



# wwPDB EM Validation Summary Report ⓘ

Aug 5, 2026 – 01:22 AM EDT

PDB ID : 8UCA / pdb\_00008uca  
EMDB ID : EMD-42122  
Title : Formation of I2+III2 supercomplex rescues respiratory chain defects  
Authors : Letts, J.A.; Padavannil, A.  
Deposited on : 2023-09-26  
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

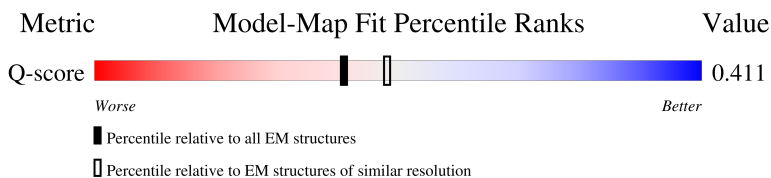
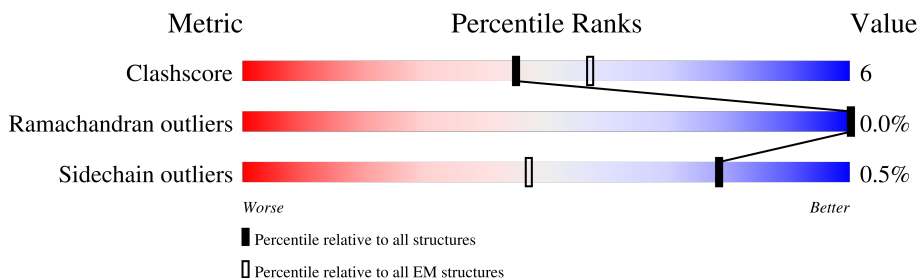
EMDB validation analysis : 0.0.1.dev133  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

