
| 28  | m     | 201 | CDL  | CA3-OA5-PA1-OA3 |
| 28  | m     | 201 | CDL  | CA3-OA5-PA1-OA4 |
| 28  | m     | 201 | CDL  | OA6-CA4-CA6-OA8 |
| 28  | m     | 201 | CDL  | CB2-OB2-PB2-OB3 |
| 28  | m     | 201 | CDL  | CB2-OB2-PB2-OB4 |
| 28  | m     | 201 | CDL  | CB2-OB2-PB2-OB5 |
| 28  | m     | 201 | CDL  | CB3-OB5-PB2-OB2 |
| 28  | m     | 201 | CDL  | CB3-OB5-PB2-OB3 |
| 28  | q     | 101 | CDL  | CA2-OA2-PA1-OA5 |
| 28  | q     | 101 | CDL  | OA5-CA3-CA4-OA6 |
| 28  | q     | 101 | CDL  | CB2-OB2-PB2-OB3 |
| 28  | q     | 101 | CDL  | CB2-OB2-PB2-OB4 |
| 28  | q     | 101 | CDL  | CB3-OB5-PB2-OB3 |
| 30  | J     | 201 | LMT  | O5'-C1'-O1'-C1  |
| 30  | J     | 201 | LMT  | C2-C1-O1'-C1'   |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 30  | j     | 204 | LMT  | O5'-C1'-O1'-C1 |
| 30  | j     | 204 | LMT  | C2-C1-O1'-C1'  |
| 32  | F     | 202 | PEE  | C1-O3P-P-O2P   |
| 32  | F     | 202 | PEE  | C1-O3P-P-O1P   |
| 32  | F     | 202 | PEE  | C1-O3P-P-O4P   |
| 32  | R     | 101 | PEE  | C4-O4P-P-O3P   |
| 32  | R     | 101 | PEE  | C4-O4P-P-O2P   |
| 32  | R     | 101 | PEE  | C4-O4P-P-O1P   |
| 32  | R     | 101 | PEE  | O4P-C4-C5-N    |
| 32  | f     | 202 | PEE  | C1-O3P-P-O2P   |
| 32  | f     | 202 | PEE  | C1-O3P-P-O1P   |
| 32  | f     | 202 | PEE  | C1-O3P-P-O4P   |
| 32  | r     | 101 | PEE  | C4-O4P-P-O3P   |
| 32  | r     | 101 | PEE  | C4-O4P-P-O2P   |
| 32  | r     | 101 | PEE  | C4-O4P-P-O1P   |
| 32  | r     | 101 | PEE  | O4P-C4-C5-N    |
| 33  | F     | 203 | PC1  | C11-O13-P-O12  |
| 33  | F     | 203 | PC1  | C11-O13-P-O11  |
| 33  | F     | 203 | PC1  | C1-O11-P-O14   |
| 33  | F     | 203 | PC1  | C1-O11-P-O13   |
| 33  | F     | 204 | PC1  | C11-O13-P-O12  |
| 33  | F     | 204 | PC1  | C11-O13-P-O11  |
| 33  | F     | 204 | PC1  | O13-C11-C12-N  |
| 33  | I     | 201 | PC1  | C11-O13-P-O12  |
| 33  | I     | 201 | PC1  | C11-O13-P-O14  |
| 33  | I     | 201 | PC1  | C11-O13-P-O11  |
| 33  | I     | 201 | PC1  | O13-C11-C12-N  |
| 33  | J     | 204 | PC1  | C11-O13-P-O14  |
| 33  | J     | 204 | PC1  | C11-O13-P-O11  |
| 33  | J     | 204 | PC1  | C1-O11-P-O12   |
| 33  | J     | 204 | PC1  | C1-O11-P-O14   |
| 33  | J     | 204 | PC1  | C1-O11-P-O13   |
| 33  | f     | 203 | PC1  | C11-O13-P-O12  |
| 33  | f     | 203 | PC1  | C11-O13-P-O11  |
| 33  | f     | 203 | PC1  | C1-O11-P-O14   |
| 33  | f     | 203 | PC1  | C1-O11-P-O13   |
| 33  | f     | 204 | PC1  | C11-O13-P-O12  |
| 33  | f     | 204 | PC1  | C11-O13-P-O11  |
| 33  | f     | 204 | PC1  | O13-C11-C12-N  |
| 33  | i     | 201 | PC1  | C11-O13-P-O12  |
| 33  | i     | 201 | PC1  | C11-O13-P-O14  |
| 33  | i     | 201 | PC1  | C11-O13-P-O11  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 33  | i     | 201 | PC1  | O13-C11-C12-N   |
| 33  | j     | 203 | PC1  | C11-O13-P-O14   |
| 33  | j     | 203 | PC1  | C11-O13-P-O11   |
| 33  | j     | 203 | PC1  | C1-O11-P-O12    |
| 33  | j     | 203 | PC1  | C1-O11-P-O14    |
| 33  | j     | 203 | PC1  | C1-O11-P-O13    |
| 34  | H1    | 201 | UTP  | C5'-O5'-PA-O2A  |
| 34  | H1    | 201 | UTP  | C5'-O5'-PA-O3A  |
| 34  | H2    | 201 | UTP  | C5'-O5'-PA-O2A  |
| 34  | H2    | 201 | UTP  | C5'-O5'-PA-O3A  |
| 28  | C     | 201 | CDL  | O1-C1-CA2-OA2   |
| 28  | J     | 202 | CDL  | O1-C1-CA2-OA2   |
| 28  | M     | 201 | CDL  | O1-C1-CB2-OB2   |
| 28  | c     | 201 | CDL  | O1-C1-CA2-OA2   |
| 28  | j     | 201 | CDL  | O1-C1-CA2-OA2   |
| 28  | m     | 201 | CDL  | O1-C1-CB2-OB2   |
| 28  | E     | 405 | CDL  | C11-CA5-OA6-CA4 |
| 28  | e     | 403 | CDL  | C11-CA5-OA6-CA4 |
| 28  | E     | 405 | CDL  | OA7-CA5-OA6-CA4 |
| 28  | e     | 403 | CDL  | OA7-CA5-OA6-CA4 |
| 31  | E     | 402 | Q7G  | O5B-C1B-O1B-C24 |
| 31  | N     | 201 | Q7G  | O5B-C1B-O1B-C24 |
| 31  | e     | 407 | Q7G  | O5B-C1B-O1B-C24 |
| 31  | n     | 201 | Q7G  | O5B-C1B-O1B-C24 |
| 28  | M     | 201 | CDL  | CA2-C1-CB2-OB2  |
| 28  | Q     | 101 | CDL  | CA2-C1-CB2-OB2  |
| 28  | m     | 201 | CDL  | CA2-C1-CB2-OB2  |
| 28  | q     | 101 | CDL  | CA2-C1-CB2-OB2  |
| 28  | E     | 403 | CDL  | C77-C78-C79-C80 |
| 28  | e     | 401 | CDL  | C77-C78-C79-C80 |
| 30  | J     | 201 | LMT  | C2'-C1'-O1'-C1  |
| 30  | j     | 204 | LMT  | C2'-C1'-O1'-C1  |
| 31  | E     | 402 | Q7G  | C2B-C1B-O1B-C24 |
| 31  | N     | 201 | Q7G  | C2B-C1B-O1B-C24 |
| 31  | e     | 407 | Q7G  | C2B-C1B-O1B-C24 |
| 31  | n     | 201 | Q7G  | C2B-C1B-O1B-C24 |
| 28  | L     | 101 | CDL  | O1-C1-CA2-OA2   |
| 28  | l     | 101 | CDL  | O1-C1-CA2-OA2   |
| 28  | E     | 404 | CDL  | C31-CA7-OA8-CA6 |
| 28  | e     | 402 | CDL  | C31-CA7-OA8-CA6 |
| 28  | M     | 201 | CDL  | C34-C35-C36-C37 |
| 28  | m     | 201 | CDL  | C34-C35-C36-C37 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 32  | R     | 101 | PEE  | C31-C32-C33-C34 |
| 32  | r     | 101 | PEE  | C31-C32-C33-C34 |
| 28  | E     | 407 | CDL  | CA7-C31-C32-C33 |
| 28  | M     | 201 | CDL  | CA5-C11-C12-C13 |
| 28  | e     | 405 | CDL  | CA7-C31-C32-C33 |
| 28  | m     | 201 | CDL  | CA5-C11-C12-C13 |
| 28  | E     | 406 | CDL  | O1-C1-CA2-OA2   |
| 28  | Q     | 101 | CDL  | O1-C1-CB2-OB2   |
| 28  | e     | 404 | CDL  | O1-C1-CA2-OA2   |
| 28  | q     | 101 | CDL  | O1-C1-CB2-OB2   |
| 28  | M     | 201 | CDL  | CB5-C51-C52-C53 |
| 28  | m     | 201 | CDL  | CB5-C51-C52-C53 |
| 28  | E     | 407 | CDL  | C11-CA5-OA6-CA4 |
| 28  | M     | 201 | CDL  | C51-CB5-OB6-CB4 |
| 28  | e     | 405 | CDL  | C11-CA5-OA6-CA4 |
| 28  | m     | 201 | CDL  | C51-CB5-OB6-CB4 |
| 28  | E     | 404 | CDL  | OA9-CA7-OA8-CA6 |
| 28  | e     | 402 | CDL  | OA9-CA7-OA8-CA6 |
| 28  | E     | 407 | CDL  | OA7-CA5-OA6-CA4 |
| 28  | e     | 405 | CDL  | OA7-CA5-OA6-CA4 |
| 28  | C     | 201 | CDL  | CB2-C1-CA2-OA2  |
| 28  | J     | 203 | CDL  | CA2-C1-CB2-OB2  |
| 28  | c     | 201 | CDL  | CB2-C1-CA2-OA2  |
| 28  | j     | 202 | CDL  | CA2-C1-CB2-OB2  |
| 28  | M     | 201 | CDL  | OB7-CB5-OB6-CB4 |
| 28  | m     | 201 | CDL  | OB7-CB5-OB6-CB4 |
| 31  | E     | 402 | Q7G  | CG1-C22-C23-C48 |
| 31  | e     | 407 | Q7G  | CG1-C22-C23-C48 |
| 28  | E     | 406 | CDL  | O1-C1-CB2-OB2   |
| 28  | J     | 203 | CDL  | O1-C1-CB2-OB2   |
| 28  | e     | 404 | CDL  | O1-C1-CB2-OB2   |
| 28  | j     | 202 | CDL  | O1-C1-CB2-OB2   |
| 28  | E     | 404 | CDL  | C74-C75-C76-C77 |
| 28  | e     | 402 | CDL  | C74-C75-C76-C77 |
| 28  | M     | 201 | CDL  | OA5-CA3-CA4-OA6 |
| 28  | m     | 201 | CDL  | OA5-CA3-CA4-OA6 |
| 28  | Q     | 101 | CDL  | C11-CA5-OA6-CA4 |
| 28  | q     | 101 | CDL  | C11-CA5-OA6-CA4 |
| 28  | Q     | 101 | CDL  | OA7-CA5-OA6-CA4 |
| 28  | q     | 101 | CDL  | OA7-CA5-OA6-CA4 |
| 28  | J     | 202 | CDL  | CA7-C31-C32-C33 |
| 28  | j     | 201 | CDL  | CA7-C31-C32-C33 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 28  | J     | 203 | CDL  | C11-CA5-OA6-CA4 |
| 28  | j     | 202 | CDL  | C11-CA5-OA6-CA4 |
| 28  | J     | 203 | CDL  | C74-C75-C76-C77 |
| 28  | j     | 202 | CDL  | C74-C75-C76-C77 |
| 28  | J     | 203 | CDL  | C78-C79-C80-C81 |
| 28  | j     | 202 | CDL  | C78-C79-C80-C81 |
| 28  | E     | 406 | CDL  | CA2-C1-CB2-OB2  |
| 28  | e     | 404 | CDL  | CA2-C1-CB2-OB2  |
| 28  | e     | 403 | CDL  | C71-C72-C73-C74 |
| 28  | E     | 405 | CDL  | C71-C72-C73-C74 |
| 28  | J     | 203 | CDL  | OA7-CA5-OA6-CA4 |
| 28  | j     | 202 | CDL  | OA7-CA5-OA6-CA4 |
| 28  | J     | 202 | CDL  | C13-C14-C15-C16 |
| 28  | j     | 201 | CDL  | C13-C14-C15-C16 |
| 28  | M     | 201 | CDL  | CA7-C31-C32-C33 |
| 28  | m     | 201 | CDL  | CA7-C31-C32-C33 |
| 28  | C     | 201 | CDL  | C55-C56-C57-C58 |
| 28  | c     | 201 | CDL  | C55-C56-C57-C58 |
| 28  | E     | 405 | CDL  | C14-C15-C16-C17 |
| 28  | e     | 403 | CDL  | C14-C15-C16-C17 |
| 28  | E     | 406 | CDL  | C11-CA5-OA6-CA4 |
| 28  | J     | 203 | CDL  | C51-CB5-OB6-CB4 |
| 28  | e     | 404 | CDL  | C11-CA5-OA6-CA4 |
| 28  | j     | 202 | CDL  | C51-CB5-OB6-CB4 |
| 32  | F     | 202 | PEE  | C11-C10-O2-C2   |
| 32  | f     | 202 | PEE  | C11-C10-O2-C2   |
| 28  | M     | 201 | CDL  | C36-C37-C38-C39 |
| 28  | m     | 201 | CDL  | C36-C37-C38-C39 |
| 28  | j     | 202 | CDL  | C15-C16-C17-C18 |
| 28  | J     | 203 | CDL  | C15-C16-C17-C18 |
| 28  | q     | 101 | CDL  | CB7-C71-C72-C73 |
| 28  | E     | 405 | CDL  | C51-CB5-OB6-CB4 |
| 28  | e     | 403 | CDL  | C51-CB5-OB6-CB4 |
| 28  | E     | 407 | CDL  | C40-C41-C42-C43 |
| 28  | e     | 405 | CDL  | C40-C41-C42-C43 |
| 28  | J     | 202 | CDL  | C81-C82-C83-C84 |
| 28  | Q     | 101 | CDL  | CA5-C11-C12-C13 |
| 28  | Q     | 101 | CDL  | CB7-C71-C72-C73 |
| 28  | q     | 101 | CDL  | CA5-C11-C12-C13 |
| 28  | j     | 201 | CDL  | C81-C82-C83-C84 |
| 31  | N     | 201 | Q7G  | O5C-C5C-C6C-O6C |
| 31  | n     | 201 | Q7G  | O5C-C5C-C6C-O6C |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 28  | E     | 406 | CDL  | OA7-CA5-OA6-CA4 |
| 28  | J     | 203 | CDL  | OB7-CB5-OB6-CB4 |
| 28  | e     | 404 | CDL  | OA7-CA5-OA6-CA4 |
| 28  | j     | 202 | CDL  | OB7-CB5-OB6-CB4 |
| 28  | C     | 201 | CDL  | C34-C35-C36-C37 |
| 28  | E     | 406 | CDL  | C17-C18-C19-C20 |
| 28  | E     | 407 | CDL  | C56-C57-C58-C59 |
| 28  | c     | 201 | CDL  | C34-C35-C36-C37 |
| 28  | e     | 404 | CDL  | C17-C18-C19-C20 |
| 28  | e     | 405 | CDL  | C56-C57-C58-C59 |
| 28  | E     | 407 | CDL  | C71-C72-C73-C74 |
| 28  | e     | 405 | CDL  | C71-C72-C73-C74 |
| 28  | E     | 405 | CDL  | C78-C79-C80-C81 |
| 28  | C     | 201 | CDL  | OA5-CA3-CA4-CA6 |
| 28  | J     | 203 | CDL  | OA5-CA3-CA4-CA6 |
| 28  | M     | 201 | CDL  | OA5-CA3-CA4-CA6 |
| 28  | Q     | 101 | CDL  | OA5-CA3-CA4-CA6 |
| 28  | c     | 201 | CDL  | OA5-CA3-CA4-CA6 |
| 28  | j     | 202 | CDL  | OA5-CA3-CA4-CA6 |
| 28  | m     | 201 | CDL  | OA5-CA3-CA4-CA6 |
| 28  | q     | 101 | CDL  | OA5-CA3-CA4-CA6 |
| 28  | e     | 403 | CDL  | C78-C79-C80-C81 |
| 32  | F     | 202 | PEE  | C42-C43-C44-C45 |
| 32  | f     | 202 | PEE  | C42-C43-C44-C45 |
| 28  | M     | 201 | CDL  | C12-C13-C14-C15 |
| 28  | m     | 201 | CDL  | C12-C13-C14-C15 |
| 30  | J     | 201 | LMT  | O5B-C5B-C6B-O6B |
| 30  | j     | 204 | LMT  | O5B-C5B-C6B-O6B |
| 28  | J     | 202 | CDL  | C62-C63-C64-C65 |
| 28  | j     | 201 | CDL  | C62-C63-C64-C65 |
| 33  | F     | 203 | PC1  | C1-C2-C3-O31    |
| 28  | m     | 201 | CDL  | C73-C74-C75-C76 |
| 28  | M     | 201 | CDL  | C73-C74-C75-C76 |
| 28  | E     | 405 | CDL  | C17-C18-C19-C20 |
| 28  | E     | 407 | CDL  | C57-C58-C59-C60 |
| 28  | e     | 403 | CDL  | C17-C18-C19-C20 |
| 28  | e     | 405 | CDL  | C57-C58-C59-C60 |
| 28  | J     | 202 | CDL  | C34-C35-C36-C37 |
| 28  | j     | 201 | CDL  | C34-C35-C36-C37 |
| 28  | E     | 404 | CDL  | C11-C12-C13-C14 |
| 32  | R     | 101 | PEE  | C31-C30-O3-C3   |
| 32  | r     | 101 | PEE  | C31-C30-O3-C3   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 28  | e     | 402 | CDL  | C11-C12-C13-C14 |
| 32  | R     | 101 | PEE  | C17-C18-C19-C20 |
| 32  | r     | 101 | PEE  | C17-C18-C19-C20 |
| 28  | e     | 405 | CDL  | C53-C54-C55-C56 |
| 33  | I     | 201 | PC1  | C32-C31-O31-C3  |
| 33  | i     | 201 | PC1  | C32-C31-O31-C3  |
| 28  | C     | 201 | CDL  | CA4-CA6-OA8-CA7 |
| 28  | c     | 201 | CDL  | CA4-CA6-OA8-CA7 |
| 28  | F     | 201 | CDL  | C11-CA5-OA6-CA4 |
| 28  | f     | 201 | CDL  | C11-CA5-OA6-CA4 |
| 28  | E     | 407 | CDL  | C53-C54-C55-C56 |
| 28  | M     | 201 | CDL  | C33-C34-C35-C36 |
| 28  | m     | 201 | CDL  | C33-C34-C35-C36 |
| 32  | R     | 101 | PEE  | C22-C23-C24-C25 |
| 28  | f     | 201 | CDL  | C77-C78-C79-C80 |
| 32  | r     | 101 | PEE  | C22-C23-C24-C25 |
| 28  | F     | 201 | CDL  | C77-C78-C79-C80 |
| 28  | E     | 406 | CDL  | OB6-CB4-CB6-OB8 |
| 28  | F     | 201 | CDL  | OB6-CB4-CB6-OB8 |
| 28  | L     | 101 | CDL  | OA6-CA4-CA6-OA8 |
| 28  | e     | 404 | CDL  | OB6-CB4-CB6-OB8 |
| 28  | f     | 201 | CDL  | OB6-CB4-CB6-OB8 |
| 28  | l     | 101 | CDL  | OA6-CA4-CA6-OA8 |
| 28  | C     | 201 | CDL  | C51-C52-C53-C54 |
| 28  | c     | 201 | CDL  | C51-C52-C53-C54 |
| 28  | e     | 401 | CDL  | C18-C19-C20-C21 |
| 28  | E     | 403 | CDL  | C18-C19-C20-C21 |
| 28  | E     | 407 | CDL  | C76-C77-C78-C79 |
| 26  | F1    | 601 | ATP  | PG-O3B-PB-O1B   |
| 26  | F2    | 601 | ATP  | PG-O3B-PB-O1B   |
| 28  | E     | 403 | CDL  | C81-C82-C83-C84 |
| 28  | e     | 401 | CDL  | C81-C82-C83-C84 |
| 28  | e     | 405 | CDL  | C76-C77-C78-C79 |
| 28  | E     | 407 | CDL  | C11-C12-C13-C14 |
| 28  | e     | 405 | CDL  | C11-C12-C13-C14 |
| 28  | J     | 203 | CDL  | C76-C77-C78-C79 |
| 28  | j     | 202 | CDL  | C76-C77-C78-C79 |
| 28  | L     | 101 | CDL  | C14-C15-C16-C17 |
| 28  | l     | 101 | CDL  | C14-C15-C16-C17 |
| 32  | F     | 202 | PEE  | O4-C10-O2-C2    |
| 32  | f     | 202 | PEE  | O4-C10-O2-C2    |
| 30  | E     | 401 | LMT  | C2-C1-O1'-C1'   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | e     | 406 | LMT  | C2-C1-O1'-C1'   |
| 28  | C     | 201 | CDL  | CA4-CA3-OA5-PA1 |
| 28  | J     | 202 | CDL  | CA4-CA3-OA5-PA1 |
| 28  | c     | 201 | CDL  | CA4-CA3-OA5-PA1 |
| 28  | j     | 201 | CDL  | CA4-CA3-OA5-PA1 |
| 33  | F     | 204 | PC1  | C37-C38-C39-C3A |
| 33  | f     | 204 | PC1  | C37-C38-C39-C3A |
| 28  | C     | 201 | CDL  | C39-C40-C41-C42 |
| 28  | c     | 201 | CDL  | C39-C40-C41-C42 |
| 32  | R     | 101 | PEE  | C23-C24-C25-C26 |
| 32  | r     | 101 | PEE  | C23-C24-C25-C26 |
| 28  | E     | 405 | CDL  | O1-C1-CA2-OA2   |
| 28  | e     | 403 | CDL  | O1-C1-CA2-OA2   |
| 28  | m     | 201 | CDL  | C83-C84-C85-C86 |
| 28  | M     | 201 | CDL  | C83-C84-C85-C86 |
| 28  | j     | 202 | CDL  | C79-C80-C81-C82 |
| 32  | R     | 101 | PEE  | O5-C30-O3-C3    |
| 32  | r     | 101 | PEE  | O5-C30-O3-C3    |
| 28  | J     | 203 | CDL  | C79-C80-C81-C82 |
| 28  | E     | 404 | CDL  | C78-C79-C80-C81 |
| 28  | e     | 402 | CDL  | C78-C79-C80-C81 |
| 28  | l     | 101 | CDL  | C31-C32-C33-C34 |
| 28  | E     | 407 | CDL  | CB3-CB4-CB6-OB8 |
| 28  | e     | 405 | CDL  | CB3-CB4-CB6-OB8 |
| 32  | F     | 202 | PEE  | C1-C2-C3-O3     |
| 32  | R     | 101 | PEE  | C1-C2-C3-O3     |
| 32  | f     | 202 | PEE  | C1-C2-C3-O3     |
| 32  | r     | 101 | PEE  | C1-C2-C3-O3     |
| 33  | f     | 203 | PC1  | C1-C2-C3-O31    |
| 28  | L     | 101 | CDL  | C31-C32-C33-C34 |
| 28  | L     | 101 | CDL  | C64-C65-C66-C67 |
| 28  | l     | 101 | CDL  | C64-C65-C66-C67 |
| 32  | r     | 101 | PEE  | C43-C44-C45-C46 |
| 32  | R     | 101 | PEE  | C43-C44-C45-C46 |
| 28  | E     | 405 | CDL  | C12-C13-C14-C15 |
| 28  | e     | 403 | CDL  | C12-C13-C14-C15 |
| 28  | E     | 407 | CDL  | CB7-C71-C72-C73 |
| 28  | e     | 405 | CDL  | CB7-C71-C72-C73 |
| 28  | C     | 201 | CDL  | OA5-CA3-CA4-OA6 |
| 28  | E     | 403 | CDL  | OB5-CB3-CB4-OB6 |
| 28  | F     | 201 | CDL  | OA5-CA3-CA4-OA6 |
| 28  | c     | 201 | CDL  | OA5-CA3-CA4-OA6 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 28  | e     | 401 | CDL  | OB5-CB3-CB4-OB6 |
| 28  | f     | 201 | CDL  | OA5-CA3-CA4-OA6 |
| 28  | L     | 101 | CDL  | CA4-CA3-OA5-PA1 |
| 28  | l     | 101 | CDL  | CA4-CA3-OA5-PA1 |
| 33  | J     | 204 | PC1  | C2-C1-O11-P     |
| 33  | j     | 203 | PC1  | C2-C1-O11-P     |
| 31  | N     | 201 | Q7G  | C24-C23-C48-O1C |
| 31  | n     | 201 | Q7G  | C24-C23-C48-O1C |
| 33  | F     | 203 | PC1  | O21-C2-C3-O31   |
| 33  | f     | 203 | PC1  | O21-C2-C3-O31   |
| 33  | I     | 201 | PC1  | O32-C31-O31-C3  |
| 33  | i     | 201 | PC1  | O32-C31-O31-C3  |
| 28  | F     | 201 | CDL  | C12-C13-C14-C15 |
| 28  | f     | 201 | CDL  | C12-C13-C14-C15 |
| 28  | E     | 405 | CDL  | C83-C84-C85-C86 |
| 28  | e     | 403 | CDL  | C83-C84-C85-C86 |
| 28  | E     | 405 | CDL  | CB5-C51-C52-C53 |
| 28  | e     | 403 | CDL  | CB5-C51-C52-C53 |
| 28  | E     | 407 | CDL  | C59-C60-C61-C62 |
| 28  | e     | 405 | CDL  | C59-C60-C61-C62 |
| 32  | R     | 101 | PEE  | C39-C40-C41-C42 |
| 32  | r     | 101 | PEE  | C39-C40-C41-C42 |
| 28  | f     | 201 | CDL  | C13-C14-C15-C16 |
| 28  | F     | 201 | CDL  | C13-C14-C15-C16 |
| 28  | E     | 403 | CDL  | C43-C44-C45-C46 |
| 28  | e     | 401 | CDL  | C43-C44-C45-C46 |
| 28  | J     | 203 | CDL  | C72-C73-C74-C75 |
| 33  | i     | 201 | PC1  | C2C-C2D-C2E-C2F |
| 33  | I     | 201 | PC1  | C2C-C2D-C2E-C2F |
| 28  | j     | 202 | CDL  | C72-C73-C74-C75 |
| 28  | Q     | 101 | CDL  | CB2-C1-CA2-OA2  |
| 28  | q     | 101 | CDL  | CB2-C1-CA2-OA2  |
| 28  | j     | 201 | CDL  | C55-C56-C57-C58 |
| 28  | J     | 202 | CDL  | C55-C56-C57-C58 |
| 28  | E     | 407 | CDL  | OB5-CB3-CB4-CB6 |
| 28  | J     | 202 | CDL  | OB5-CB3-CB4-CB6 |
| 28  | e     | 405 | CDL  | OB5-CB3-CB4-CB6 |
| 28  | j     | 201 | CDL  | OB5-CB3-CB4-CB6 |
| 28  | m     | 201 | CDL  | C78-C79-C80-C81 |
| 28  | E     | 407 | CDL  | C78-C79-C80-C81 |
| 28  | M     | 201 | CDL  | C78-C79-C80-C81 |
| 28  | e     | 405 | CDL  | C78-C79-C80-C81 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 28  | E     | 407 | CDL  | C52-C53-C54-C55 |
| 28  | e     | 405 | CDL  | C52-C53-C54-C55 |
| 28  | e     | 401 | CDL  | C56-C57-C58-C59 |
| 28  | E     | 405 | CDL  | OB7-CB5-OB6-CB4 |
| 28  | F     | 201 | CDL  | OA7-CA5-OA6-CA4 |
| 28  | e     | 403 | CDL  | OB7-CB5-OB6-CB4 |
| 28  | f     | 201 | CDL  | OA7-CA5-OA6-CA4 |
| 28  | E     | 403 | CDL  | C56-C57-C58-C59 |
| 31  | N     | 201 | Q7G  | C16-C17-O20-CG1 |
| 31  | N     | 201 | Q7G  | C18-C17-O20-CG1 |
| 31  | n     | 201 | Q7G  | C16-C17-O20-CG1 |
| 31  | n     | 201 | Q7G  | C18-C17-O20-CG1 |
| 26  | B1    | 601 | ATP  | PB-O3B-PG-O2G   |
| 26  | B2    | 601 | ATP  | PB-O3B-PG-O2G   |
| 28  | E     | 404 | CDL  | CA6-CA4-OA6-CA5 |
| 28  | Q     | 101 | CDL  | CB3-CB4-OB6-CB5 |
| 28  | e     | 402 | CDL  | CA6-CA4-OA6-CA5 |
| 28  | q     | 101 | CDL  | CB3-CB4-OB6-CB5 |
| 28  | L     | 101 | CDL  | C31-CA7-OA8-CA6 |
| 28  | E     | 404 | CDL  | OB5-CB3-CB4-OB6 |
| 28  | E     | 407 | CDL  | OA5-CA3-CA4-OA6 |
| 28  | e     | 402 | CDL  | OB5-CB3-CB4-OB6 |
| 28  | e     | 405 | CDL  | OA5-CA3-CA4-OA6 |
| 28  | E     | 406 | CDL  | CB3-CB4-CB6-OB8 |
| 28  | e     | 404 | CDL  | CB3-CB4-CB6-OB8 |
| 28  | E     | 404 | CDL  | C34-C35-C36-C37 |
| 28  | e     | 402 | CDL  | C34-C35-C36-C37 |
| 28  | j     | 201 | CDL  | C77-C78-C79-C80 |
| 28  | l     | 101 | CDL  | C31-CA7-OA8-CA6 |
| 28  | C     | 201 | CDL  | C83-C84-C85-C86 |
| 28  | J     | 202 | CDL  | C77-C78-C79-C80 |
| 28  | c     | 201 | CDL  | C83-C84-C85-C86 |
| 28  | E     | 405 | CDL  | OA6-CA4-CA6-OA8 |
| 28  | e     | 403 | CDL  | OA6-CA4-CA6-OA8 |
| 32  | R     | 101 | PEE  | O2-C2-C3-O3     |
| 32  | r     | 101 | PEE  | O2-C2-C3-O3     |
| 28  | E     | 403 | CDL  | C13-C14-C15-C16 |
| 28  | e     | 401 | CDL  | C13-C14-C15-C16 |
| 28  | J     | 203 | CDL  | C61-C62-C63-C64 |
| 28  | j     | 202 | CDL  | C61-C62-C63-C64 |
| 28  | M     | 201 | CDL  | C42-C43-C44-C45 |
| 28  | m     | 201 | CDL  | C42-C43-C44-C45 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 30  | j     | 204 | LMT  | C2-C3-C4-C5     |
| 30  | J     | 201 | LMT  | C2-C3-C4-C5     |
| 26  | B2    | 601 | ATP  | PA-O3A-PB-O1B   |
| 26  | C1    | 601 | ATP  | PA-O3A-PB-O2B   |
| 26  | C2    | 601 | ATP  | PA-O3A-PB-O2B   |
| 33  | F     | 203 | PC1  | O13-C11-C12-N   |
| 33  | J     | 204 | PC1  | O13-C11-C12-N   |
| 33  | f     | 203 | PC1  | O13-C11-C12-N   |
| 33  | j     | 203 | PC1  | O13-C11-C12-N   |
| 28  | e     | 402 | CDL  | C81-C82-C83-C84 |
| 28  | E     | 406 | CDL  | CB2-C1-CA2-OA2  |
| 28  | e     | 404 | CDL  | CB2-C1-CA2-OA2  |
| 28  | E     | 404 | CDL  | C81-C82-C83-C84 |
| 28  | E     | 403 | CDL  | OB5-CB3-CB4-CB6 |
| 28  | E     | 406 | CDL  | OA5-CA3-CA4-CA6 |
| 28  | e     | 401 | CDL  | OB5-CB3-CB4-CB6 |
| 28  | e     | 404 | CDL  | OA5-CA3-CA4-CA6 |
| 32  | R     | 101 | PEE  | O4-C10-O2-C2    |
| 32  | r     | 101 | PEE  | O4-C10-O2-C2    |
| 33  | J     | 204 | PC1  | C3C-C3D-C3E-C3F |
| 33  | j     | 203 | PC1  | C3C-C3D-C3E-C3F |
| 28  | e     | 402 | CDL  | C75-C76-C77-C78 |
| 28  | E     | 404 | CDL  | C75-C76-C77-C78 |
| 28  | L     | 101 | CDL  | OA9-CA7-OA8-CA6 |
| 28  | l     | 101 | CDL  | OA9-CA7-OA8-CA6 |
| 28  | E     | 404 | CDL  | C1-CB2-OB2-PB2  |
| 28  | F     | 201 | CDL  | CB4-CB3-OB5-PB2 |
| 28  | J     | 203 | CDL  | CB4-CB3-OB5-PB2 |
| 28  | e     | 402 | CDL  | C1-CB2-OB2-PB2  |
| 28  | f     | 201 | CDL  | CB4-CB3-OB5-PB2 |
| 28  | j     | 202 | CDL  | CB4-CB3-OB5-PB2 |
| 32  | R     | 101 | PEE  | C2-C1-O3P-P     |
| 32  | r     | 101 | PEE  | C2-C1-O3P-P     |
| 32  | r     | 101 | PEE  | C13-C14-C15-C16 |
| 28  | E     | 406 | CDL  | OA5-CA3-CA4-OA6 |
| 28  | J     | 202 | CDL  | OB5-CB3-CB4-OB6 |
| 28  | J     | 203 | CDL  | OA5-CA3-CA4-OA6 |
| 28  | e     | 404 | CDL  | OA5-CA3-CA4-OA6 |
| 28  | j     | 201 | CDL  | OB5-CB3-CB4-OB6 |
| 28  | j     | 202 | CDL  | OA5-CA3-CA4-OA6 |
| 32  | R     | 101 | PEE  | C13-C14-C15-C16 |
| 28  | M     | 201 | CDL  | C20-C21-C22-C23 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 28  | m     | 201 | CDL  | C20-C21-C22-C23 |
| 28  | C     | 201 | CDL  | C62-C63-C64-C65 |
| 28  | c     | 201 | CDL  | C62-C63-C64-C65 |
| 28  | E     | 407 | CDL  | OB6-CB4-CB6-OB8 |
| 28  | e     | 405 | CDL  | OB6-CB4-CB6-OB8 |
| 32  | F     | 202 | PEE  | O2-C2-C3-O3     |
| 32  | f     | 202 | PEE  | O2-C2-C3-O3     |
| 28  | C     | 201 | CDL  | CA3-CA4-CA6-OA8 |
| 28  | M     | 201 | CDL  | CA3-CA4-CA6-OA8 |
| 28  | c     | 201 | CDL  | CA3-CA4-CA6-OA8 |
| 28  | m     | 201 | CDL  | CA3-CA4-CA6-OA8 |
| 31  | E     | 402 | Q7G  | CG1-C22-C23-C24 |
| 31  | e     | 407 | Q7G  | CG1-C22-C23-C24 |
| 31  | E     | 402 | Q7G  | C23-C24-O1B-C1B |
| 31  | e     | 407 | Q7G  | C23-C24-O1B-C1B |
| 32  | R     | 101 | PEE  | C38-C39-C40-C41 |
| 32  | r     | 101 | PEE  | C38-C39-C40-C41 |
| 28  | q     | 101 | CDL  | C77-C78-C79-C80 |
| 28  | E     | 404 | CDL  | C17-C18-C19-C20 |
| 28  | Q     | 101 | CDL  | C77-C78-C79-C80 |
| 28  | e     | 402 | CDL  | C17-C18-C19-C20 |
| 28  | e     | 402 | CDL  | C79-C80-C81-C82 |
| 28  | E     | 404 | CDL  | C53-C54-C55-C56 |
| 26  | A1    | 601 | ATP  | C5'-O5'-PA-O1A  |
| 26  | A2    | 601 | ATP  | C5'-O5'-PA-O1A  |
| 26  | C1    | 601 | ATP  | C5'-O5'-PA-O1A  |
| 26  | C2    | 601 | ATP  | C5'-O5'-PA-O1A  |
| 26  | F1    | 601 | ATP  | C5'-O5'-PA-O1A  |
| 26  | F2    | 601 | ATP  | C5'-O5'-PA-O1A  |
| 28  | C     | 201 | CDL  | CA3-OA5-PA1-OA3 |
| 28  | C     | 201 | CDL  | CB2-OB2-PB2-OB3 |
| 28  | E     | 403 | CDL  | CB3-OB5-PB2-OB4 |
| 28  | E     | 405 | CDL  | CB2-OB2-PB2-OB3 |
| 28  | E     | 407 | CDL  | CB3-OB5-PB2-OB3 |
| 28  | F     | 201 | CDL  | CB3-OB5-PB2-OB3 |
| 28  | J     | 202 | CDL  | CA2-OA2-PA1-OA4 |
| 28  | J     | 203 | CDL  | CA2-OA2-PA1-OA3 |
| 28  | L     | 101 | CDL  | CA3-OA5-PA1-OA3 |
| 28  | Q     | 101 | CDL  | CA2-OA2-PA1-OA3 |
| 28  | Q     | 101 | CDL  | CA3-OA5-PA1-OA3 |
| 28  | Q     | 101 | CDL  | CB2-OB2-PB2-OB5 |
| 28  | c     | 201 | CDL  | CA3-OA5-PA1-OA3 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 28  | c     | 201 | CDL  | CB2-OB2-PB2-OB3 |
| 28  | e     | 401 | CDL  | CB3-OB5-PB2-OB4 |
| 28  | e     | 403 | CDL  | CB2-OB2-PB2-OB3 |
| 28  | e     | 405 | CDL  | CB3-OB5-PB2-OB3 |
| 28  | f     | 201 | CDL  | CB3-OB5-PB2-OB3 |
| 28  | j     | 201 | CDL  | CA2-OA2-PA1-OA4 |
| 28  | j     | 202 | CDL  | CA2-OA2-PA1-OA3 |
| 28  | l     | 101 | CDL  | CA3-OA5-PA1-OA3 |
| 28  | l     | 101 | CDL  | CB2-OB2-PB2-OB4 |
| 28  | q     | 101 | CDL  | CA2-OA2-PA1-OA3 |
| 28  | q     | 101 | CDL  | CA3-OA5-PA1-OA3 |
| 28  | q     | 101 | CDL  | CB2-OB2-PB2-OB5 |
| 32  | F     | 202 | PEE  | C4-O4P-P-O3P    |
| 32  | F     | 202 | PEE  | C4-O4P-P-O2P    |
| 32  | F     | 202 | PEE  | C4-O4P-P-O1P    |
| 32  | f     | 202 | PEE  | C4-O4P-P-O3P    |
| 32  | f     | 202 | PEE  | C4-O4P-P-O2P    |
| 32  | f     | 202 | PEE  | C4-O4P-P-O1P    |
| 33  | F     | 203 | PC1  | C1-O11-P-O12    |
| 33  | f     | 203 | PC1  | C1-O11-P-O12    |
| 28  | e     | 402 | CDL  | C53-C54-C55-C56 |
| 28  | E     | 404 | CDL  | C79-C80-C81-C82 |
| 28  | J     | 202 | CDL  | C72-C73-C74-C75 |
| 28  | e     | 403 | CDL  | C62-C63-C64-C65 |
| 28  | j     | 201 | CDL  | C72-C73-C74-C75 |
| 28  | E     | 405 | CDL  | C62-C63-C64-C65 |
| 28  | E     | 403 | CDL  | CB4-CB3-OB5-PB2 |
| 28  | E     | 404 | CDL  | CA4-CA3-OA5-PA1 |
| 28  | E     | 407 | CDL  | CA4-CA3-OA5-PA1 |
| 28  | e     | 401 | CDL  | CB4-CB3-OB5-PB2 |
| 28  | e     | 402 | CDL  | CA4-CA3-OA5-PA1 |
| 28  | e     | 405 | CDL  | CA4-CA3-OA5-PA1 |
| 28  | E     | 403 | CDL  | C53-C54-C55-C56 |
| 29  | D1    | 601 | ADP  | PA-O3A-PB-O1B   |
| 29  | D2    | 601 | ADP  | PA-O3A-PB-O1B   |
| 28  | e     | 401 | CDL  | C53-C54-C55-C56 |
| 28  | E     | 406 | CDL  | CA6-CA4-OA6-CA5 |
| 28  | J     | 203 | CDL  | CB3-CB4-OB6-CB5 |
| 28  | e     | 404 | CDL  | CA6-CA4-OA6-CA5 |
| 28  | j     | 202 | CDL  | CB3-CB4-OB6-CB5 |
| 32  | r     | 101 | PEE  | C34-C35-C36-C37 |
| 32  | R     | 101 | PEE  | C34-C35-C36-C37 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 28  | E     | 404 | CDL  | OB5-CB3-CB4-CB6 |
| 28  | E     | 407 | CDL  | OA5-CA3-CA4-CA6 |
| 28  | e     | 402 | CDL  | OB5-CB3-CB4-CB6 |
| 28  | e     | 405 | CDL  | OA5-CA3-CA4-CA6 |
| 32  | r     | 101 | PEE  | C36-C37-C38-C39 |
| 33  | F     | 204 | PC1  | C21-C22-C23-C24 |
| 33  | f     | 204 | PC1  | C21-C22-C23-C24 |
| 28  | J     | 202 | CDL  | C1-CB2-OB2-PB2  |
| 28  | j     | 201 | CDL  | C1-CB2-OB2-PB2  |
| 33  | i     | 201 | PC1  | C2A-C2B-C2C-C2D |
| 28  | C     | 201 | CDL  | OA6-CA4-CA6-OA8 |
| 28  | E     | 405 | CDL  | OB6-CB4-CB6-OB8 |
| 28  | c     | 201 | CDL  | OA6-CA4-CA6-OA8 |
| 28  | e     | 403 | CDL  | OB6-CB4-CB6-OB8 |
| 33  | I     | 201 | PC1  | C2A-C2B-C2C-C2D |
| 32  | R     | 101 | PEE  | C11-C10-O2-C2   |
| 32  | r     | 101 | PEE  | C11-C10-O2-C2   |
| 32  | R     | 101 | PEE  | C36-C37-C38-C39 |
| 28  | E     | 405 | CDL  | C51-C52-C53-C54 |
| 28  | e     | 403 | CDL  | C51-C52-C53-C54 |
| 28  | F     | 201 | CDL  | CB3-CB4-CB6-OB8 |
| 28  | L     | 101 | CDL  | CA3-CA4-CA6-OA8 |
| 28  | f     | 201 | CDL  | CB3-CB4-CB6-OB8 |
| 28  | l     | 101 | CDL  | CA3-CA4-CA6-OA8 |
| 26  | A1    | 601 | ATP  | PG-O3B-PB-O2B   |
| 26  | A2    | 601 | ATP  | PG-O3B-PB-O2B   |
| 26  | B1    | 601 | ATP  | PA-O3A-PB-O1B   |
| 26  | B1    | 601 | ATP  | PA-O3A-PB-O2B   |
| 26  | B2    | 601 | ATP  | PA-O3A-PB-O2B   |
| 26  | C1    | 601 | ATP  | PG-O3B-PB-O2B   |
| 26  | C2    | 601 | ATP  | PG-O3B-PB-O2B   |
| 26  | F1    | 601 | ATP  | PG-O3B-PB-O2B   |
| 26  | F2    | 601 | ATP  | PG-O3B-PB-O2B   |
| 28  | M     | 201 | CDL  | C72-C73-C74-C75 |
| 28  | m     | 201 | CDL  | C72-C73-C74-C75 |
| 32  | F     | 202 | PEE  | C16-C17-C18-C19 |
| 32  | f     | 202 | PEE  | C16-C17-C18-C19 |
| 28  | e     | 402 | CDL  | C55-C56-C57-C58 |
| 28  | E     | 404 | CDL  | C55-C56-C57-C58 |
| 28  | C     | 201 | CDL  | C35-C36-C37-C38 |
| 28  | c     | 201 | CDL  | C35-C36-C37-C38 |
| 33  | J     | 204 | PC1  | O11-C1-C2-O21   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 33  | j     | 203 | PC1  | O11-C1-C2-O21   |
| 33  | F     | 204 | PC1  | O31-C31-C32-C33 |
| 33  | f     | 204 | PC1  | O31-C31-C32-C33 |
| 28  | F     | 201 | CDL  | C78-C79-C80-C81 |
| 28  | E     | 403 | CDL  | C80-C81-C82-C83 |
| 28  | f     | 201 | CDL  | C78-C79-C80-C81 |
| 28  | e     | 401 | CDL  | C80-C81-C82-C83 |
| 28  | E     | 405 | CDL  | CA3-CA4-CA6-OA8 |
| 28  | E     | 405 | CDL  | CB3-CB4-CB6-OB8 |
| 28  | e     | 403 | CDL  | CA3-CA4-CA6-OA8 |
| 28  | e     | 403 | CDL  | CB3-CB4-CB6-OB8 |
| 28  | j     | 202 | CDL  | CB3-CB4-CB6-OB8 |
| 28  | L     | 101 | CDL  | C36-C37-C38-C39 |
| 28  | l     | 101 | CDL  | C36-C37-C38-C39 |
| 28  | c     | 201 | CDL  | C40-C41-C42-C43 |
| 28  | J     | 202 | CDL  | CA3-CA4-OA6-CA5 |
| 28  | j     | 201 | CDL  | CA3-CA4-OA6-CA5 |
| 28  | C     | 201 | CDL  | C40-C41-C42-C43 |
| 32  | R     | 101 | PEE  | C33-C34-C35-C36 |
| 28  | e     | 402 | CDL  | C54-C55-C56-C57 |
| 32  | r     | 101 | PEE  | C33-C34-C35-C36 |
| 28  | E     | 404 | CDL  | C54-C55-C56-C57 |
| 28  | m     | 201 | CDL  | C21-C22-C23-C24 |
| 28  | M     | 201 | CDL  | C21-C22-C23-C24 |
| 28  | E     | 405 | CDL  | C1-CA2-OA2-PA1  |
| 28  | e     | 403 | CDL  | C1-CA2-OA2-PA1  |
| 28  | C     | 201 | CDL  | C42-C43-C44-C45 |
| 28  | E     | 406 | CDL  | C78-C79-C80-C81 |
| 28  | c     | 201 | CDL  | C42-C43-C44-C45 |
| 28  | e     | 404 | CDL  | C78-C79-C80-C81 |
| 33  | J     | 204 | PC1  | O11-C1-C2-C3    |
| 33  | j     | 203 | PC1  | O11-C1-C2-C3    |
| 28  | M     | 201 | CDL  | C75-C76-C77-C78 |
| 28  | m     | 201 | CDL  | C75-C76-C77-C78 |
| 28  | E     | 403 | CDL  | C16-C17-C18-C19 |
| 28  | e     | 401 | CDL  | C16-C17-C18-C19 |
| 28  | E     | 404 | CDL  | OA7-CA5-OA6-CA4 |
| 28  | e     | 402 | CDL  | OA7-CA5-OA6-CA4 |
| 28  | L     | 101 | CDL  | C39-C40-C41-C42 |
| 28  | l     | 101 | CDL  | C39-C40-C41-C42 |
| 28  | q     | 101 | CDL  | C75-C76-C77-C78 |
| 28  | F     | 201 | CDL  | O1-C1-CB2-OB2   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 28  | f     | 201 | CDL  | O1-C1-CB2-OB2   |
| 28  | Q     | 101 | CDL  | C75-C76-C77-C78 |
| 28  | Q     | 101 | CDL  | C1-CB2-OB2-PB2  |
| 28  | q     | 101 | CDL  | C1-CB2-OB2-PB2  |
| 28  | C     | 201 | CDL  | C38-C39-C40-C41 |
| 28  | E     | 404 | CDL  | C77-C78-C79-C80 |
| 28  | e     | 402 | CDL  | C77-C78-C79-C80 |
| 33  | f     | 204 | PC1  | O22-C21-O21-C2  |
| 28  | c     | 201 | CDL  | C38-C39-C40-C41 |
| 28  | E     | 403 | CDL  | C11-C12-C13-C14 |
| 28  | e     | 401 | CDL  | C11-C12-C13-C14 |
| 28  | j     | 201 | CDL  | C71-C72-C73-C74 |
| 28  | J     | 203 | CDL  | CB3-CB4-CB6-OB8 |
| 28  | C     | 201 | CDL  | C56-C57-C58-C59 |
| 28  | c     | 201 | CDL  | C56-C57-C58-C59 |
| 28  | J     | 202 | CDL  | C71-C72-C73-C74 |
| 28  | E     | 403 | CDL  | C37-C38-C39-C40 |
| 33  | F     | 204 | PC1  | O22-C21-O21-C2  |
| 28  | e     | 401 | CDL  | C37-C38-C39-C40 |
| 28  | e     | 403 | CDL  | C18-C19-C20-C21 |
| 28  | E     | 405 | CDL  | C18-C19-C20-C21 |
| 28  | j     | 202 | CDL  | C37-C38-C39-C40 |
| 33  | f     | 204 | PC1  | C24-C25-C26-C27 |
| 28  | L     | 101 | CDL  | CB2-C1-CA2-OA2  |
| 28  | l     | 101 | CDL  | CB2-C1-CA2-OA2  |
| 33  | F     | 204 | PC1  | C24-C25-C26-C27 |
| 28  | J     | 203 | CDL  | C37-C38-C39-C40 |
| 33  | F     | 204 | PC1  | C22-C21-O21-C2  |
| 33  | f     | 204 | PC1  | C22-C21-O21-C2  |
| 28  | C     | 201 | CDL  | C1-CB2-OB2-PB2  |
| 28  | c     | 201 | CDL  | C1-CB2-OB2-PB2  |
| 28  | E     | 403 | CDL  | C17-C18-C19-C20 |
| 28  | e     | 403 | CDL  | C23-C24-C25-C26 |
| 32  | R     | 101 | PEE  | C18-C19-C20-C21 |
| 32  | r     | 101 | PEE  | C18-C19-C20-C21 |
| 28  | E     | 405 | CDL  | C23-C24-C25-C26 |
| 26  | C1    | 601 | ATP  | PB-O3B-PG-O1G   |
| 26  | C2    | 601 | ATP  | PB-O3B-PG-O1G   |
| 26  | F1    | 601 | ATP  | PB-O3B-PG-O1G   |
| 26  | F2    | 601 | ATP  | PB-O3B-PG-O1G   |
| 28  | e     | 401 | CDL  | C17-C18-C19-C20 |
| 28  | E     | 405 | CDL  | C71-CB7-OB8-CB6 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 28  | e     | 403 | CDL  | C71-CB7-OB8-CB6 |
| 28  | F     | 201 | CDL  | C37-C38-C39-C40 |
| 26  | A1    | 601 | ATP  | PB-O3B-PG-O3G   |
| 26  | A2    | 601 | ATP  | PB-O3B-PG-O3G   |
| 32  | F     | 202 | PEE  | C36-C37-C38-C39 |
| 32  | f     | 202 | PEE  | C36-C37-C38-C39 |
| 28  | f     | 201 | CDL  | C37-C38-C39-C40 |
| 28  | M     | 201 | CDL  | C19-C20-C21-C22 |
| 28  | m     | 201 | CDL  | C19-C20-C21-C22 |
| 28  | E     | 405 | CDL  | OB9-CB7-OB8-CB6 |
| 28  | Q     | 101 | CDL  | OB5-CB3-CB4-OB6 |
| 28  | q     | 101 | CDL  | OB5-CB3-CB4-OB6 |
| 28  | e     | 403 | CDL  | OB9-CB7-OB8-CB6 |
| 28  | E     | 407 | CDL  | C79-C80-C81-C82 |
| 28  | L     | 101 | CDL  | C60-C61-C62-C63 |
| 28  | e     | 405 | CDL  | C79-C80-C81-C82 |
| 32  | F     | 202 | PEE  | C18-C19-C20-C21 |
| 32  | f     | 202 | PEE  | C18-C19-C20-C21 |
| 32  | F     | 202 | PEE  | O2-C10-C11-C12  |
| 28  | l     | 101 | CDL  | C60-C61-C62-C63 |
| 32  | f     | 202 | PEE  | O2-C10-C11-C12  |
| 28  | E     | 407 | CDL  | O1-C1-CA2-OA2   |
| 28  | e     | 405 | CDL  | O1-C1-CA2-OA2   |
| 32  | R     | 101 | PEE  | C16-C17-C18-C19 |
| 32  | r     | 101 | PEE  | C16-C17-C18-C19 |
| 33  | F     | 203 | PC1  | O22-C21-O21-C2  |
| 33  | f     | 203 | PC1  | O22-C21-O21-C2  |
| 33  | I     | 201 | PC1  | C3B-C3C-C3D-C3E |
| 33  | i     | 201 | PC1  | C3B-C3C-C3D-C3E |
| 28  | E     | 406 | CDL  | C18-C19-C20-C21 |
| 28  | e     | 404 | CDL  | C18-C19-C20-C21 |
| 33  | F     | 203 | PC1  | C22-C21-O21-C2  |
| 33  | f     | 203 | PC1  | C22-C21-O21-C2  |
| 28  | E     | 403 | CDL  | C32-C31-CA7-OA8 |
| 28  | F     | 201 | CDL  | C12-C11-CA5-OA6 |
| 28  | e     | 401 | CDL  | C32-C31-CA7-OA8 |
| 28  | f     | 201 | CDL  | C12-C11-CA5-OA6 |
| 26  | A1    | 601 | ATP  | PA-O3A-PB-O2B   |
| 26  | A2    | 601 | ATP  | PA-O3A-PB-O2B   |
| 26  | C1    | 601 | ATP  | PA-O3A-PB-O1B   |
| 26  | C2    | 601 | ATP  | PA-O3A-PB-O1B   |
| 34  | H1    | 201 | UTP  | PG-O3B-PB-O2B   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | H2    | 201 | UTP  | PG-O3B-PB-O1B   |
| 34  | H2    | 201 | UTP  | PG-O3B-PB-O2B   |
| 28  | E     | 404 | CDL  | C52-C51-CB5-OB6 |
| 28  | e     | 402 | CDL  | C52-C51-CB5-OB6 |
| 28  | L     | 101 | CDL  | OA7-CA5-OA6-CA4 |
| 28  | l     | 101 | CDL  | OA7-CA5-OA6-CA4 |
| 28  | E     | 404 | CDL  | C11-CA5-OA6-CA4 |
| 28  | e     | 402 | CDL  | C11-CA5-OA6-CA4 |
| 28  | J     | 203 | CDL  | C12-C11-CA5-OA6 |
| 28  | j     | 202 | CDL  | C12-C11-CA5-OA6 |
| 28  | M     | 201 | CDL  | C12-C11-CA5-OA6 |
| 28  | M     | 201 | CDL  | C72-C71-CB7-OB8 |
| 28  | m     | 201 | CDL  | C12-C11-CA5-OA6 |
| 28  | m     | 201 | CDL  | C72-C71-CB7-OB8 |
| 28  | F     | 201 | CDL  | C72-C71-CB7-OB8 |
| 28  | f     | 201 | CDL  | C72-C71-CB7-OB8 |
| 28  | j     | 202 | CDL  | C38-C39-C40-C41 |
| 28  | J     | 203 | CDL  | C38-C39-C40-C41 |
| 28  | E     | 407 | CDL  | C12-C11-CA5-OA6 |
| 28  | e     | 405 | CDL  | C12-C11-CA5-OA6 |
| 28  | m     | 201 | CDL  | C53-C54-C55-C56 |
| 28  | M     | 201 | CDL  | C53-C54-C55-C56 |
| 33  | J     | 204 | PC1  | O31-C31-C32-C33 |
| 33  | j     | 203 | PC1  | O31-C31-C32-C33 |
| 32  | R     | 101 | PEE  | C35-C36-C37-C38 |
| 32  | r     | 101 | PEE  | C35-C36-C37-C38 |
| 28  | F     | 201 | CDL  | OA5-CA3-CA4-CA6 |
| 28  | Q     | 101 | CDL  | OB5-CB3-CB4-CB6 |
| 28  | f     | 201 | CDL  | OA5-CA3-CA4-CA6 |
| 28  | q     | 101 | CDL  | OB5-CB3-CB4-CB6 |
| 28  | J     | 202 | CDL  | C52-C51-CB5-OB6 |
| 28  | Q     | 101 | CDL  | C72-C71-CB7-OB8 |
| 28  | j     | 201 | CDL  | C52-C51-CB5-OB6 |
| 28  | q     | 101 | CDL  | C72-C71-CB7-OB8 |
| 32  | R     | 101 | PEE  | O2-C10-C11-C12  |
| 32  | r     | 101 | PEE  | O2-C10-C11-C12  |
| 28  | l     | 101 | CDL  | C58-C59-C60-C61 |
| 28  | e     | 405 | CDL  | C81-C82-C83-C84 |
| 28  | E     | 407 | CDL  | C81-C82-C83-C84 |
| 28  | L     | 101 | CDL  | C58-C59-C60-C61 |
| 28  | E     | 407 | CDL  | CA3-CA4-OA6-CA5 |
| 28  | J     | 202 | CDL  | CA6-CA4-OA6-CA5 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 28  | j     | 201 | CDL  | CA6-CA4-OA6-CA5 |
| 28  | m     | 201 | CDL  | C51-C52-C53-C54 |
| 28  | Q     | 101 | CDL  | O1-C1-CA2-OA2   |
| 28  | e     | 402 | CDL  | O1-C1-CA2-OA2   |
| 28  | q     | 101 | CDL  | O1-C1-CA2-OA2   |
| 33  | F     | 204 | PC1  | C2B-C2C-C2D-C2E |
| 33  | f     | 204 | PC1  | C2B-C2C-C2D-C2E |
| 28  | M     | 201 | CDL  | C51-C52-C53-C54 |
| 32  | F     | 202 | PEE  | O4-C10-C11-C12  |
| 32  | f     | 202 | PEE  | O4-C10-C11-C12  |
| 28  | E     | 404 | CDL  | CB4-CB3-OB5-PB2 |
| 28  | e     | 402 | CDL  | CB4-CB3-OB5-PB2 |
| 28  | e     | 402 | CDL  | C24-C25-C26-C27 |
| 28  | Q     | 101 | CDL  | C73-C74-C75-C76 |
| 28  | E     | 405 | CDL  | C32-C31-CA7-OA8 |
| 28  | e     | 403 | CDL  | C32-C33-C34-C35 |
| 28  | q     | 101 | CDL  | C73-C74-C75-C76 |
| 28  | E     | 405 | CDL  | C32-C33-C34-C35 |
| 28  | j     | 202 | CDL  | C59-C60-C61-C62 |
| 28  | E     | 405 | CDL  | C52-C51-CB5-OB6 |
| 28  | e     | 403 | CDL  | C32-C31-CA7-OA8 |
| 28  | e     | 403 | CDL  | C52-C51-CB5-OB6 |
| 28  | J     | 203 | CDL  | C12-C11-CA5-OA7 |
| 28  | M     | 201 | CDL  | C72-C71-CB7-OB9 |
| 28  | e     | 405 | CDL  | C12-C11-CA5-OA7 |
| 28  | J     | 203 | CDL  | C59-C60-C61-C62 |
| 28  | E     | 404 | CDL  | C24-C25-C26-C27 |
| 28  | E     | 404 | CDL  | O1-C1-CA2-OA2   |
| 28  | E     | 407 | CDL  | C12-C11-CA5-OA7 |
| 28  | f     | 201 | CDL  | C72-C71-CB7-OB9 |
| 28  | j     | 202 | CDL  | C12-C11-CA5-OA7 |
| 28  | m     | 201 | CDL  | C72-C71-CB7-OB9 |
| 28  | M     | 201 | CDL  | OB9-CB7-OB8-CB6 |
| 28  | m     | 201 | CDL  | OB9-CB7-OB8-CB6 |
| 28  | F     | 201 | CDL  | C72-C71-CB7-OB9 |
| 28  | L     | 101 | CDL  | C80-C81-C82-C83 |
| 28  | l     | 101 | CDL  | C80-C81-C82-C83 |
| 28  | E     | 407 | CDL  | C32-C31-CA7-OA8 |
| 28  | e     | 405 | CDL  | C32-C31-CA7-OA8 |
| 28  | m     | 201 | CDL  | C71-CB7-OB8-CB6 |
| 28  | L     | 101 | CDL  | C11-CA5-OA6-CA4 |
| 28  | F     | 201 | CDL  | C12-C11-CA5-OA7 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 28  | f     | 201 | CDL  | C12-C11-CA5-OA7 |
| 28  | m     | 201 | CDL  | C12-C11-CA5-OA7 |
| 28  | E     | 403 | CDL  | C32-C31-CA7-OA9 |
| 28  | M     | 201 | CDL  | C12-C11-CA5-OA7 |
| 28  | e     | 401 | CDL  | C32-C31-CA7-OA9 |
| 28  | E     | 404 | CDL  | C32-C31-CA7-OA8 |
| 28  | e     | 402 | CDL  | C32-C31-CA7-OA8 |
| 28  | q     | 101 | CDL  | C72-C71-CB7-OB9 |
| 28  | Q     | 101 | CDL  | C72-C71-CB7-OB9 |
| 33  | j     | 203 | PC1  | O32-C31-C32-C33 |
| 28  | l     | 101 | CDL  | C11-CA5-OA6-CA4 |
| 32  | R     | 101 | PEE  | O4-C10-C11-C12  |
| 33  | J     | 204 | PC1  | O32-C31-C32-C33 |
| 28  | j     | 202 | CDL  | C71-C72-C73-C74 |
| 28  | E     | 405 | CDL  | OA5-CA3-CA4-CA6 |
| 28  | e     | 403 | CDL  | OA5-CA3-CA4-CA6 |
| 28  | M     | 201 | CDL  | C71-CB7-OB8-CB6 |
| 28  | J     | 203 | CDL  | C71-C72-C73-C74 |
| 28  | M     | 201 | CDL  | C14-C15-C16-C17 |
| 32  | r     | 101 | PEE  | O4-C10-C11-C12  |
| 32  | R     | 101 | PEE  | C41-C42-C43-C44 |
| 32  | r     | 101 | PEE  | C41-C42-C43-C44 |
| 28  | m     | 201 | CDL  | C14-C15-C16-C17 |
| 33  | i     | 201 | PC1  | O21-C21-C22-C23 |
| 26  | A1    | 601 | ATP  | PA-O3A-PB-O1B   |
| 26  | A2    | 601 | ATP  | PA-O3A-PB-O1B   |
| 34  | H1    | 201 | UTP  | PG-O3B-PB-O1B   |
| 28  | E     | 404 | CDL  | C32-C31-CA7-OA9 |
| 28  | e     | 405 | CDL  | C32-C31-CA7-OA9 |
| 33  | I     | 201 | PC1  | O21-C21-C22-C23 |
| 28  | E     | 405 | CDL  | C32-C31-CA7-OA9 |
| 28  | E     | 407 | CDL  | C32-C31-CA7-OA9 |
| 28  | e     | 402 | CDL  | C32-C31-CA7-OA9 |
| 28  | e     | 403 | CDL  | C52-C51-CB5-OB7 |