# 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 3.70 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 11569 ( 3.20 - 4.20 )                                    |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 3     | 115    |                  |
| 1   | 3a    | 115    |                  |
| 2   | S3    | 263    |                  |
| 2   | s3    | 263    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | S2    | 463    |                  |
| 3   | s2    | 463    |                  |
| 4   | 1     | 318    |                  |
| 4   | 1a    | 318    |                  |
| 5   | 6     | 172    |                  |
| 5   | 6a    | 172    |                  |
| 6   | 4L    | 98     |                  |
| 6   | 4l    | 98     |                  |
| 7   | 5     | 607    |                  |
| 7   | 5a    | 607    |                  |
| 8   | 4     | 459    |                  |
| 8   | 4a    | 459    |                  |
| 9   | 2     | 345    |                  |
| 9   | 2a    | 345    |                  |
| 10  | AL    | 355    |                  |
| 10  | al    | 355    |                  |
| 11  | A9    | 377    |                  |
| 11  | a9    | 377    |                  |
| 12  | S4    | 175    |                  |
| 12  | s4    | 175    |                  |
| 13  | S6    | 116    |                  |
| 13  | s6    | 116    |                  |
| 14  | A2    | 99     |                  |
| 14  | a2    | 99     |                  |
| 15  | AB    | 156    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15  | AC    | 156    |                  |
| 15  | ab    | 156    |                  |
| 15  | ac    | 156    |                  |
| 16  | A5    | 116    |                  |
| 16  | a5    | 116    |                  |
| 17  | A6    | 131    |                  |
| 17  | a6    | 131    |                  |
| 18  | A8    | 172    |                  |
| 18  | a8    | 172    |                  |
| 19  | AM    | 142    |                  |
| 19  | am    | 142    |                  |
| 20  | AO    | 144    |                  |
| 20  | ao    | 144    |                  |
| 21  | A1    | 70     |                  |
| 21  | a1    | 70     |                  |
| 22  | A3    | 84     |                  |
| 22  | a3    | 84     |                  |
| 23  | C1    | 76     |                  |
| 23  | c1    | 76     |                  |
| 24  | C2    | 120    |                  |
| 24  | c2    | 120    |                  |
| 25  | S5    | 106    |                  |
| 25  | s5    | 106    |                  |
| 26  | B1    | 57     |                  |
| 26  | b1    | 57     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 27  | BM    | 151    |                  |
| 27  | bm    | 151    |                  |
| 28  | B5    | 189    |                  |
| 28  | b5    | 189    |                  |
| 29  | B6    | 127    |                  |
| 29  | b6    | 127    |                  |
| 30  | B2    | 105    |                  |
| 30  | b2    | 105    |                  |
| 31  | B3    | 104    |                  |
| 31  | b3    | 104    |                  |
| 32  | B8    | 186    |                  |
| 32  | b8    | 186    |                  |
| 33  | B4    | 129    |                  |
| 33  | b4    | 129    |                  |
| 34  | B9    | 179    |                  |
| 34  | b9    | 179    |                  |
| 35  | B7    | 136    |                  |
| 35  | b7    | 136    |                  |
| 36  | BL    | 176    |                  |
| 36  | bl    | 176    |                  |
| 37  | AN    | 145    |                  |
| 37  | an    | 145    |                  |
| 38  | A7    | 112    |                  |
| 38  | a7    | 112    |                  |
| 39  | V3    | 104    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 39  | v3    | 104    |                  |
| 40  | 3A    | 446    |                  |
| 40  | 3L    | 446    |                  |
| 41  | 3B    | 439    |                  |
| 41  | 3M    | 439    |                  |
| 42  | 3C    | 380    |                  |
| 42  | 3N    | 380    |                  |
| 43  | 3D    | 241    |                  |
| 43  | 3O    | 241    |                  |
| 44  | 3E    | 196    |                  |
| 44  | 3P    | 196    |                  |
| 45  | 3F    | 110    |                  |
| 45  | 3Q    | 110    |                  |
| 46  | 3G    | 81     |                  |
| 46  | 3R    | 81     |                  |
| 47  | 3H    | 76     |                  |
| 47  | 3S    | 76     |                  |
| 48  | 3J    | 63     |                  |
| 48  | 3U    | 63     |                  |
| 49  | 3K    | 56     |                  |
| 49  | 3V    | 56     |                  |
| 50  | 3T    | 78     |                  |
| 51  | V1    | 457    |                  |
| 51  | v1    | 457    |                  |
| 52  | V2    | 244    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 52  | v2    | 244    |                  |
| 53  | S1    | 716    |                  |
| 53  | s1    | 716    |                  |
| 54  | S7    | 224    |                  |
| 54  | s7    | 224    |                  |
| 55  | S8    | 212    |                  |
| 55  | s8    | 212    |                  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 62  | HEC  | 3D    | 401 | X         | -        | -       | -                |
| 62  | HEC  | 3O    | 401 | X         | -        | -       | -                |
| 64  | SF4  | S7    | 301 | -         | -        | X       | -                |
| 64  | SF4  | s7    | 301 | -         | -        | X       | -                |
| 64  | SF4  | s8    | 301 | -         | -        | X       | -                |

## 2 Entry composition

There are 65 unique types of molecules in this entry. The entry contains 162102 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | 3     | 113      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 914   | 622 | 131 | 155 | 6 |         |       |
| 1   | 3a    | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 893   | 607 | 128 | 152 | 6 |         |       |

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | S3    | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1712  | 1105 | 294 | 310 | 3 |         |       |
| 2   | s3    | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1701  | 1099 | 290 | 309 | 3 |         |       |

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | S2    | 423      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3410  | 2180 | 586 | 620 | 24 |         |       |
| 3   | s2    | 421      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3386  | 2165 | 581 | 616 | 24 |         |       |

- Molecule 4 is a protein called NADH-ubiquinone oxidoreductase chain 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | 1     | 317      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2530  | 1700 | 383 | 426 | 21 |         |       |
| 4   | 1a    | 316      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2522  | 1695 | 382 | 425 | 20 |         |       |

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase chain 6.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 5   | 6     | 170      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1290  | 868 | 184 | 224 | 14 |         |       |
| 5   | 6a    | 171      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1298  | 873 | 185 | 225 | 15 |         |       |