There are no ring outliers.

16 monomers are involved in 19 short contacts:

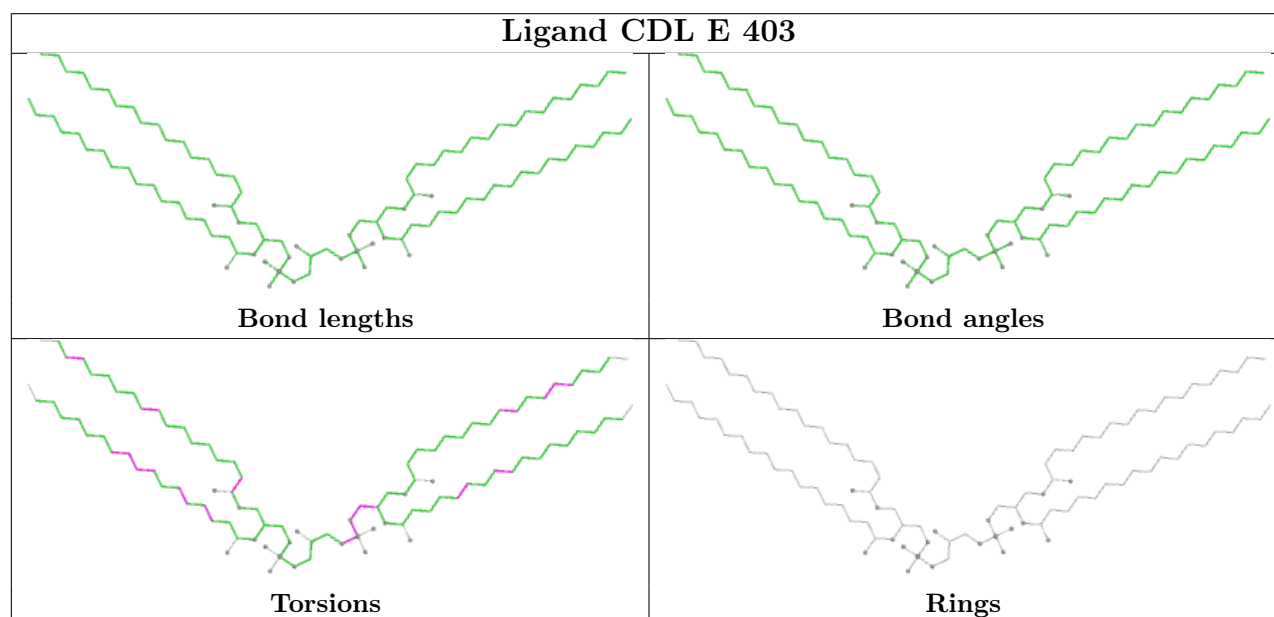
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 28  | M     | 201 | CDL  | 1       | 0            |
| 32  | r     | 101 | PEE  | 1       | 0            |
| 28  | C     | 201 | CDL  | 1       | 0            |

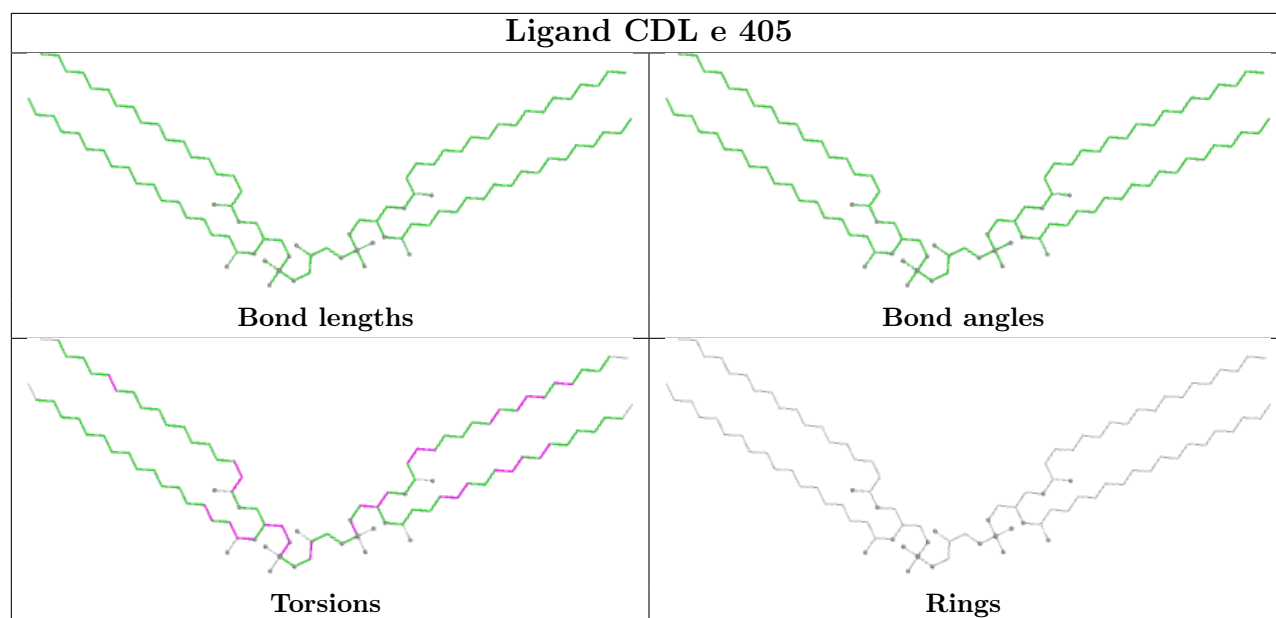
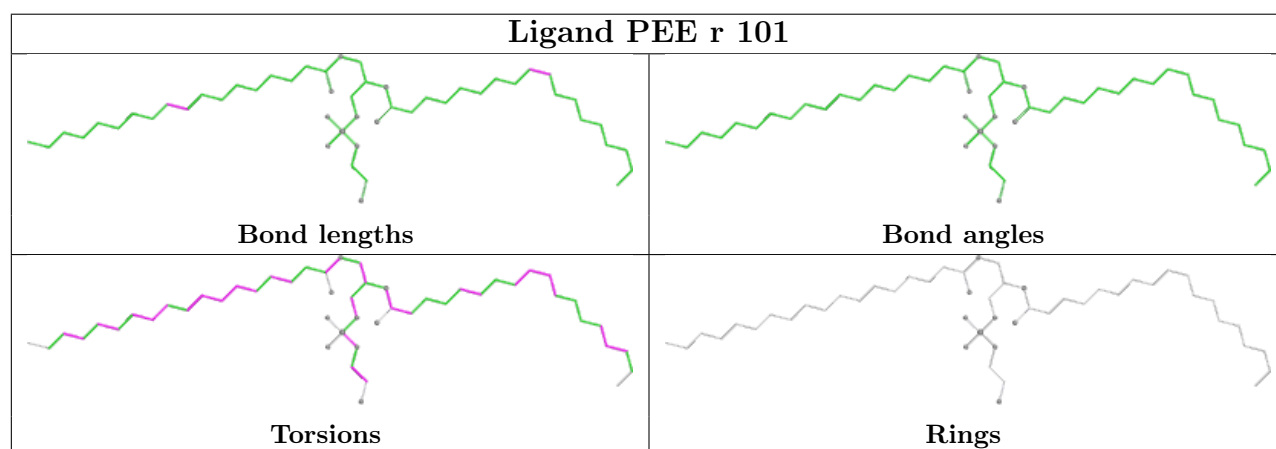
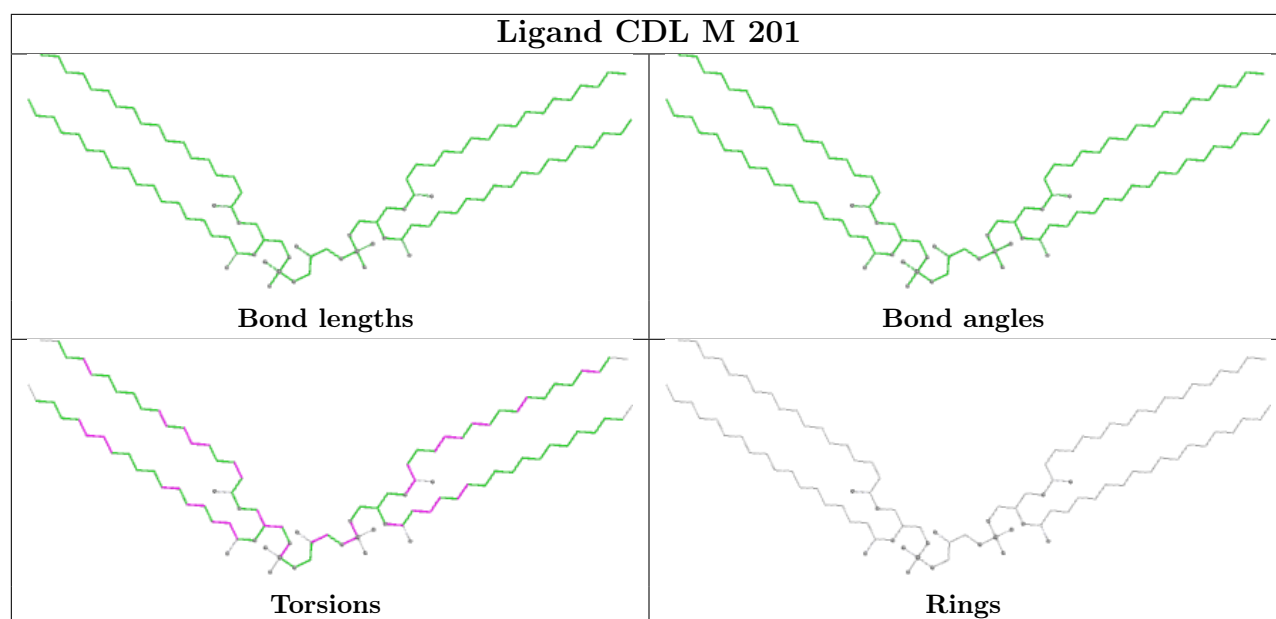
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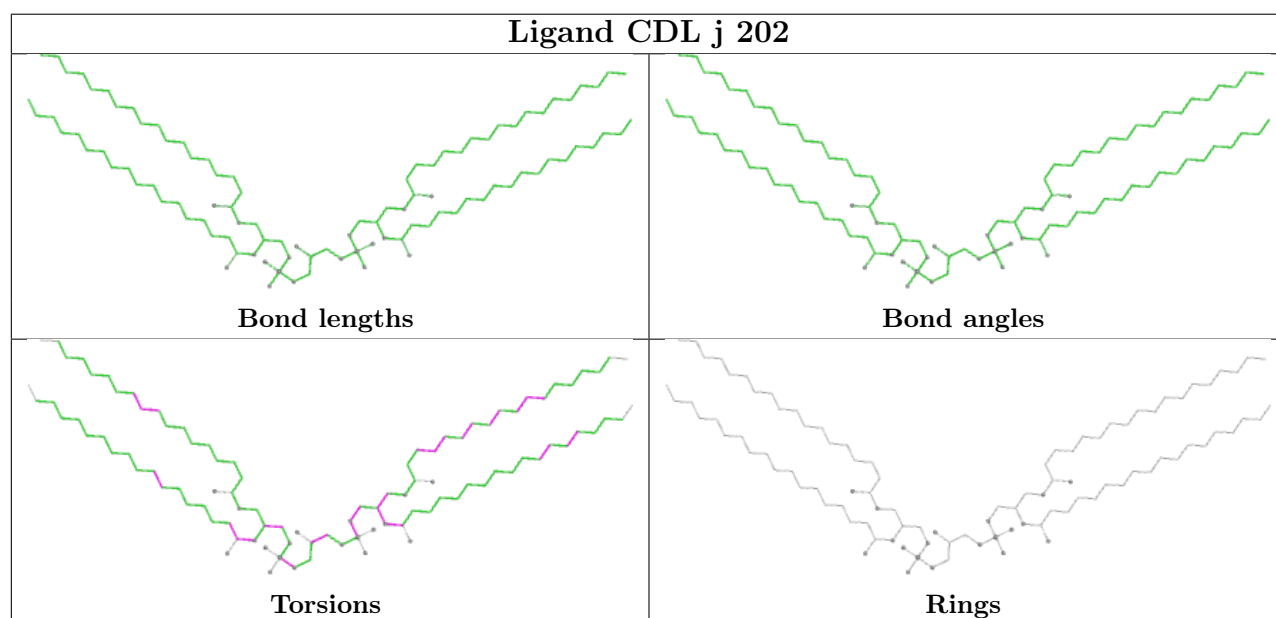
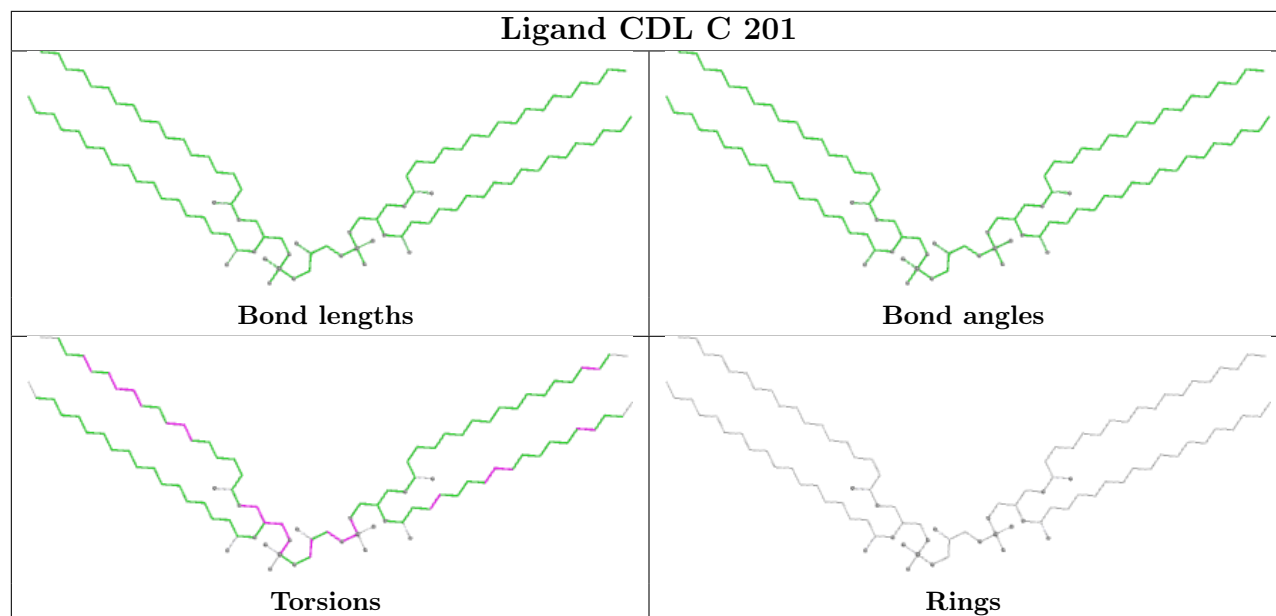
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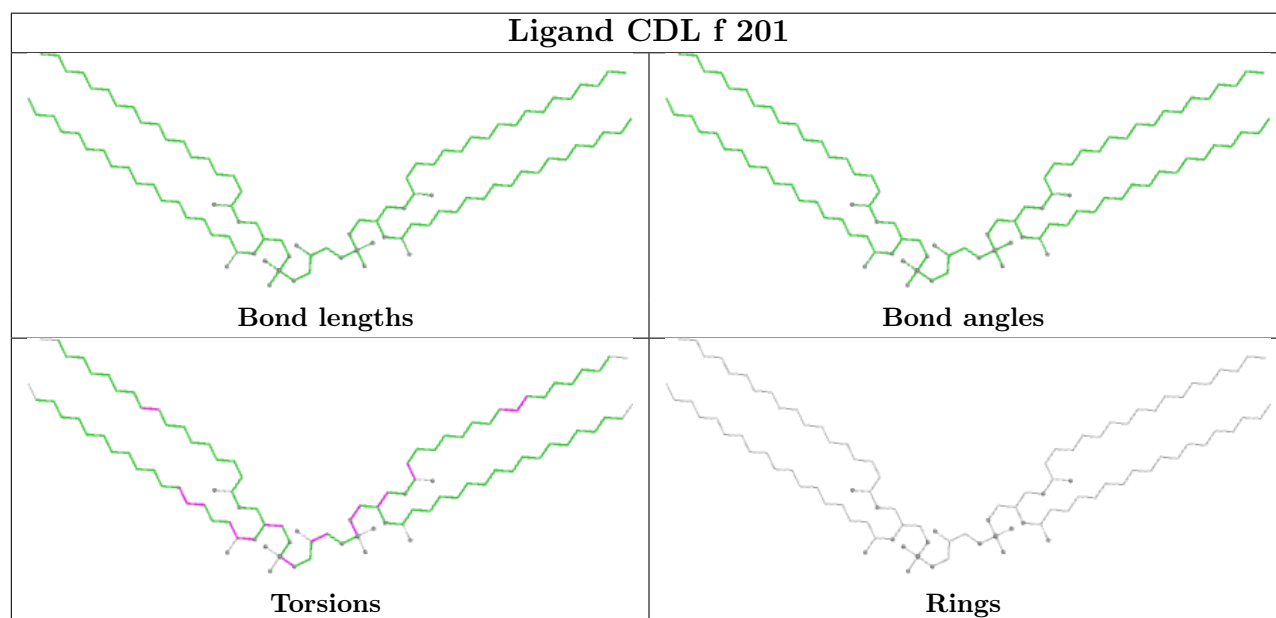
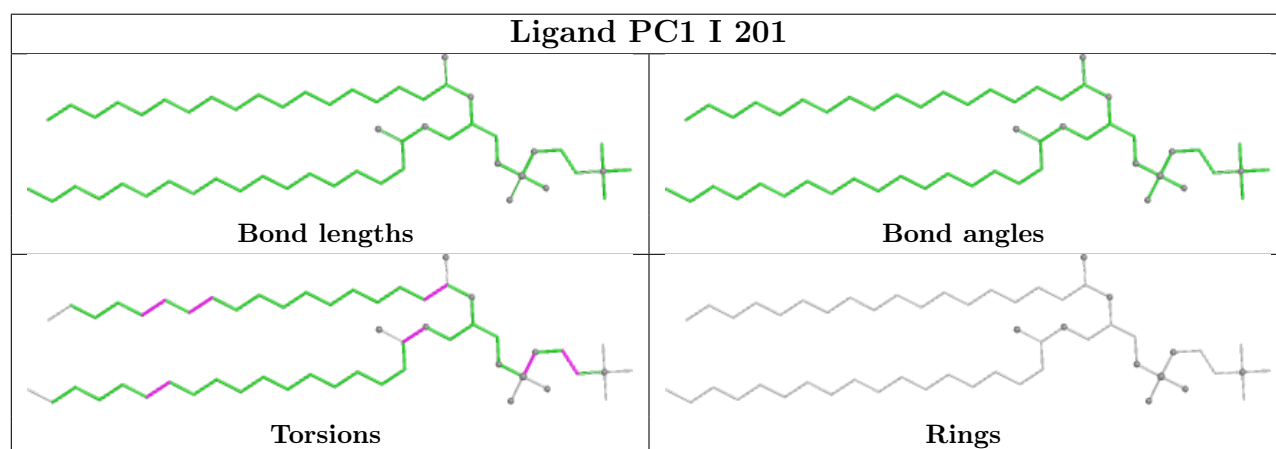
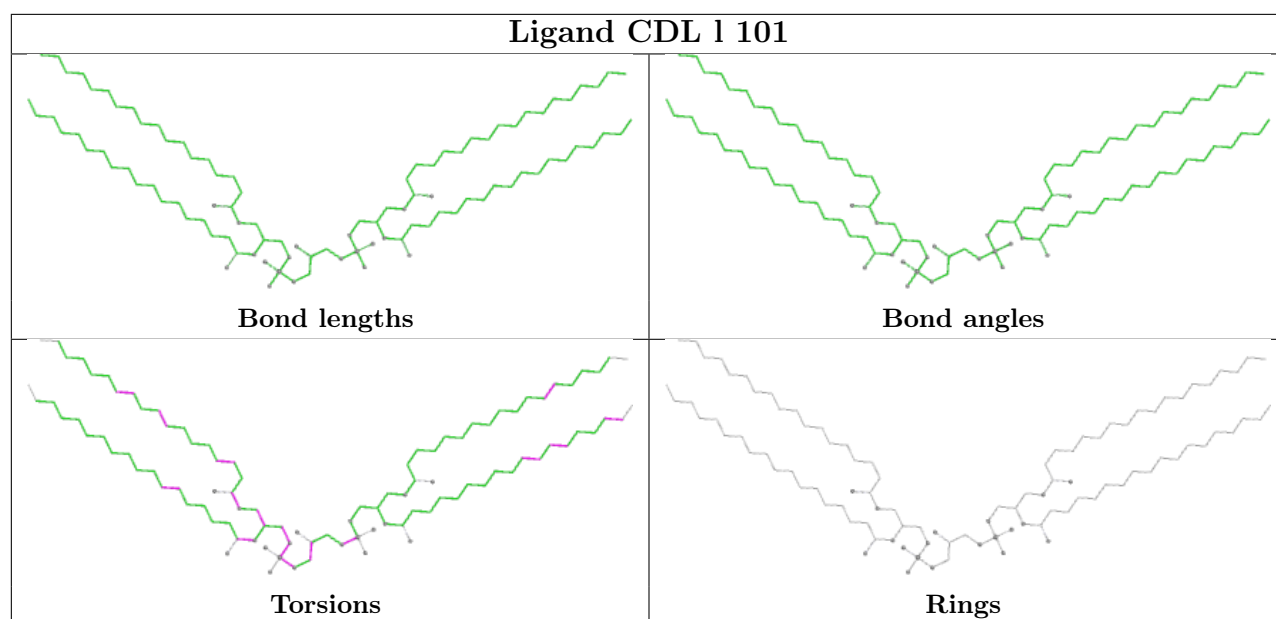
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 28  | j     | 202 | CDL  | 1       | 0            |
| 34  | H2    | 201 | UTP  | 2       | 0            |
| 28  | Q     | 101 | CDL  | 1       | 0            |
| 28  | e     | 402 | CDL  | 3       | 0            |
| 28  | e     | 403 | CDL  | 2       | 0            |
| 26  | B2    | 601 | ATP  | 1       | 0            |
| 34  | H1    | 201 | UTP  | 2       | 0            |
| 28  | J     | 203 | CDL  | 1       | 0            |
| 28  | E     | 404 | CDL  | 3       | 0            |
| 33  | F     | 204 | PC1  | 1       | 0            |
| 33  | f     | 204 | PC1  | 1       | 0            |
| 28  | E     | 405 | CDL  | 2       | 0            |
| 28  | c     | 201 | CDL  | 1       | 0            |

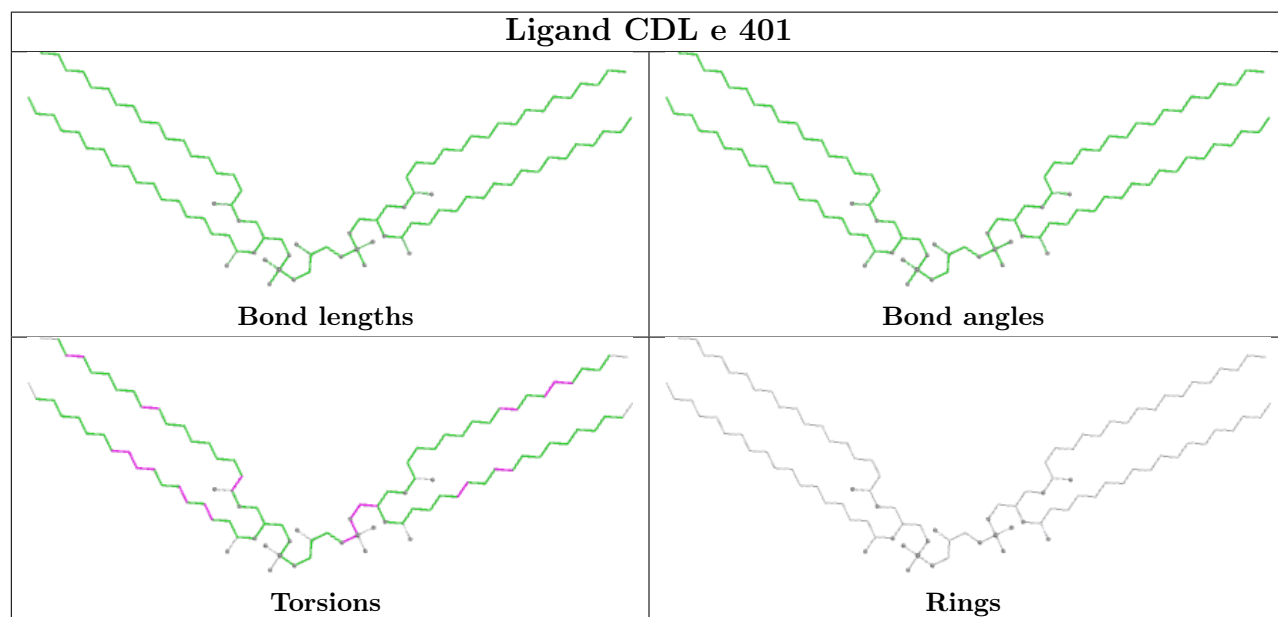
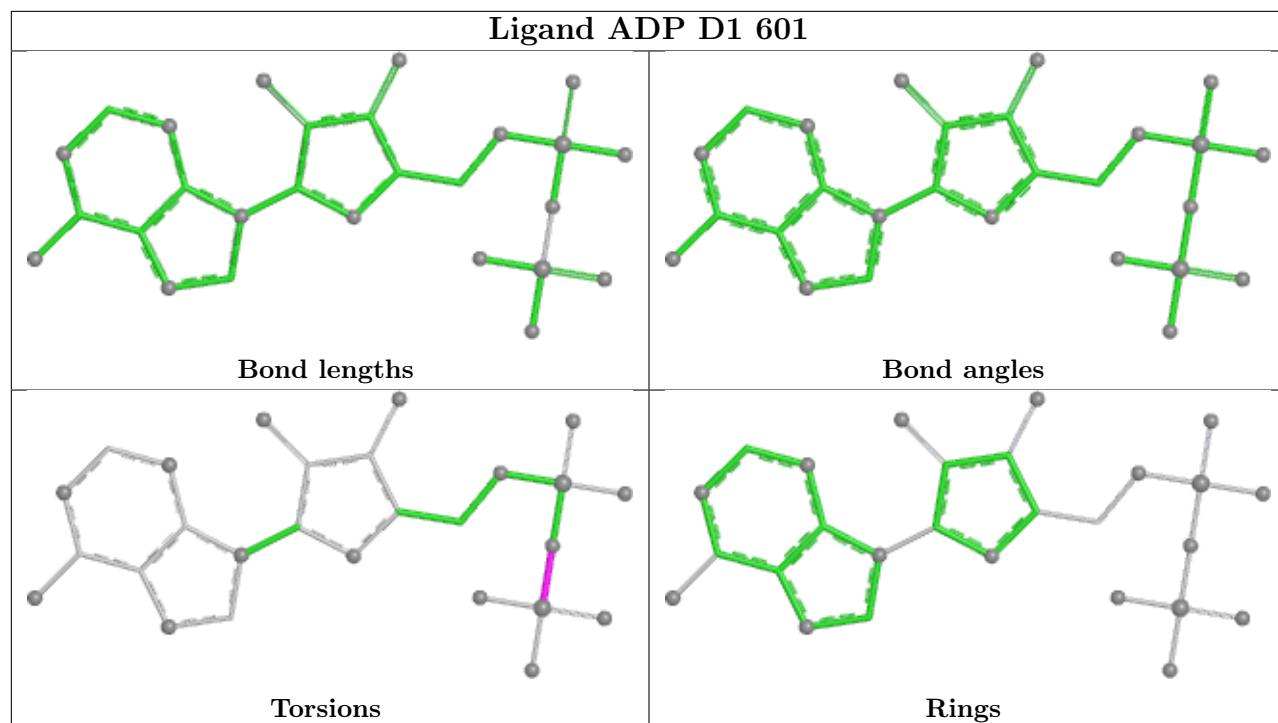
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

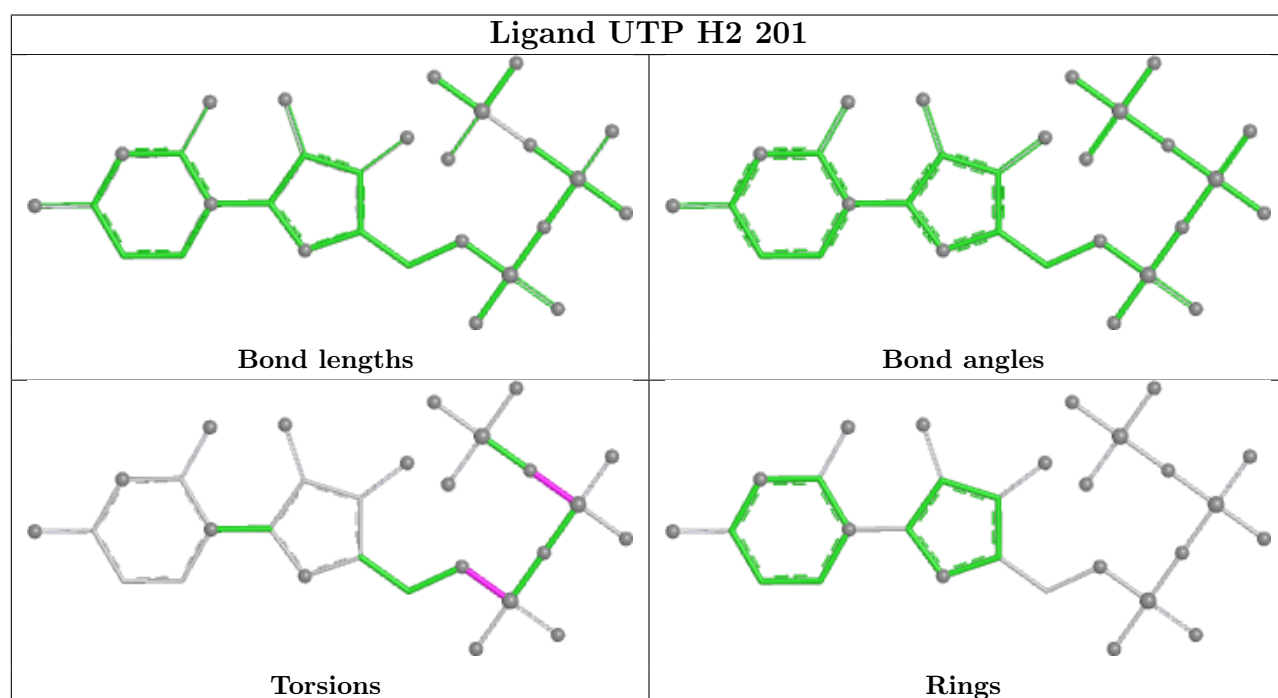
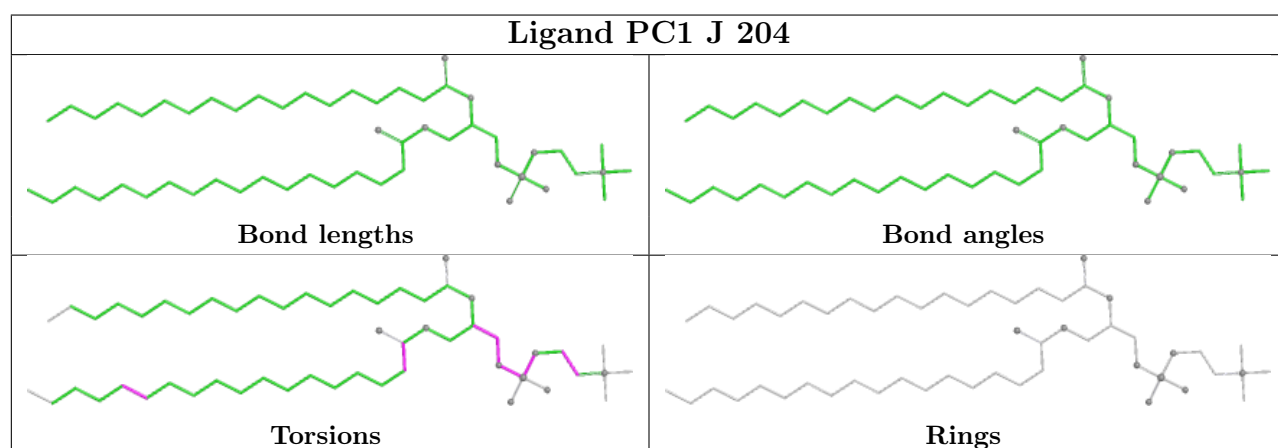
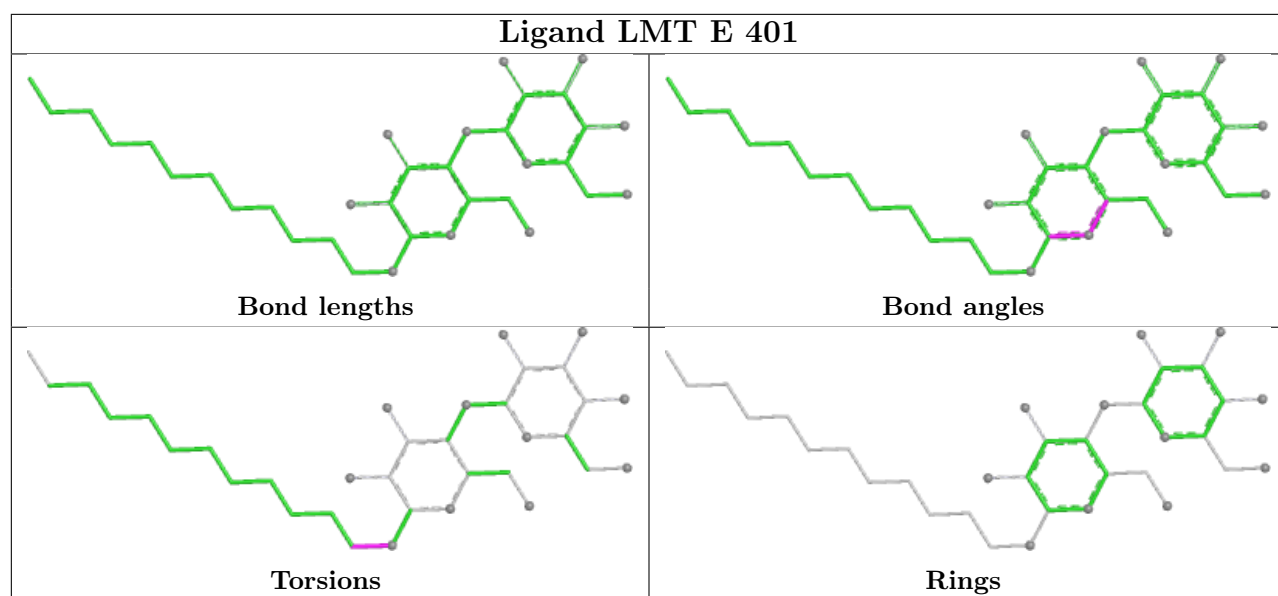


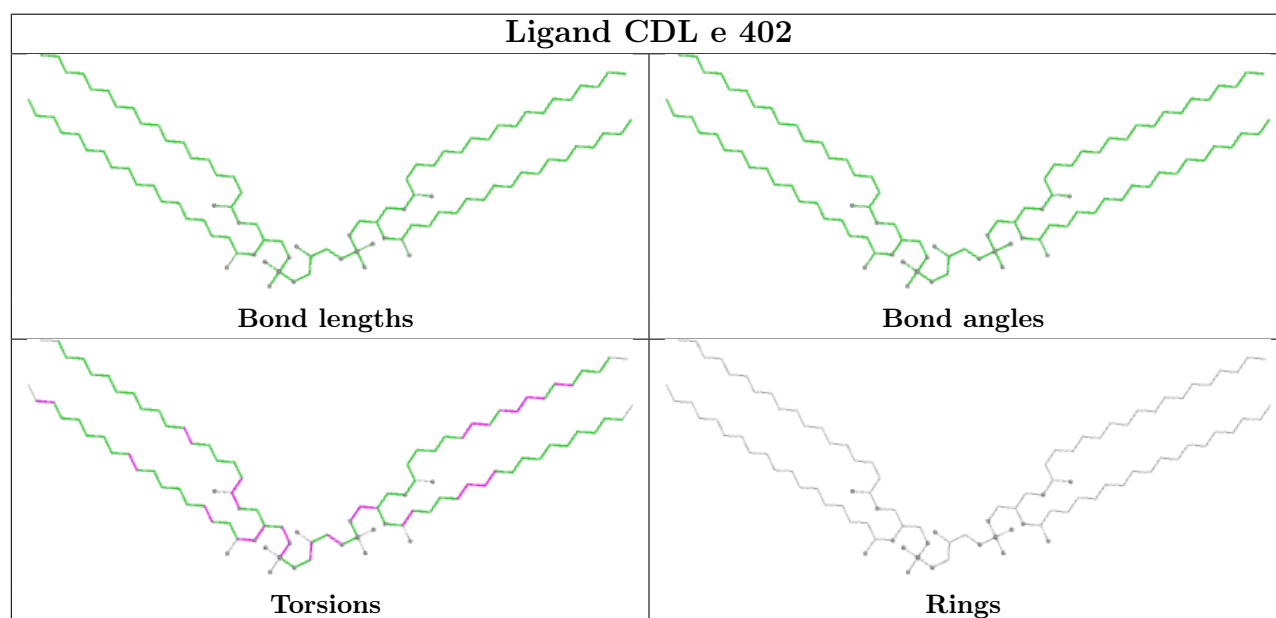
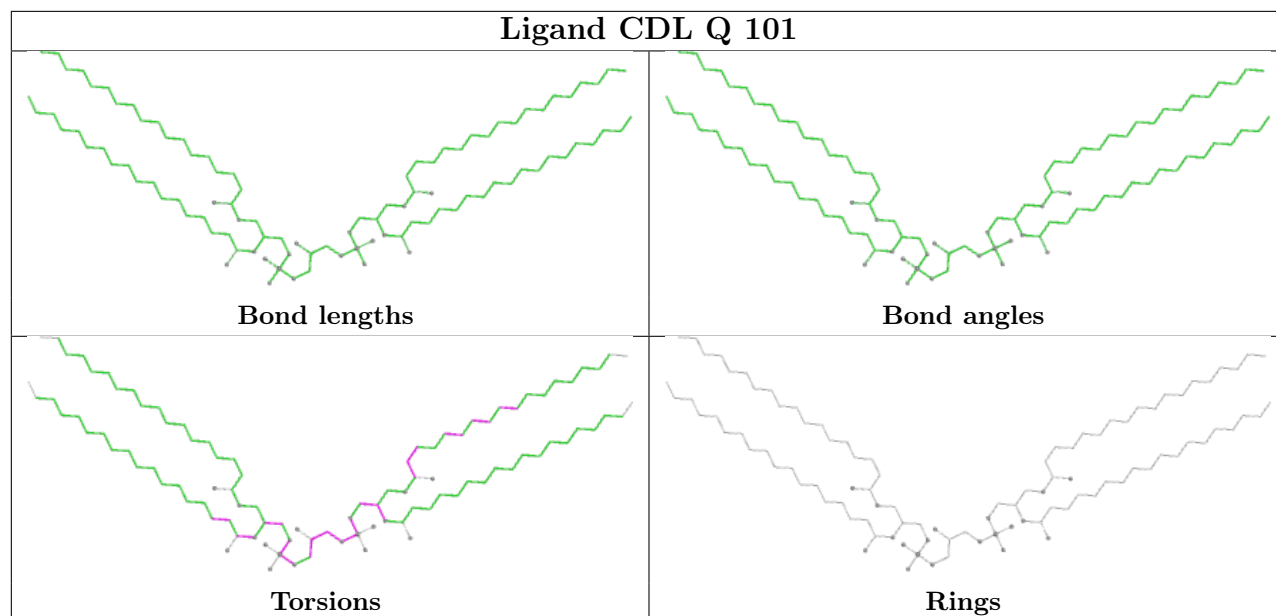