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 6   | 4L    | 97       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 729   | 473 | 111 | 135 | 10 |         |       |
| 6   | 4l    | 97       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 727   | 471 | 111 | 135 | 10 |         |       |

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase chain 5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7   | 5     | 605      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4790  | 3175 | 745 | 825 | 45 |         |       |
| 7   | 5a    | 605      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4790  | 3175 | 745 | 825 | 45 |         |       |

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 8   | 4     | 459      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3630  | 2407 | 567 | 616 | 40 |         |       |
| 8   | 4a    | 459      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3630  | 2407 | 567 | 616 | 40 |         |       |

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase chain 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9   | 2     | 344      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2694  | 1790 | 416 | 451 | 37 |         |       |
| 9   | 2a    | 344      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2694  | 1790 | 416 | 451 | 37 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 10  | AL    | 320      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2607  | 1674 | 431 | 492 | 10 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 10  | al    | 320      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2607  | 1674 | 431 | 492 | 10 |         |       |

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 11  | A9    | 342      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2748  | 1777 | 483 | 481 | 7 |         |       |
| 11  | a9    | 342      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2748  | 1777 | 483 | 481 | 7 |         |       |

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | S4    | 126      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1021  | 646 | 179 | 192 | 4 |         |       |
| 12  | s4    | 126      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1021  | 646 | 179 | 192 | 4 |         |       |

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | S6    | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 748   | 464 | 138 | 143 | 3 |         |       |
| 13  | s6    | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 748   | 464 | 138 | 143 | 3 |         |       |

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | A2    | 84       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 671   | 421 | 127 | 120 | 3 |         |       |
| 14  | a2    | 84       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 671   | 421 | 127 | 120 | 3 |         |       |

- Molecule 15 is a protein called Acyl carrier protein, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | AB    | 78       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 628   | 404 | 93  | 126 | 5 |         |       |
| 15  | AC    | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 706   | 453 | 104 | 144 | 5 |         |       |
| 15  | ab    | 78       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 628   | 404 | 93  | 126 | 5 |         |       |
| 15  | ac    | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 706   | 453 | 104 | 144 | 5 |         |       |

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | A5    | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 927   | 604 | 154 | 166 | 3 |         |       |
| 16  | a5    | 113      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 923   | 602 | 153 | 165 | 3 |         |       |

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | A6    | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 957   | 612 | 178 | 161 | 6 |         |       |
| 17  | a6    | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 950   | 607 | 177 | 160 | 6 |         |       |

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 18  | A8    | 169      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1385  | 882 | 248 | 245 | 10 |         |       |
| 18  | a8    | 170      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1389  | 884 | 249 | 246 | 10 |         |       |

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | AM    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1045  | 667 | 176 | 193 | 9 |         |       |
| 19  | am    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1045  | 667 | 176 | 193 | 9 |         |       |

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | AO    | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1161  | 747 | 206 | 200 | 8 |         |       |
| 20  | ao    | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1161  | 747 | 206 | 200 | 8 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 21  | A1    | 69       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 564   | 366 | 100 | 94 | 4 |         |       |
| 21  | a1    | 69       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 564   | 366 | 100 | 94 | 4 |         |       |

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | A3    | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 648   | 425 | 105 | 114 | 4 |         |       |
| 22  | a3    | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 648   | 425 | 105 | 114 | 4 |         |       |

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 23  | C1    | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 407   | 266 | 70 | 70 | 1 |         |       |
| 23  | c1    | 45       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 377   | 247 | 65 | 64 | 1 |         |       |

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | C2    | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 996   | 651 | 171 | 165 | 9 |         |       |
| 24  | c2    | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 996   | 651 | 171 | 165 | 9 |         |       |

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | S5    | 105      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 877   | 555 | 162 | 152 | 8 |         |       |
| 25  | s5    | 105      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 877   | 555 | 162 | 152 | 8 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 26  | B1    | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 482   | 314 | 85 | 81 | 2 |         |       |
| 26  | b1    | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 482   | 314 | 85 | 81 | 2 |         |       |