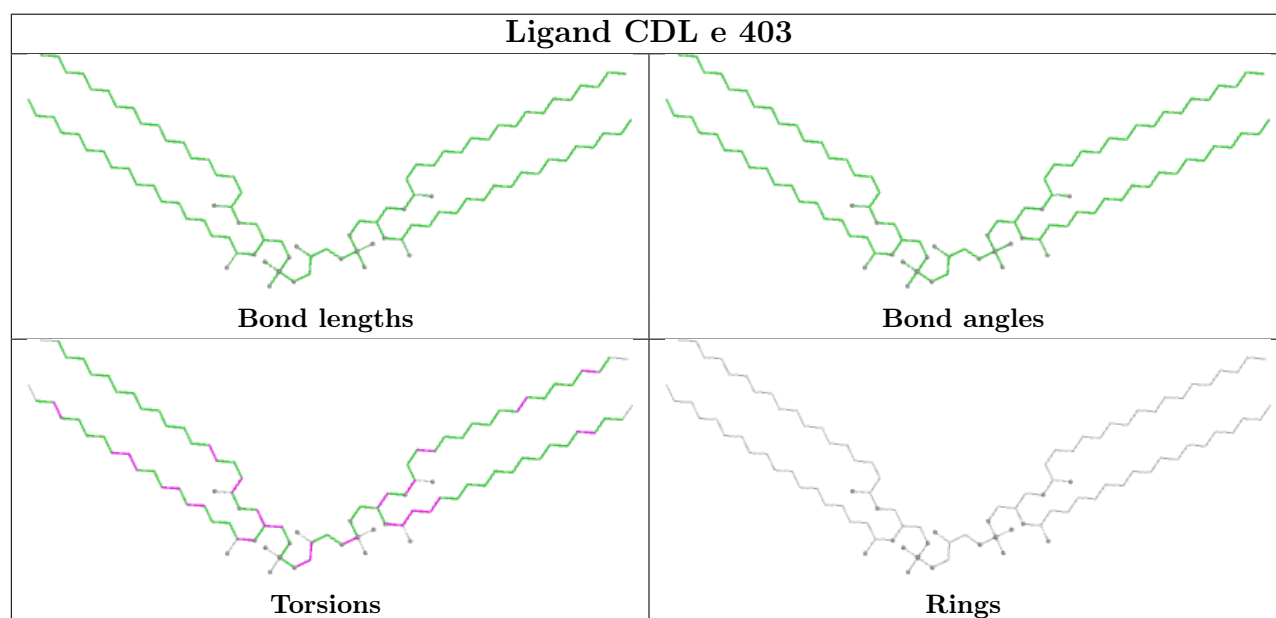
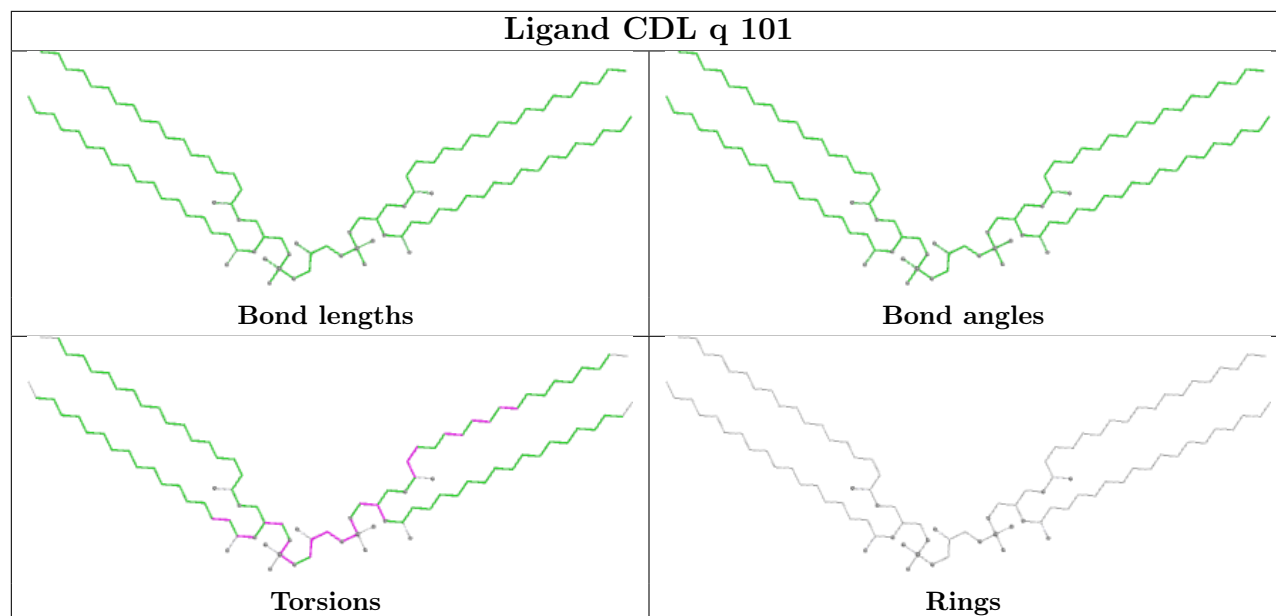


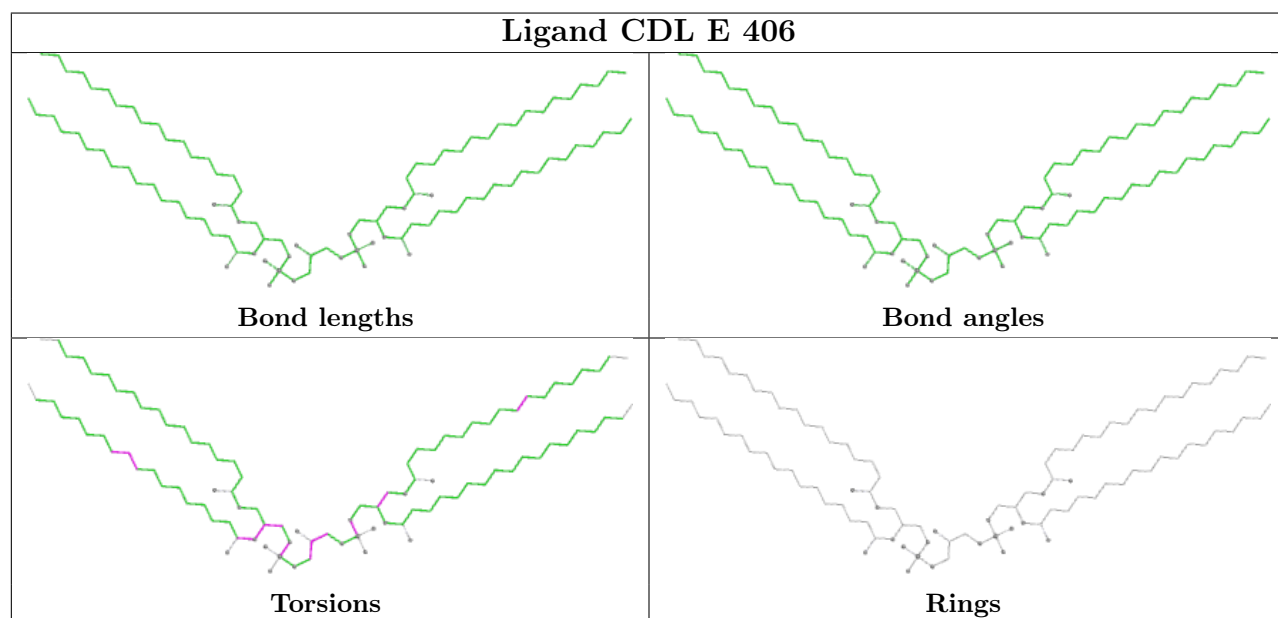
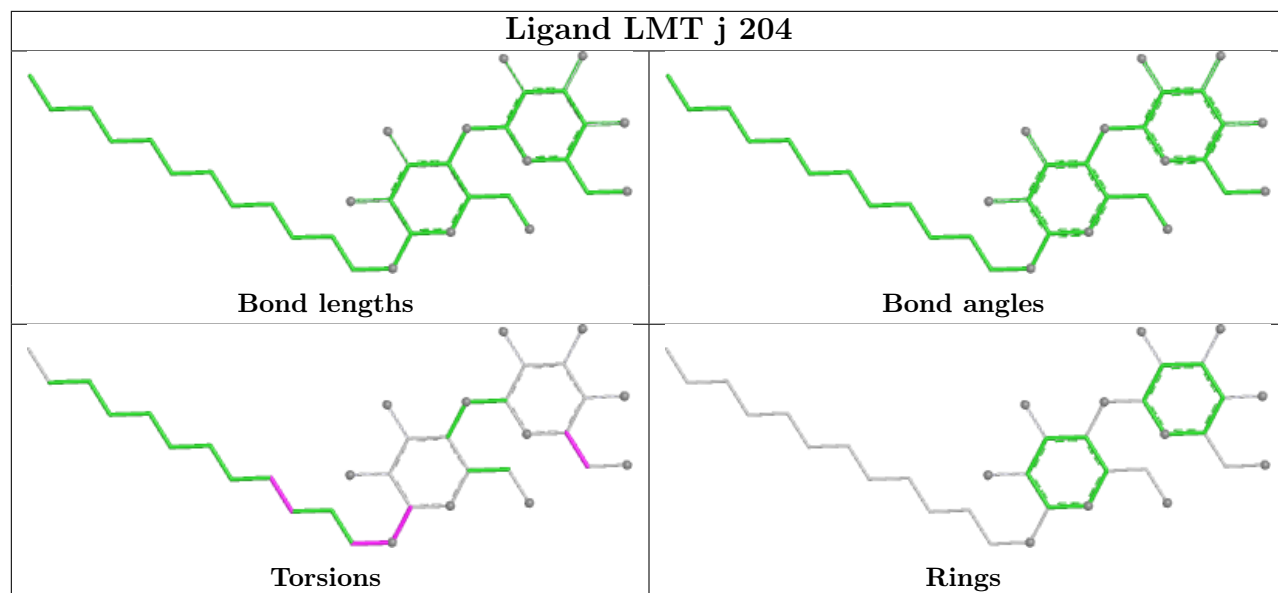


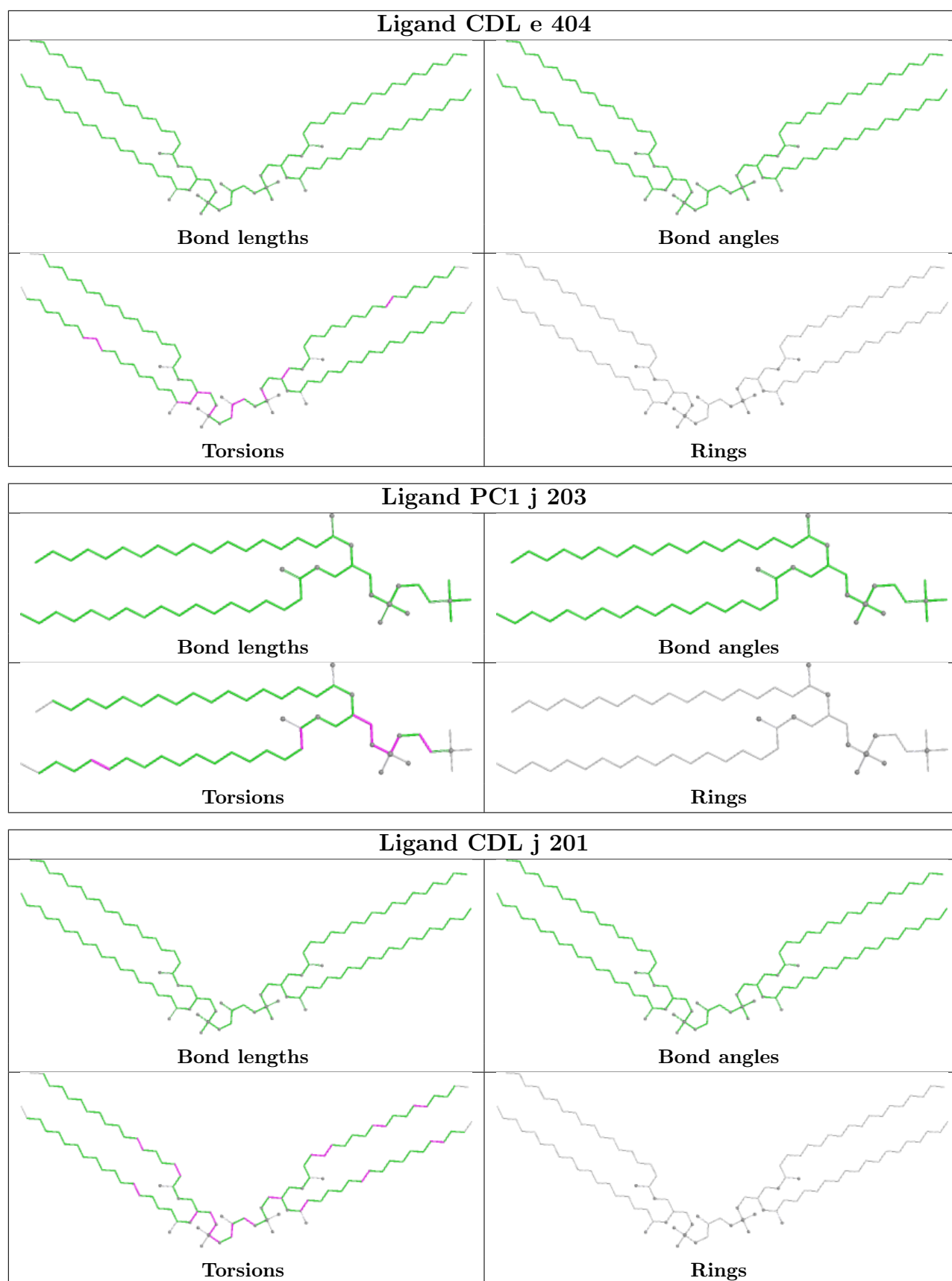


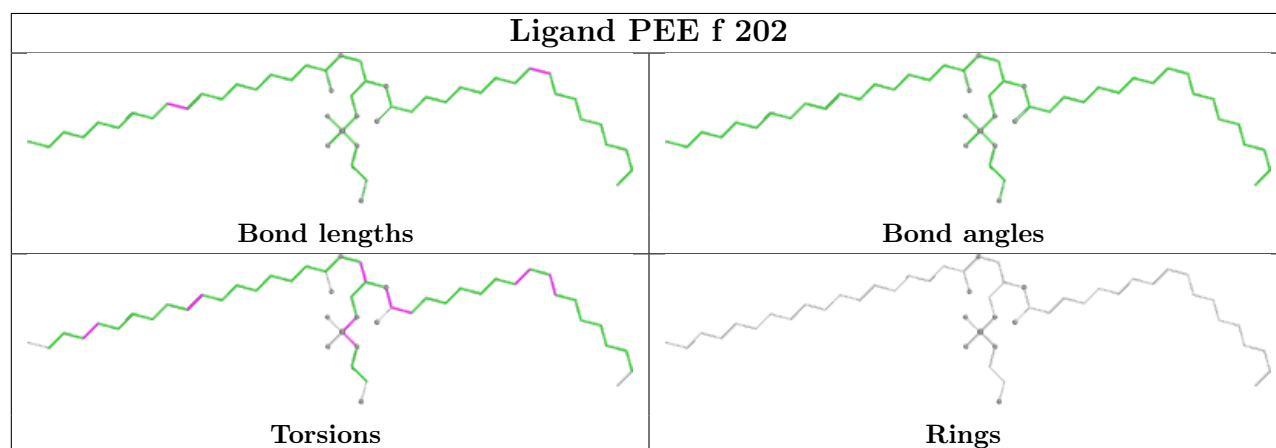
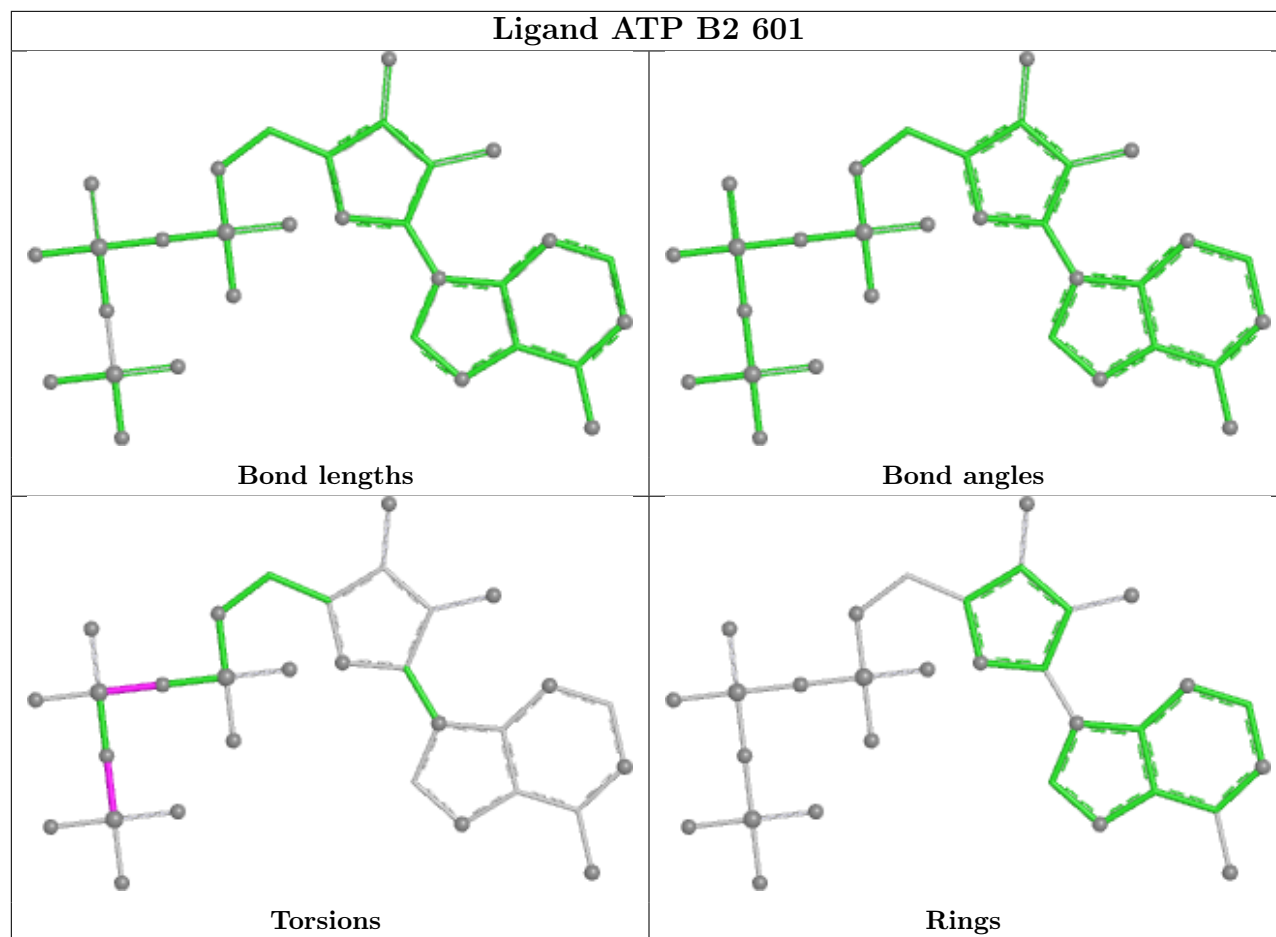


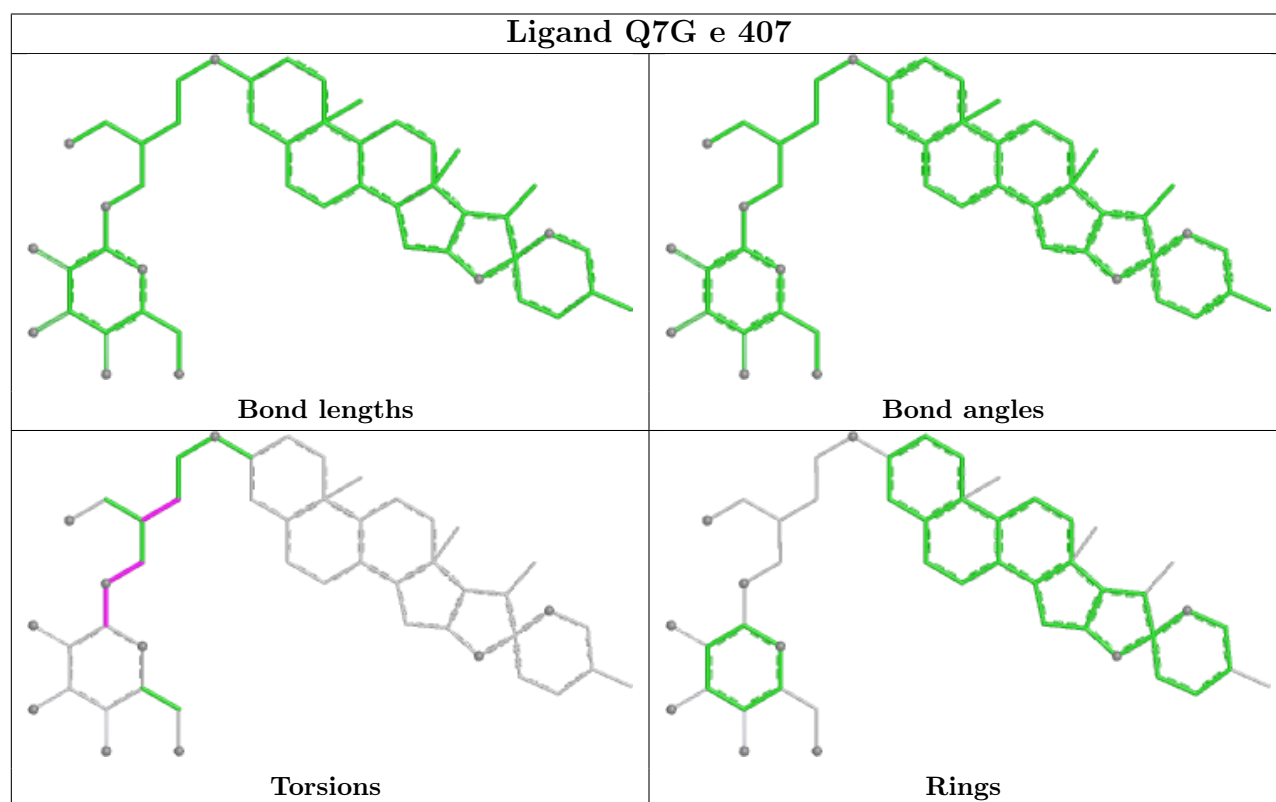
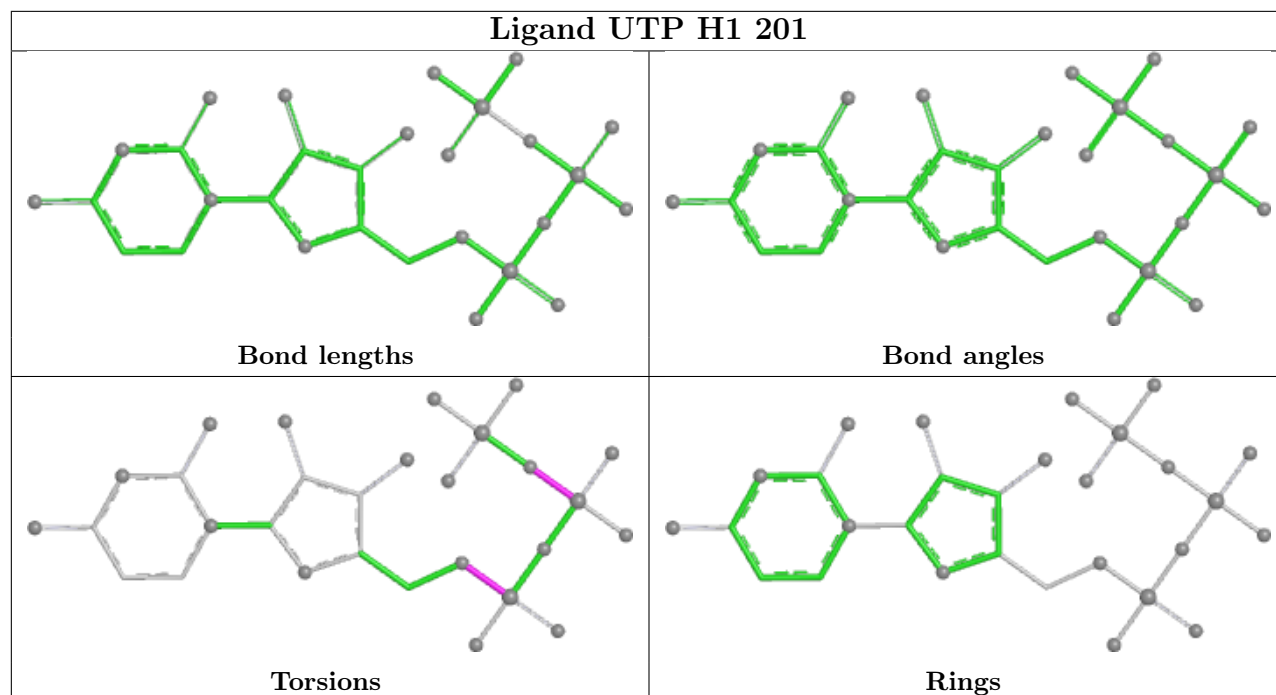


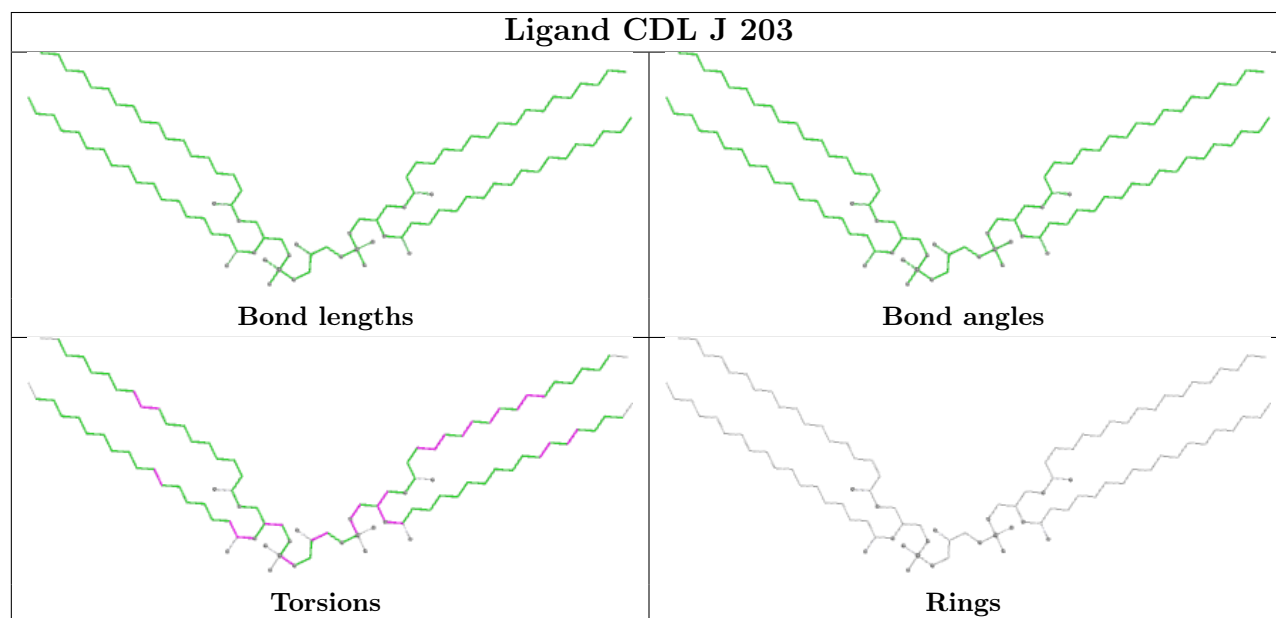
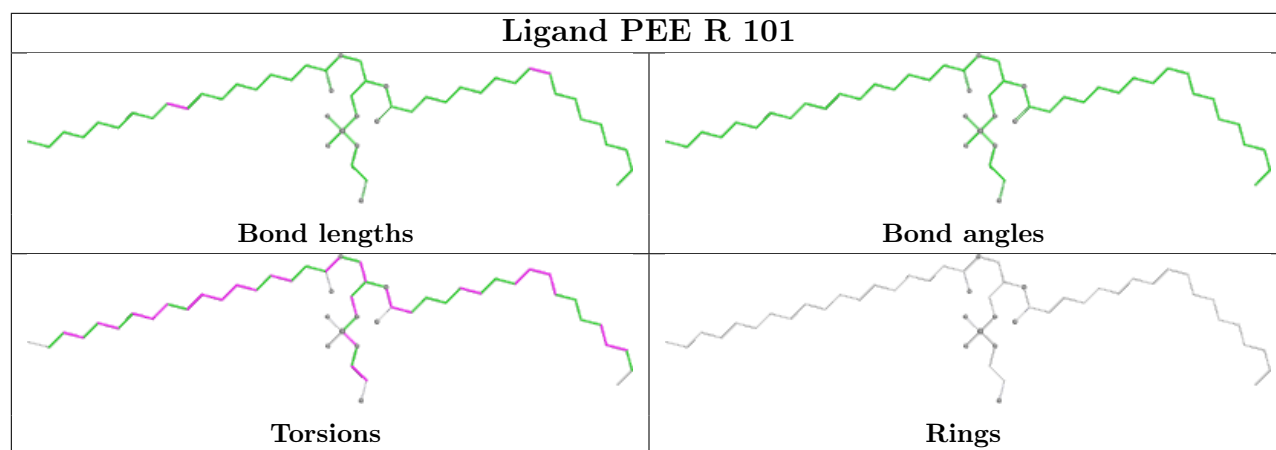
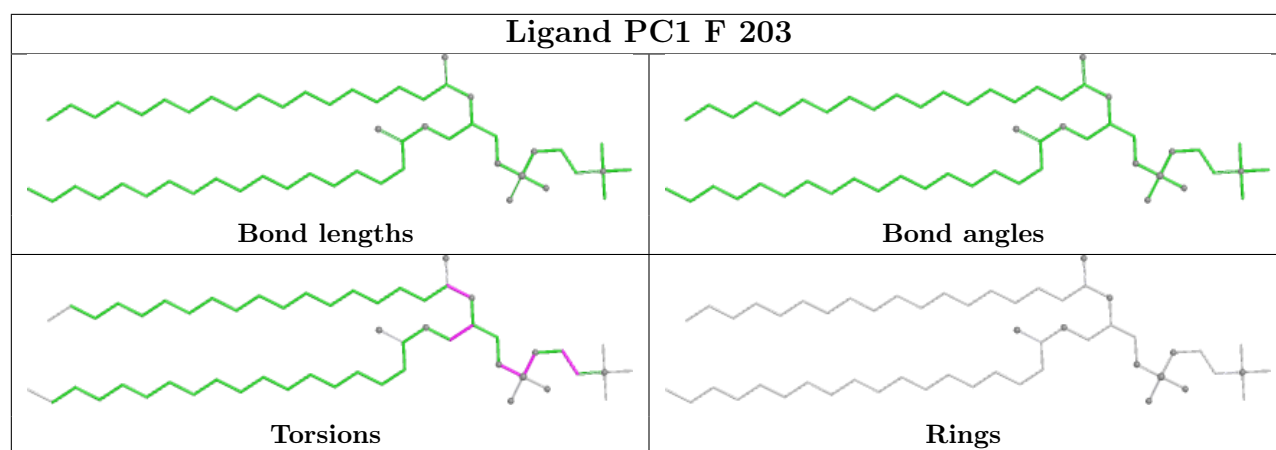


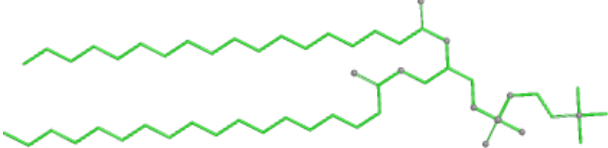
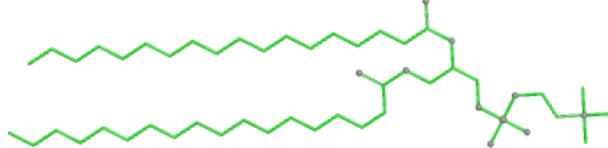
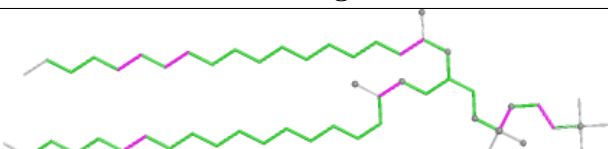
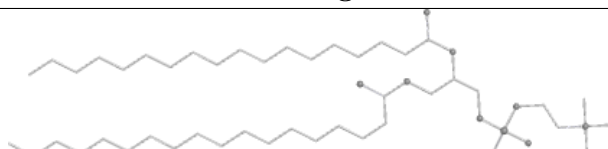
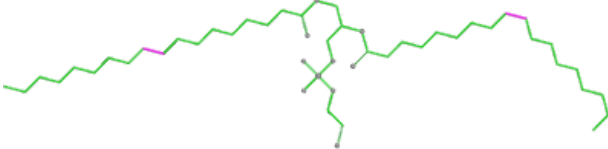
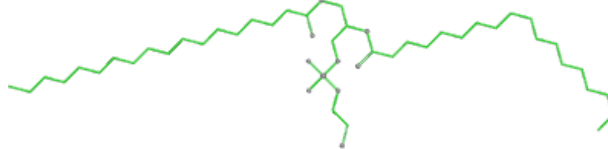
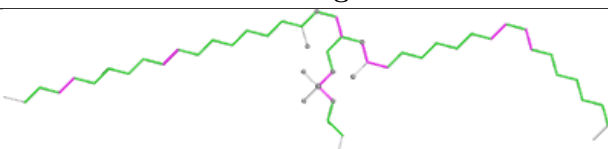
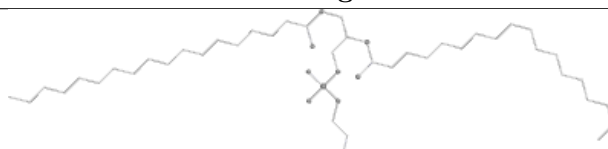


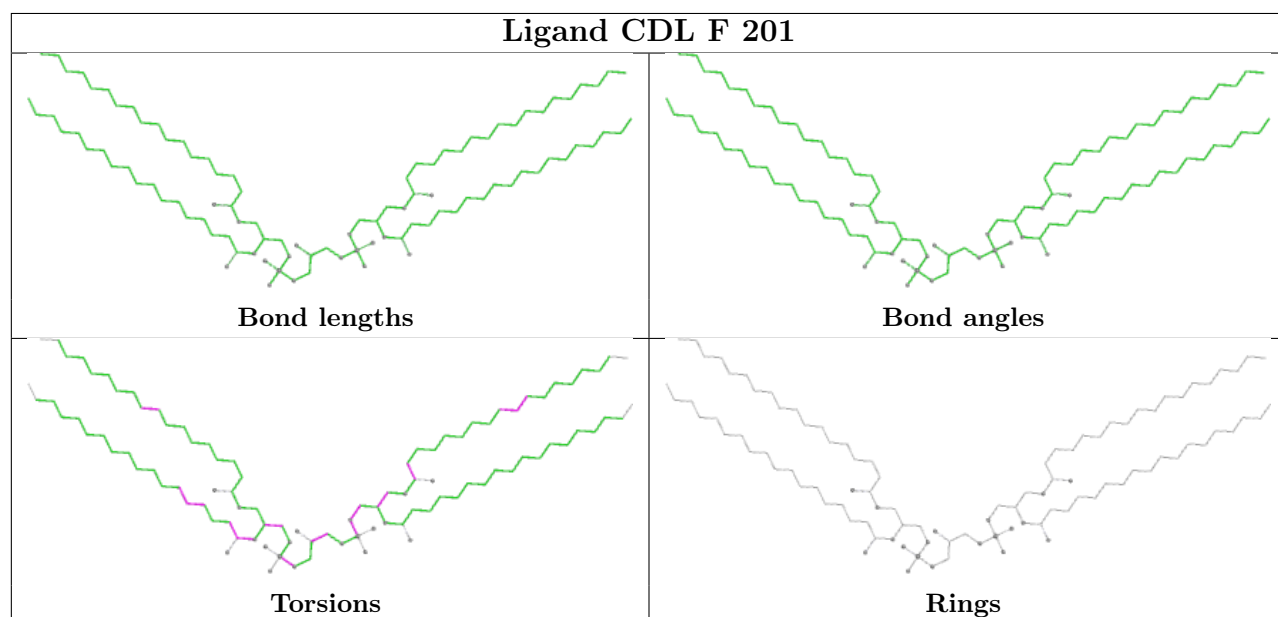
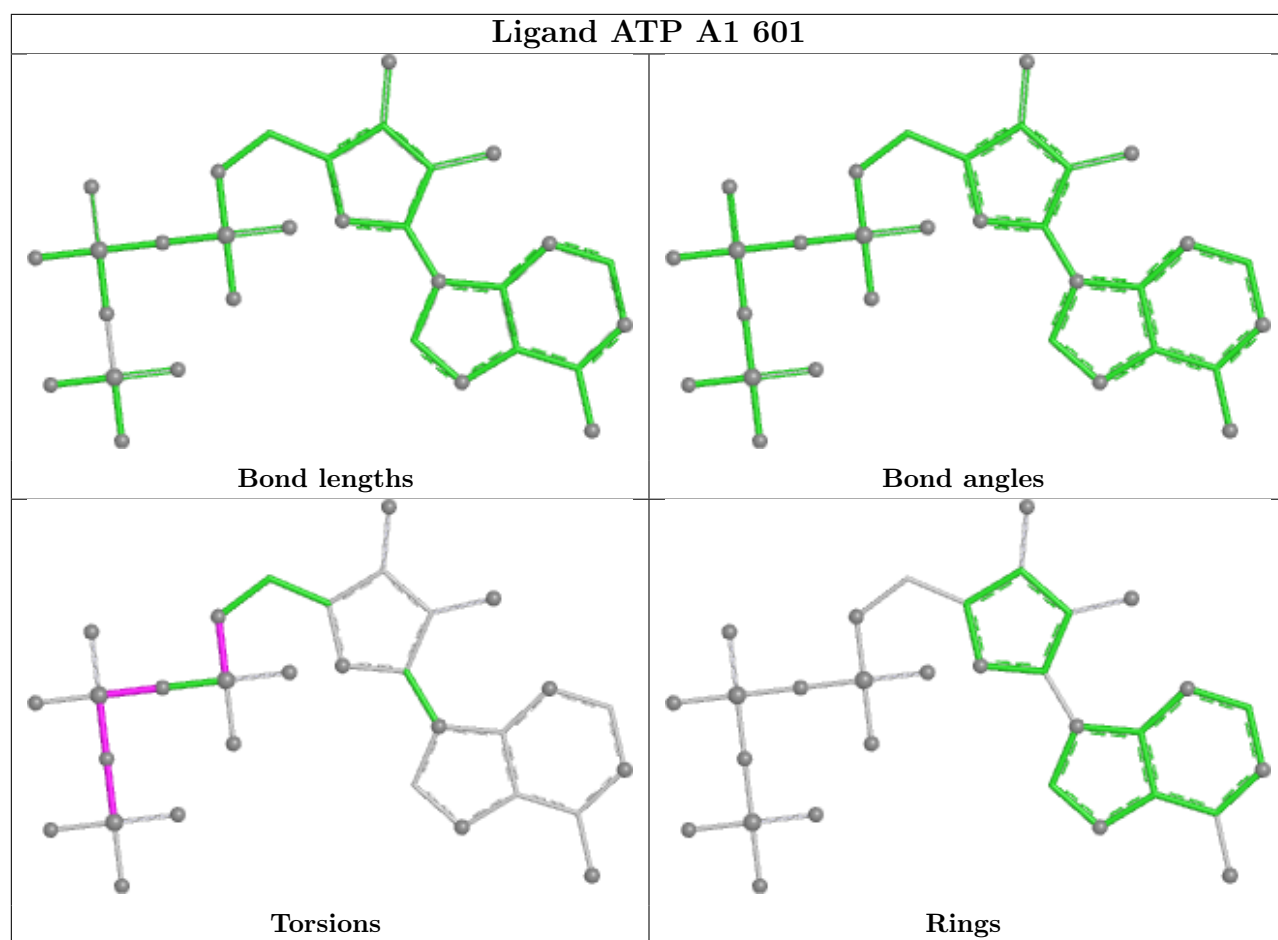


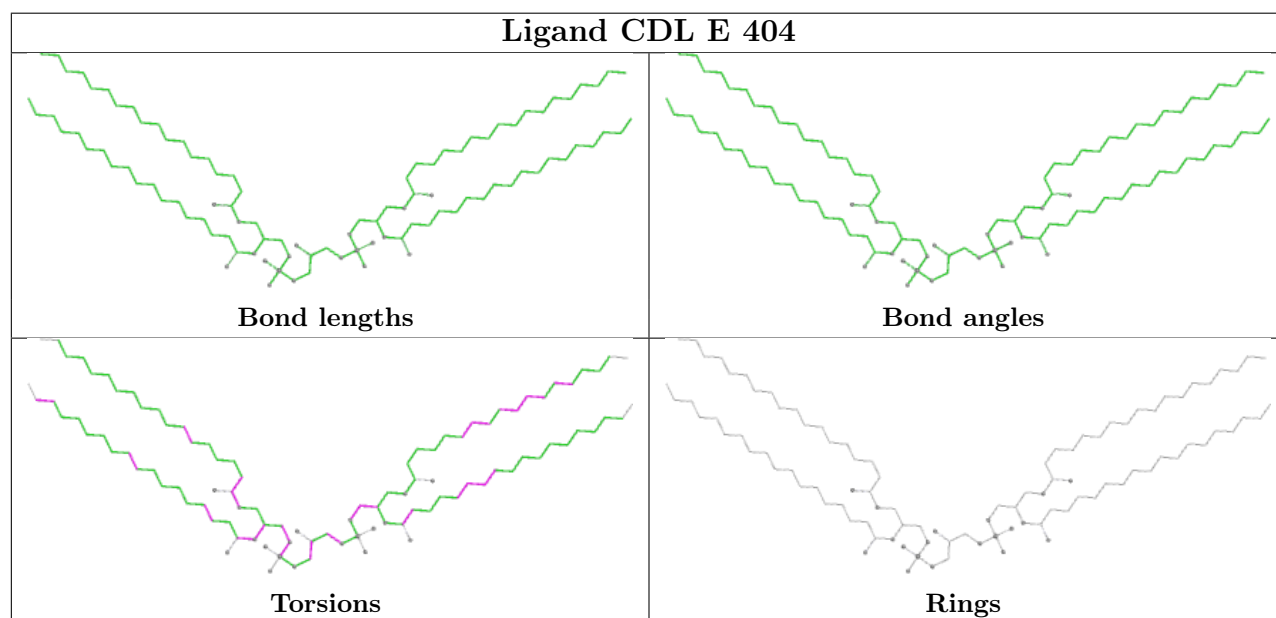
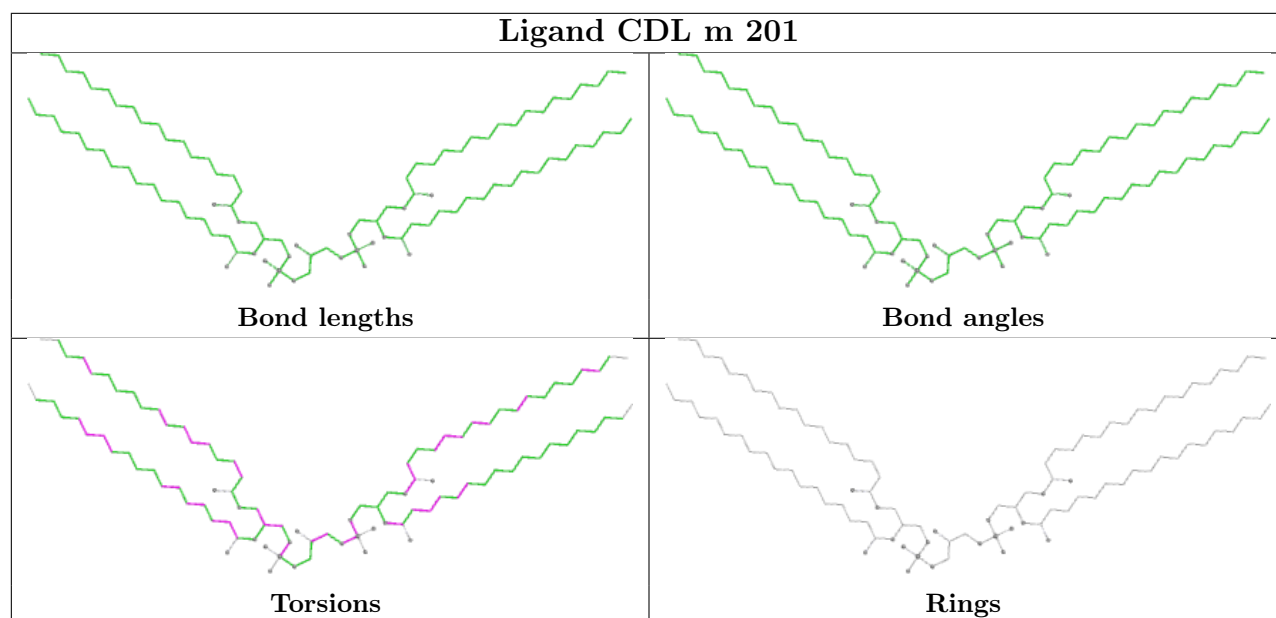
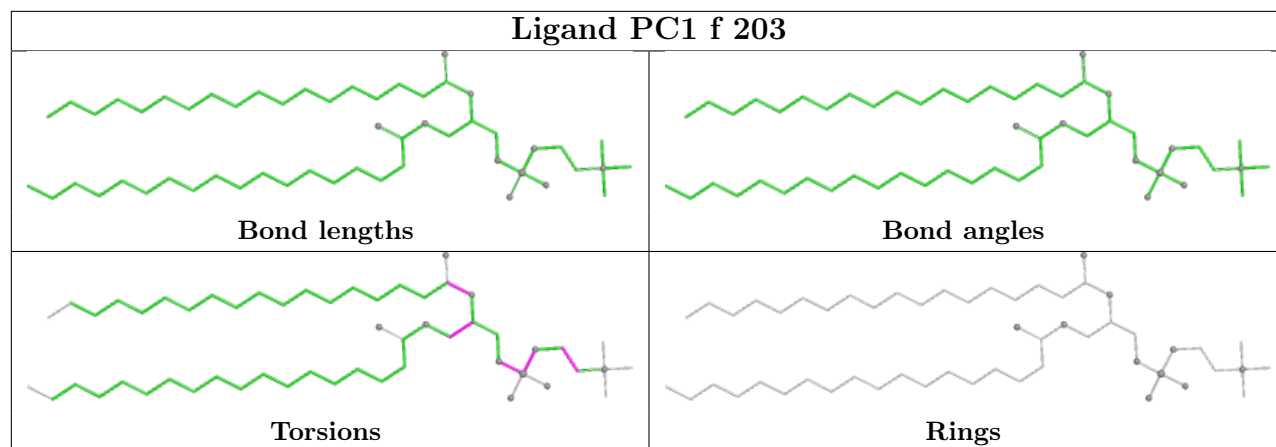


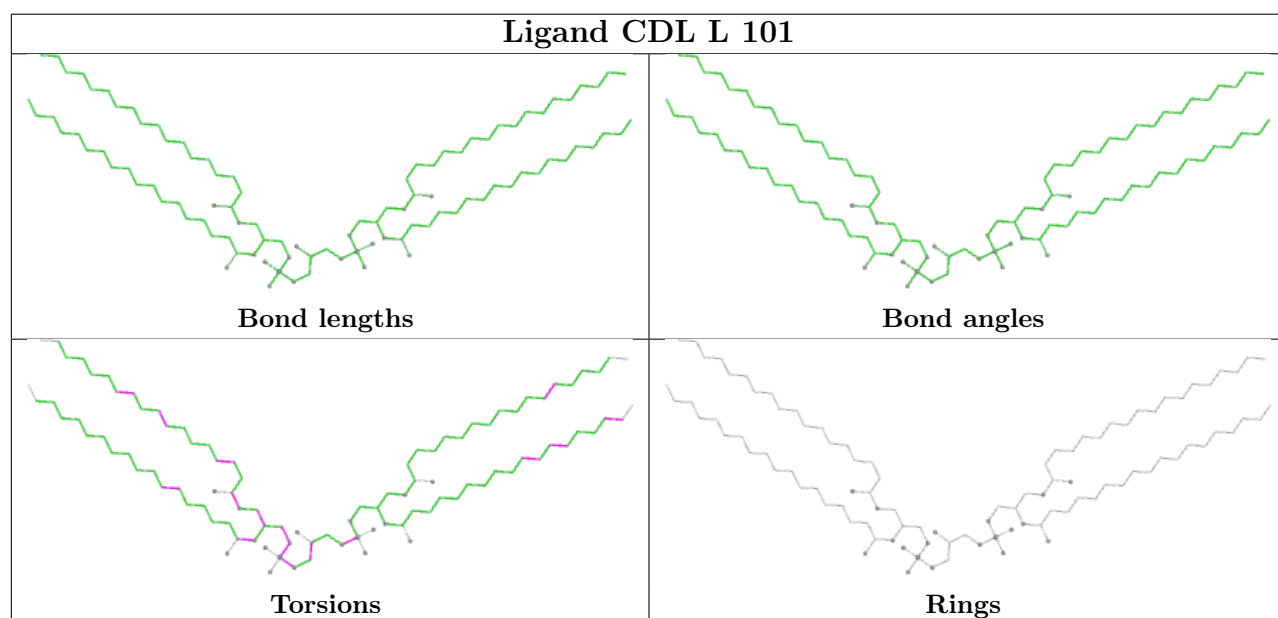
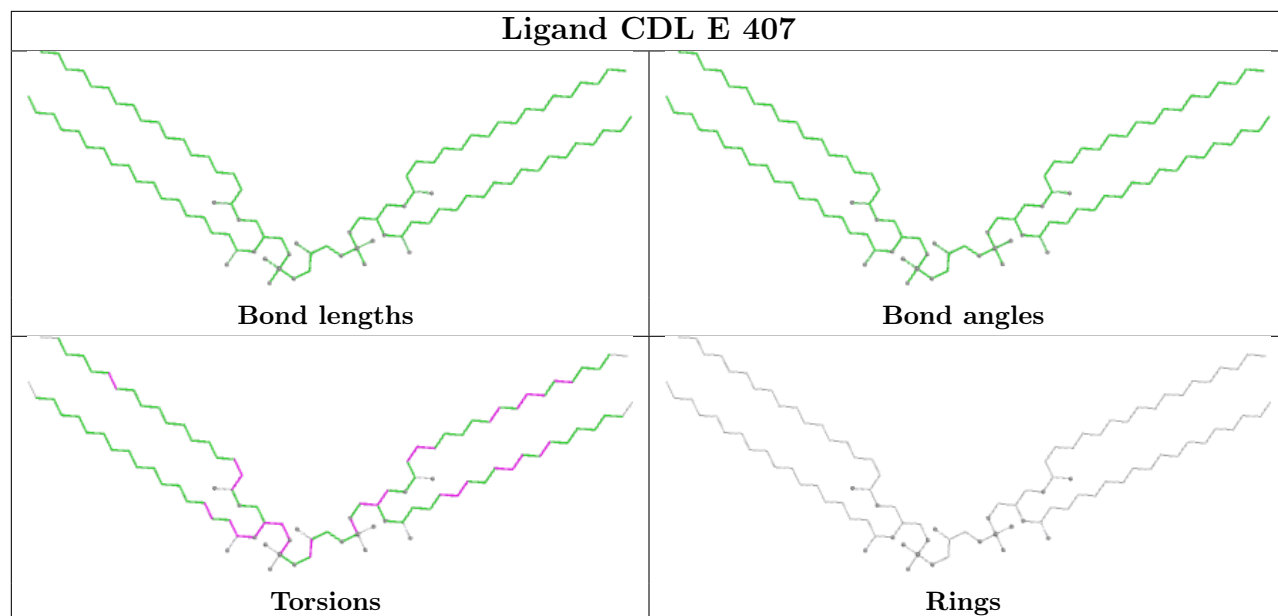


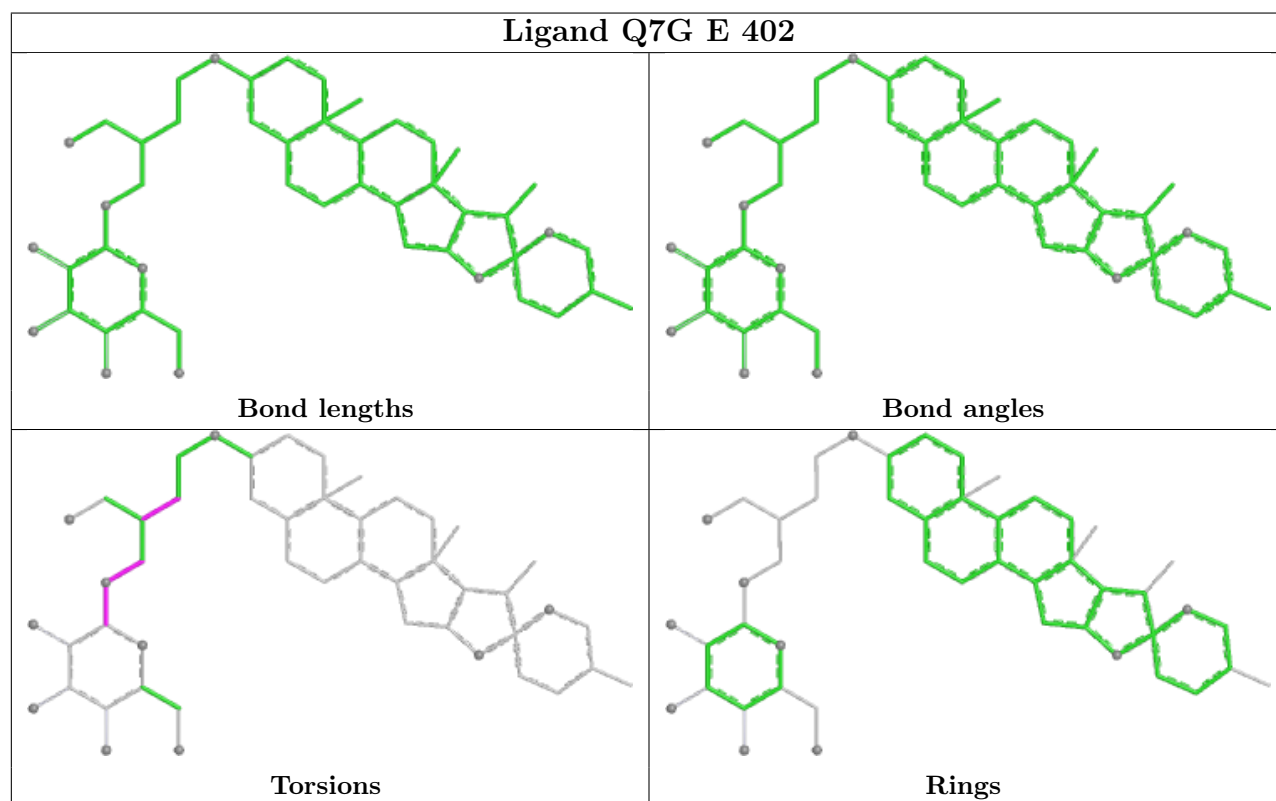
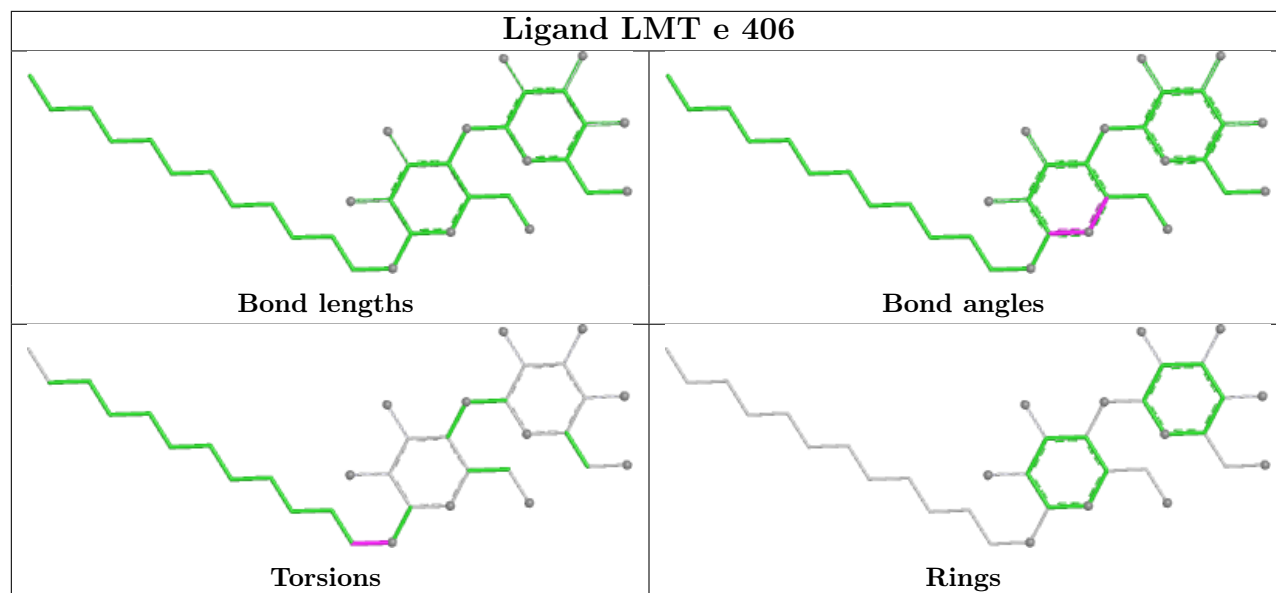


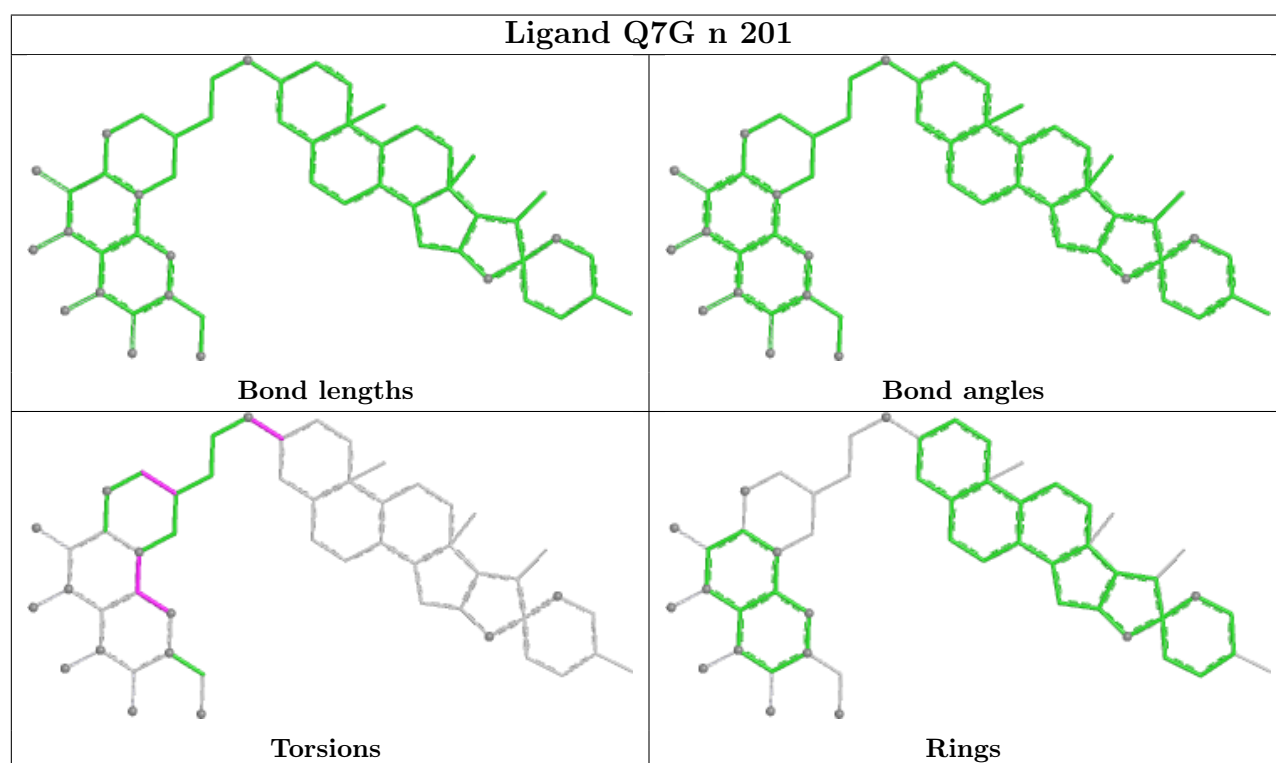
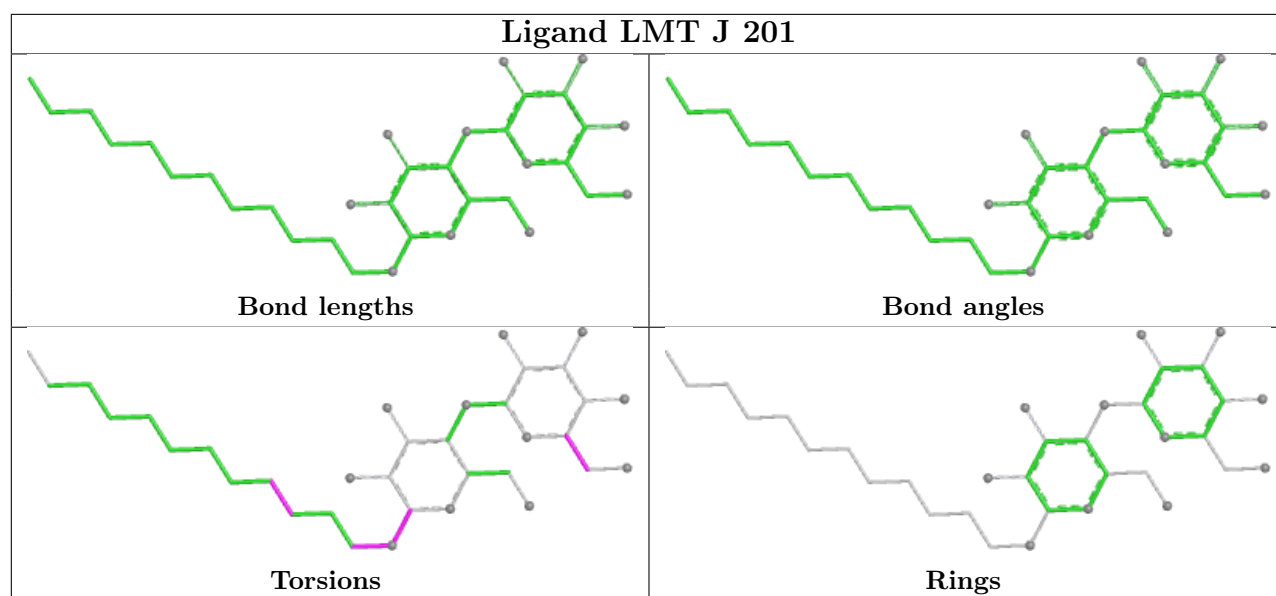
| Ligand PC1 i 201                                                                                      |                                                                                                       |
|-------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |
| Ligand PEE F 202                                                                                      |                                                                                                       |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |

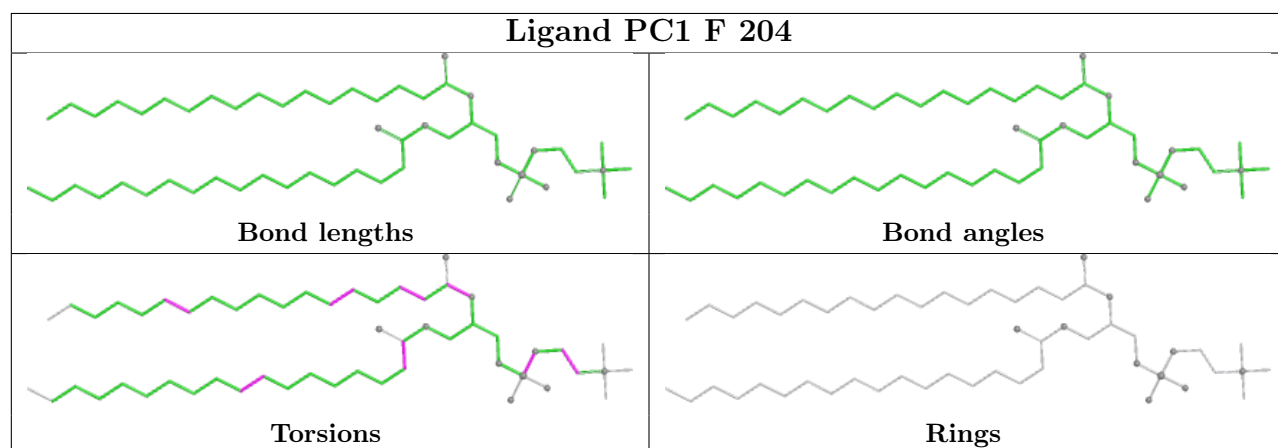
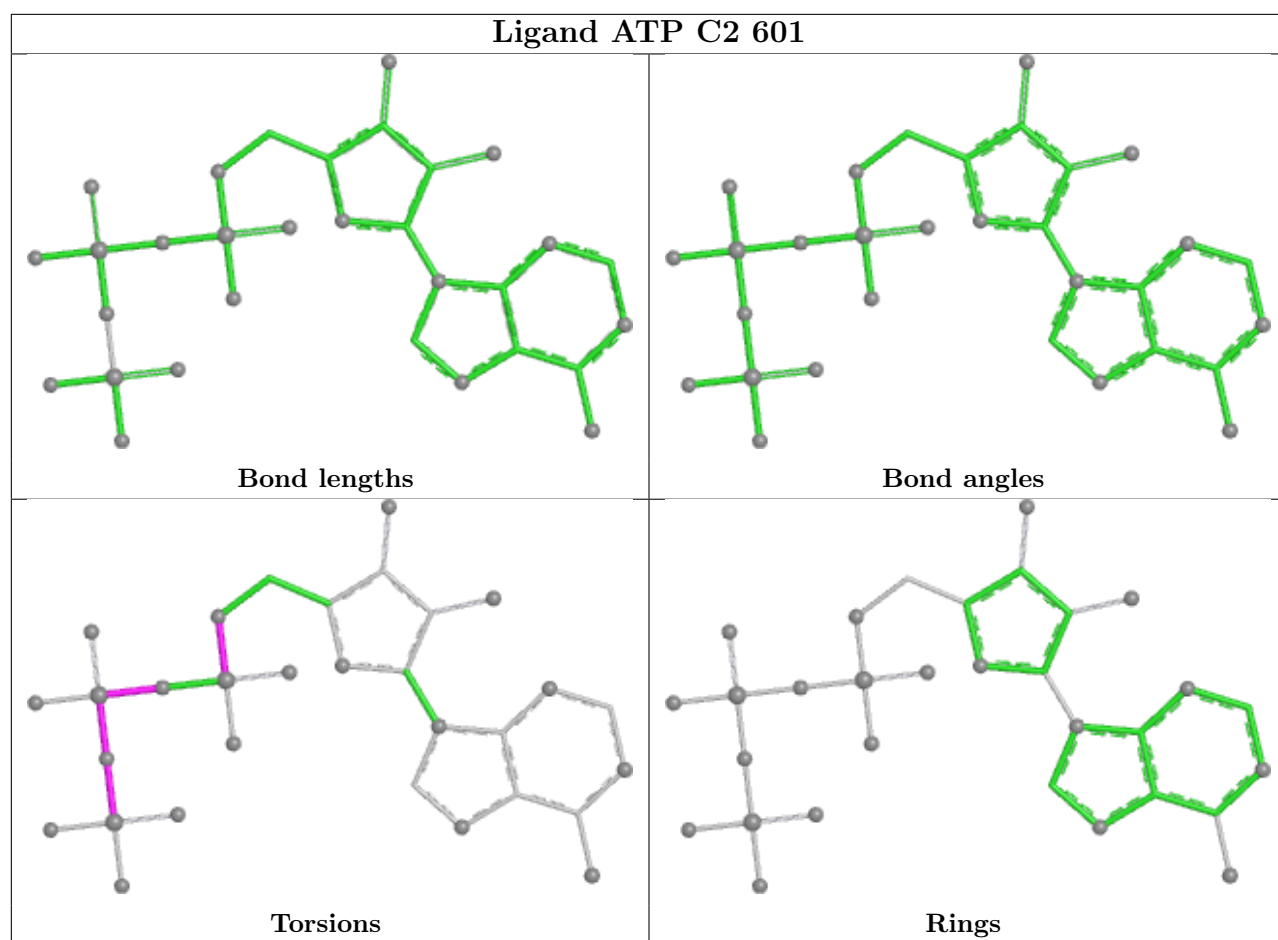


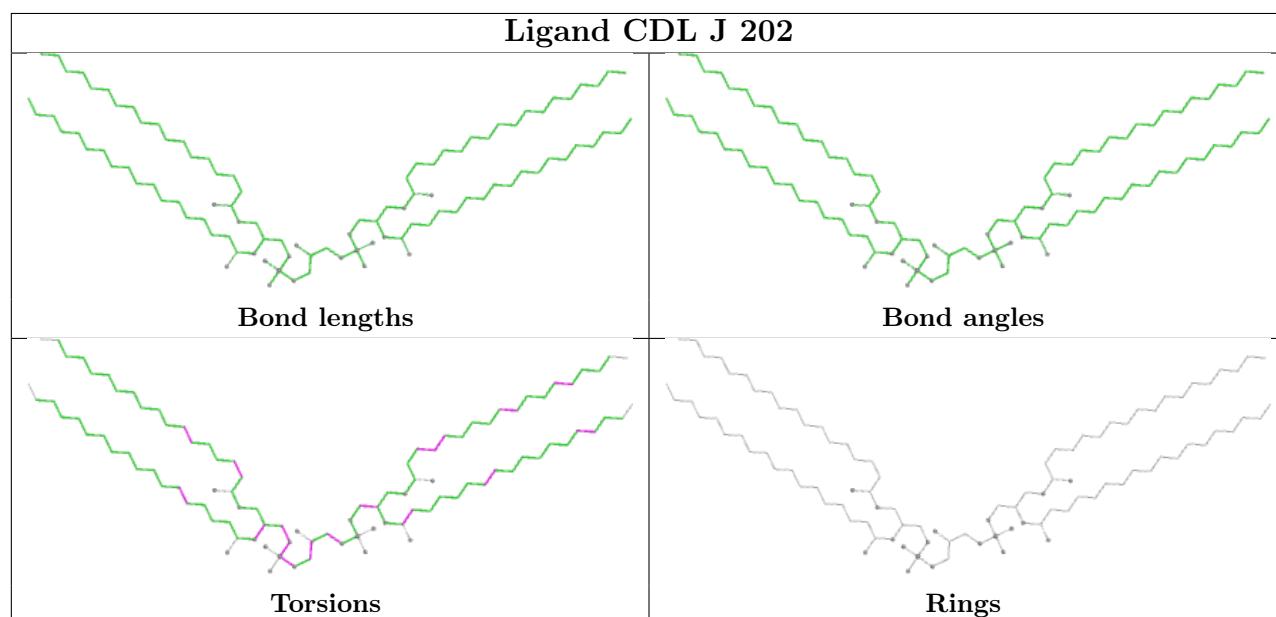
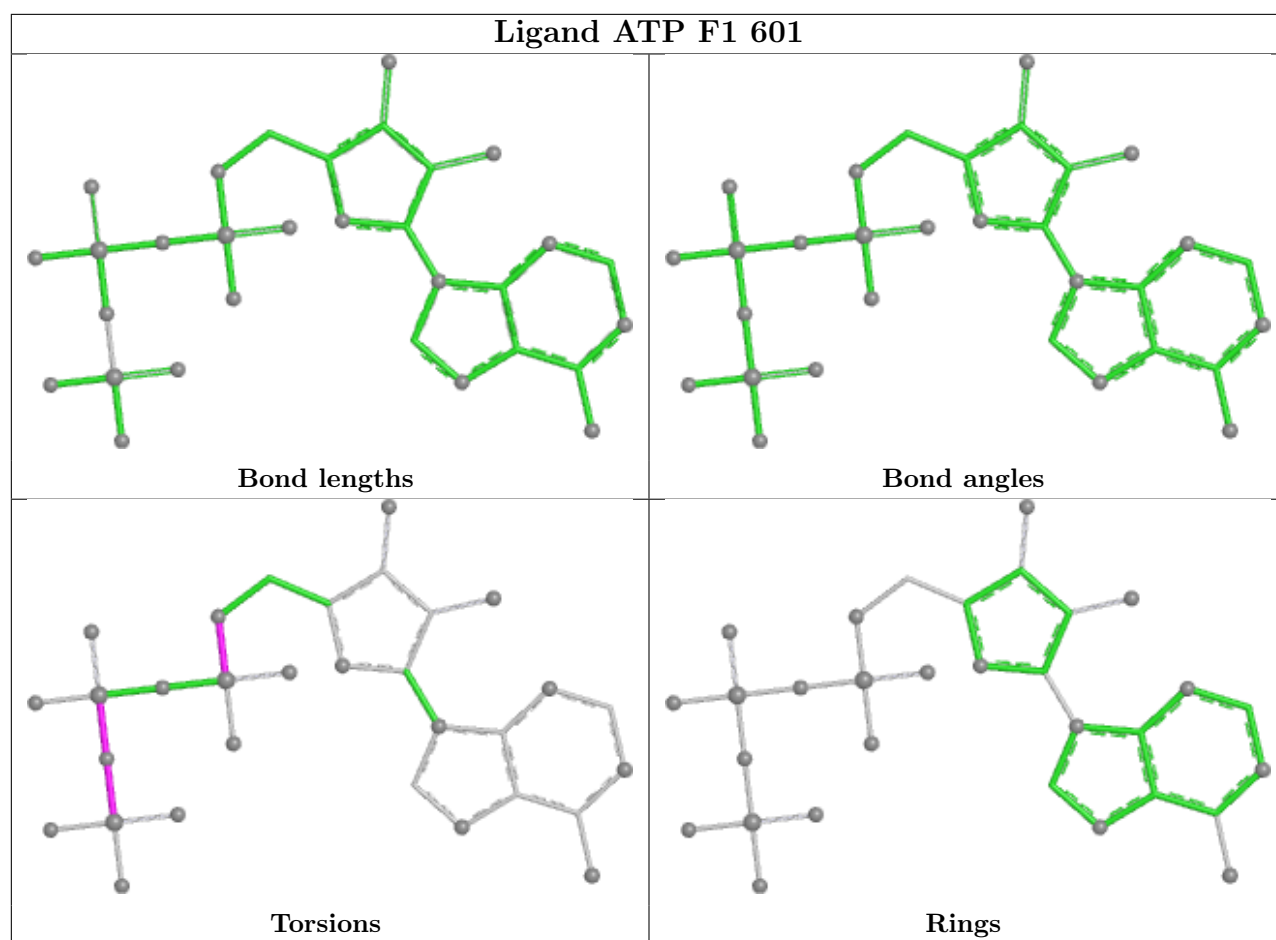


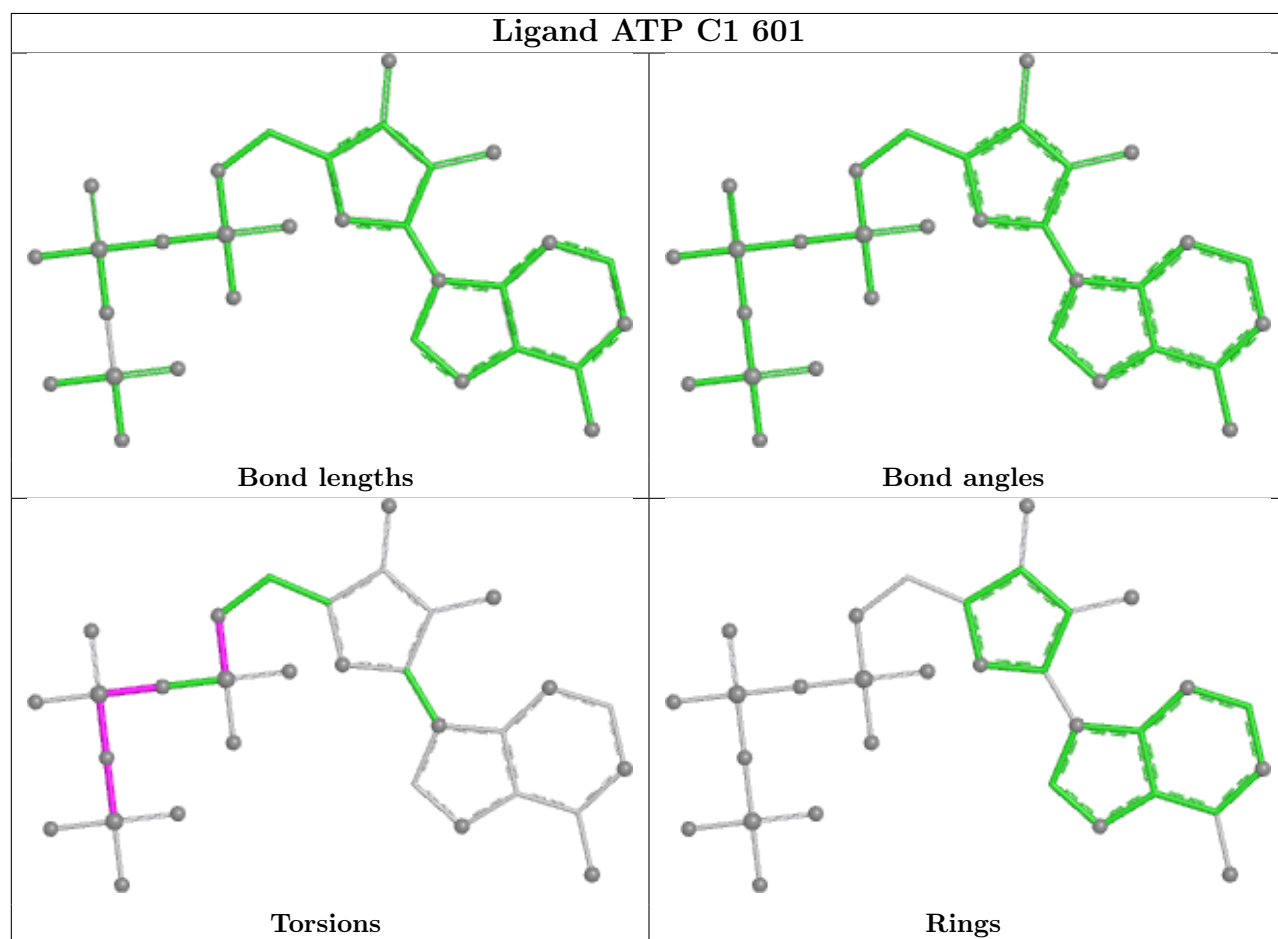
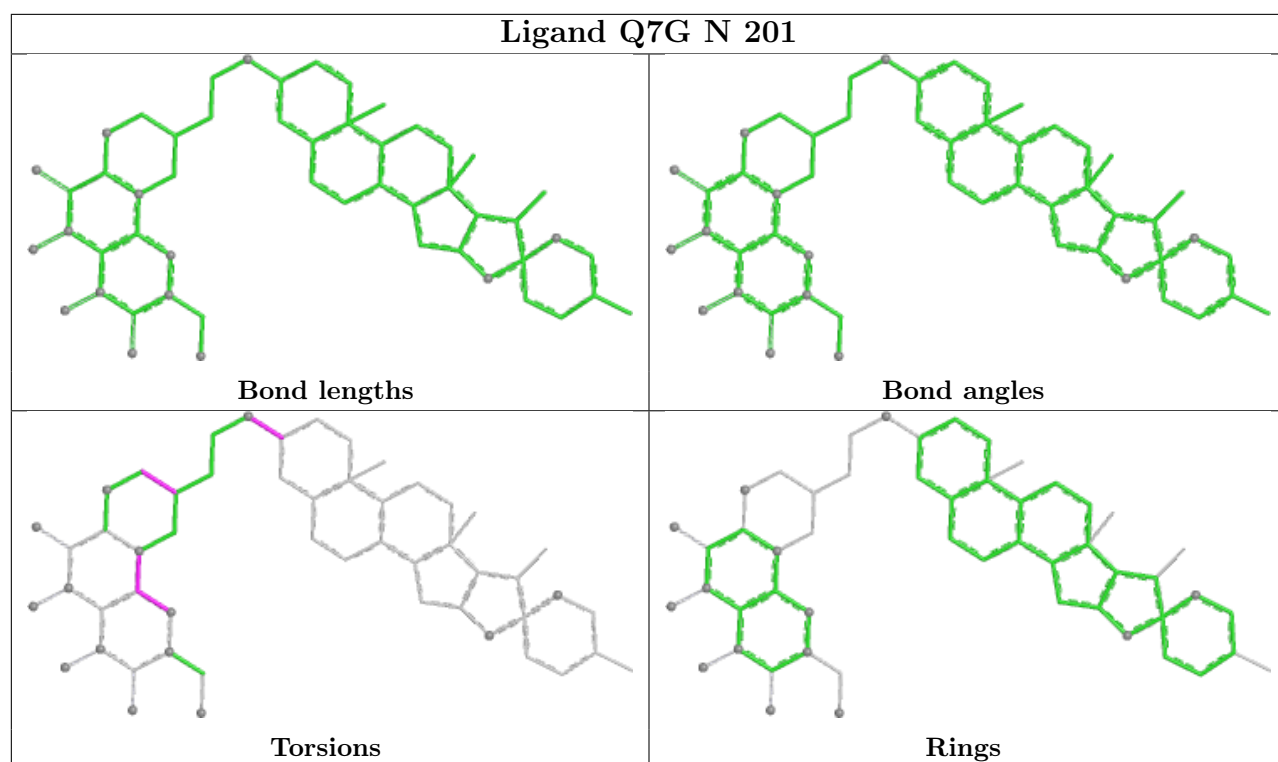


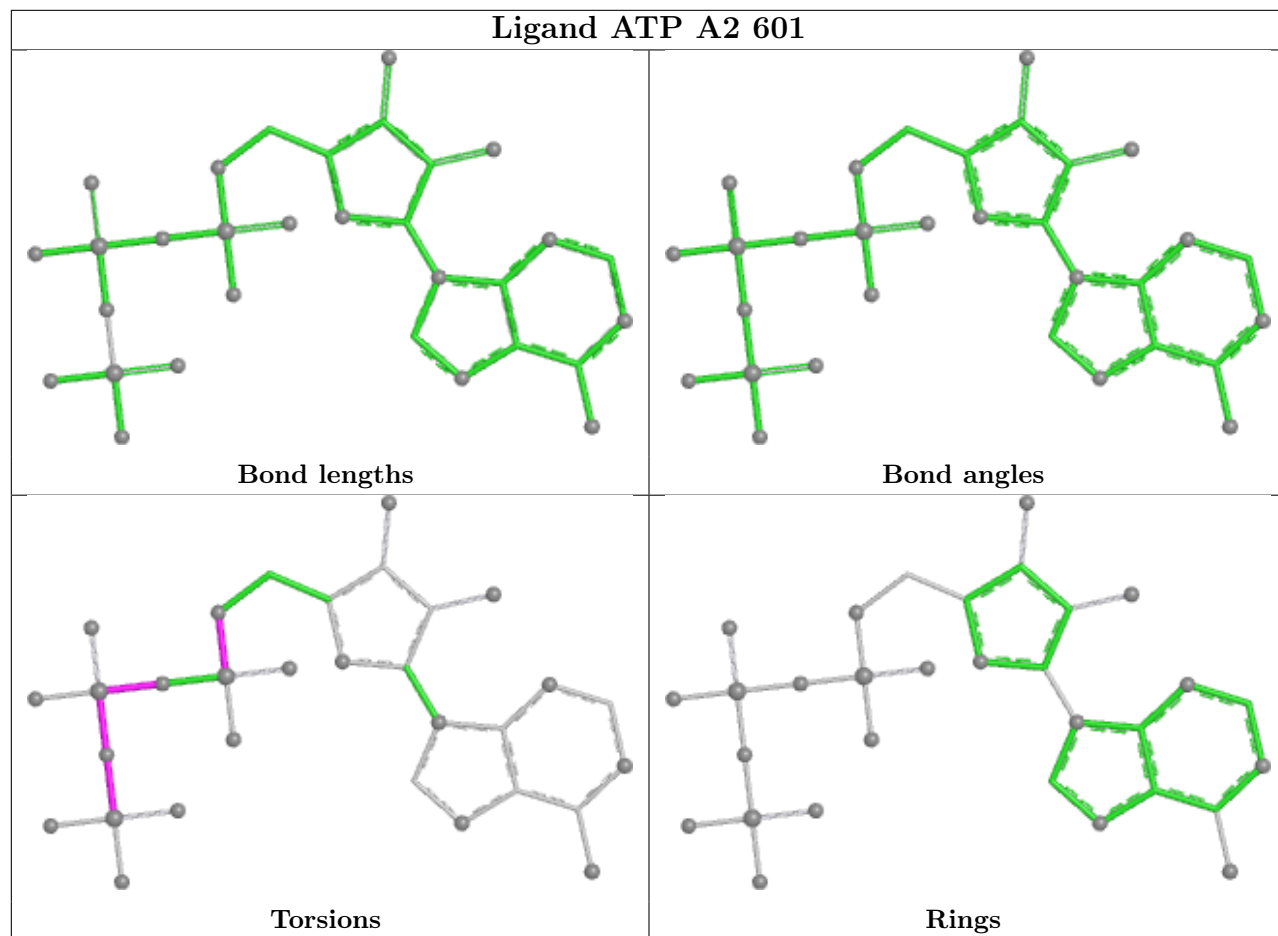
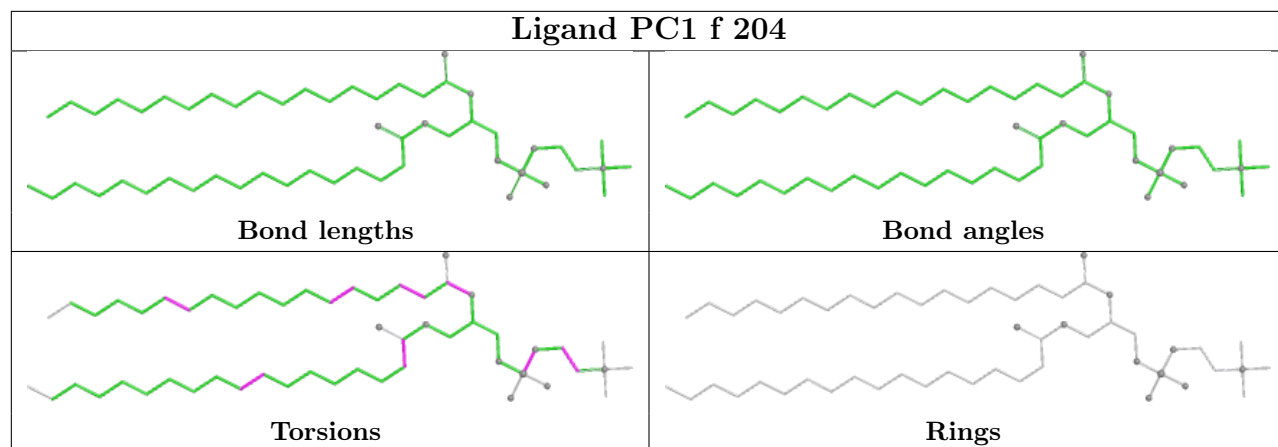


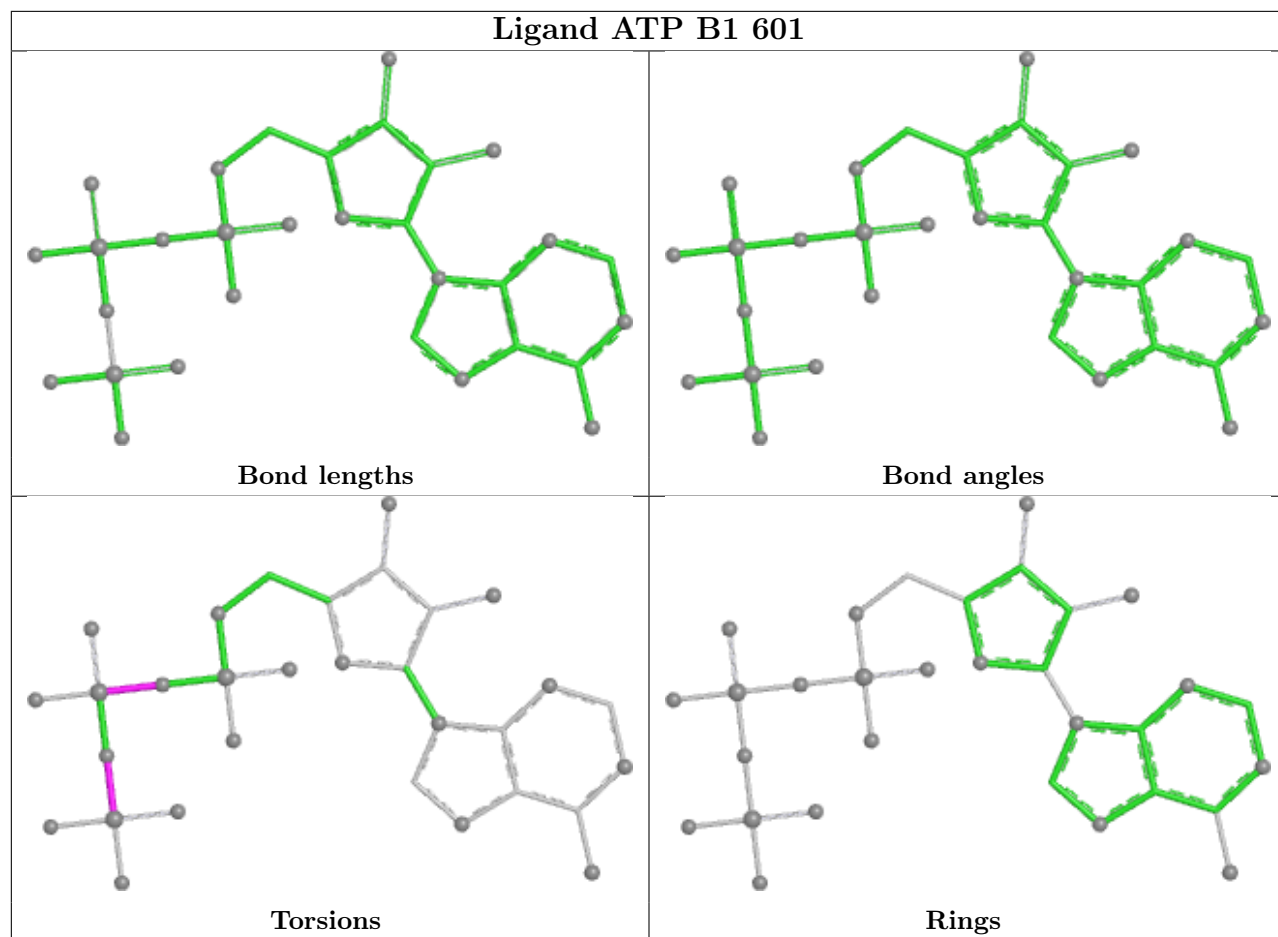


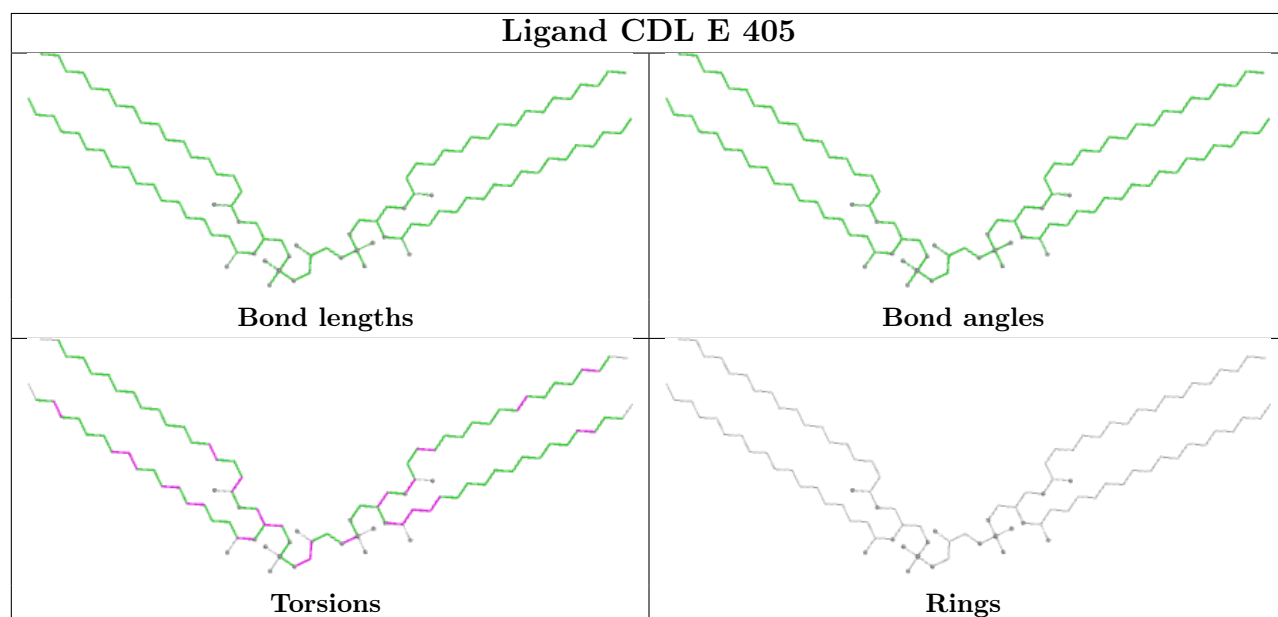
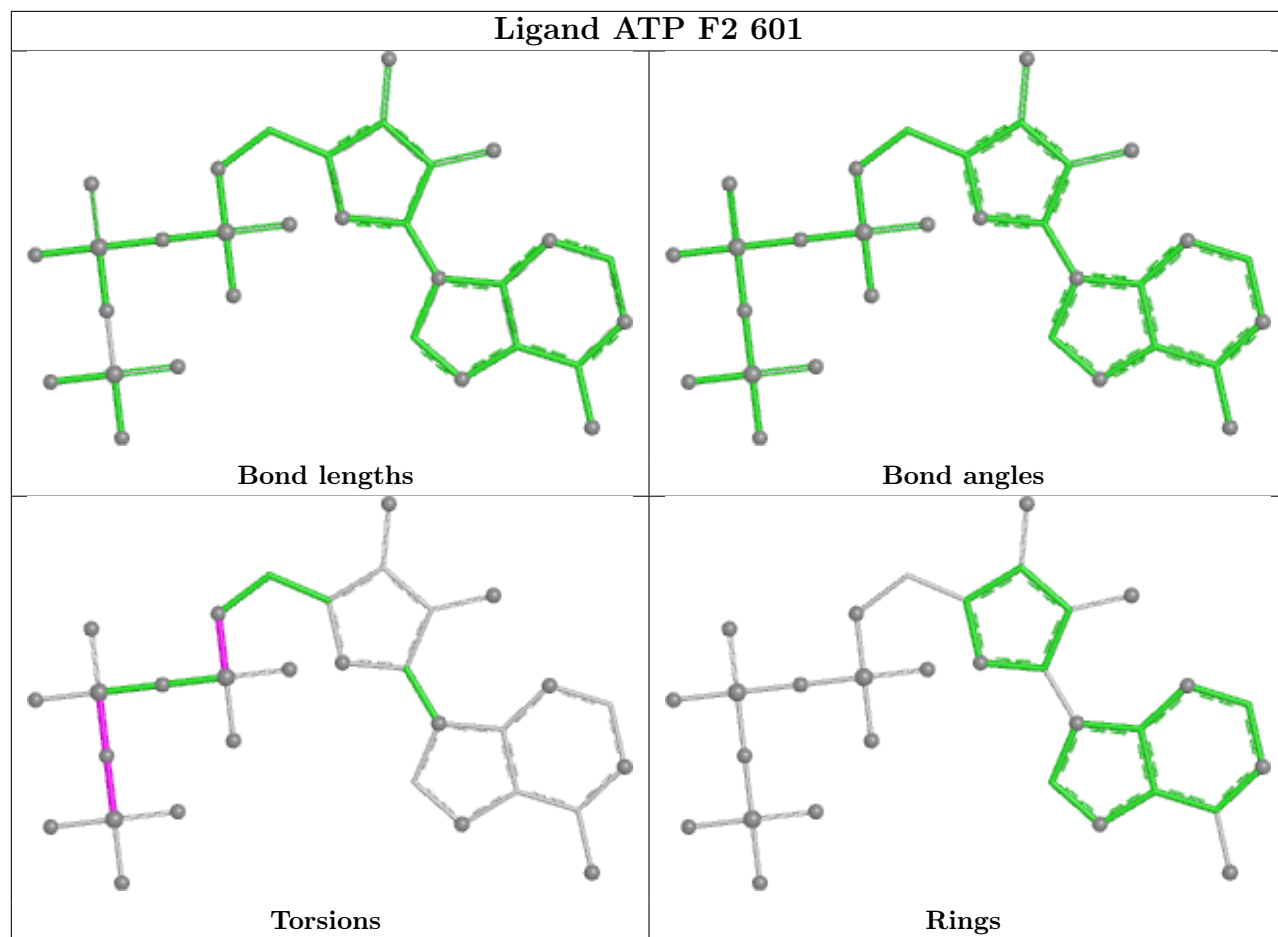


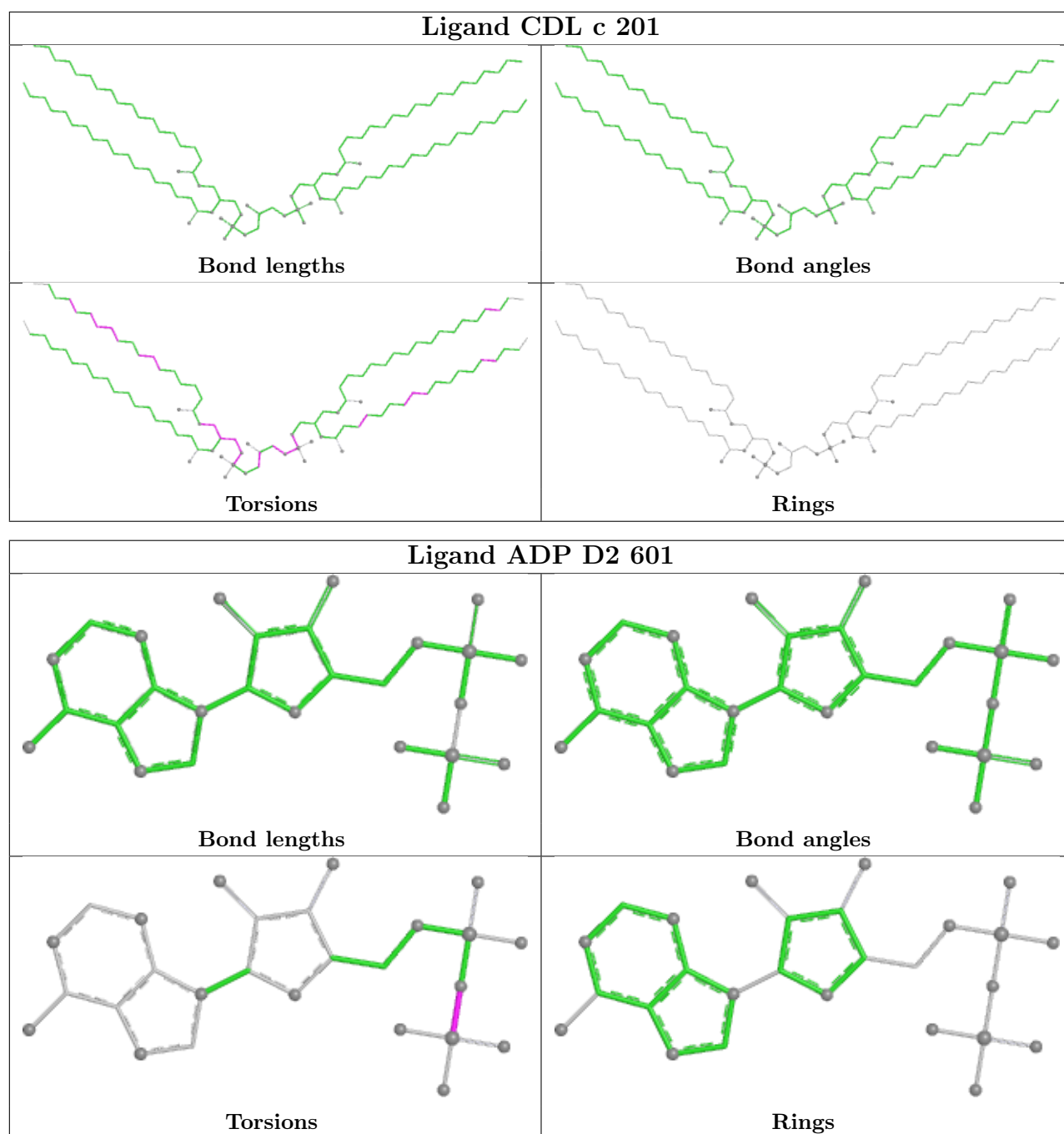












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15559. 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

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

### 6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

### 6.5 Orthogonal surface views

This section was not generated.

### 6.6 Mask visualisation

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

## 7 Map analysis ⓘ

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

### 7.1 Map-value distribution ⓘ

This section was not generated.

### 7.2 Volume estimate versus contour level ⓘ

This section was not generated.

### 7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

## 8 Fourier-Shell correlation

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

## 9 Map-model fit

This section was not generated.