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | BM    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 826   | 536 | 133 | 153 | 4 |         |       |
| 27  | bm    | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 835   | 541 | 134 | 156 | 4 |         |       |

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | B5    | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1166  | 764 | 195 | 204 | 3 |         |       |
| 28  | b5    | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1158  | 760 | 193 | 202 | 3 |         |       |

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | B6    | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 783   | 511 | 137 | 132 | 3 |         |       |
| 29  | b6    | 90       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 761   | 495 | 133 | 130 | 3 |         |       |

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 30  | B2    | 64       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 555   | 365 | 92 | 97 | 1 |         |       |
| 30  | b2    | 63       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 545   | 359 | 89 | 96 | 1 |         |       |

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 31  | B3    | 70       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 569   | 376 | 99  | 92 | 2 |         |       |
| 31  | b3    | 71       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 573   | 378 | 100 | 93 | 2 |         |       |

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 32  | B8    | 155      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1302  | 840 | 216 | 235 | 11 |         |       |
| 32  | b8    | 155      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1302  | 840 | 216 | 235 | 11 |         |       |

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 33  | B4    | 125      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 1044  | 673 | 188 | 183 |  |         |       |
| 33  | b4    | 125      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 1044  | 673 | 188 | 183 |  |         |       |

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 34  | B9    | 178      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1541  | 985 | 276 | 269 | 11 |         |       |
| 34  | b9    | 177      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1534  | 981 | 275 | 267 | 11 |         |       |

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | B7    | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 984   | 620 | 185 | 171 | 8 |         |       |
| 35  | b7    | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1005  | 634 | 189 | 174 | 8 |         |       |

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | BL    | 167      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1410  | 888 | 251 | 263 | 8 |         |       |
| 36  | bl    | 169      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1430  | 899 | 257 | 266 | 8 |         |       |

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | AN    | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1201  | 772 | 214 | 211 | 4 |         |       |
| 37  | an    | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1201  | 772 | 214 | 211 | 4 |         |       |

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | A7    | 92       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 741   | 469 | 139 | 130 | 3 |         |       |
| 38  | a7    | 70       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 560   | 350 | 108 | 100 | 2 |         |       |

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 39  | V3    | 40       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 339   | 213 | 62 | 64 |         |       |
| 39  | v3    | 36       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 303   | 190 | 56 | 57 |         |       |

- Molecule 40 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 40  | 3A    | 445      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3459  | 2163 | 610 | 669 | 17 |         |       |
| 40  | 3L    | 445      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3460  | 2163 | 610 | 670 | 17 |         |       |

- Molecule 41 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 41  | 3B    | 420      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3154  | 1980 | 555 | 610 | 9 |         |       |
| 41  | 3M    | 420      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3154  | 1980 | 555 | 610 | 9 |         |       |

- Molecule 42 is a protein called Cytochrome b.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 42  | 3C    | 380      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3046  | 2052 | 473 | 499 | 22 |         |       |
| 42  | 3N    | 380      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3046  | 2052 | 473 | 499 | 22 |         |       |

- Molecule 43 is a protein called Cytochrome c1, heme protein, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 43  | 3D    | 241      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1919  | 1224 | 329 | 352 | 14 |         |       |
| 43  | 3O    | 240      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1909  | 1218 | 327 | 350 | 14 |         |       |

- Molecule 44 is a protein called Cytochrome b-c1 complex subunit 9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | 3E    | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 602   | 374 | 100 | 126 | 2 |         |       |
| 44  | 3P    | 81       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 610   | 380 | 101 | 127 | 2 |         |       |

- Molecule 45 is a protein called Cytochrome b-c1 complex subunit 7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | 3F    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 900   | 575 | 160 | 162 | 3 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | 3Q    | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 879   | 563 | 156 | 157 | 3 |         |       |

- Molecule 46 is a protein called Cytochrome b-c1 complex subunit 8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | 3G    | 79       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 670   | 432 | 123 | 114 | 1 |         |       |
| 46  | 3R    | 71       | Total | C   | N   | O   |   | 0       | 0     |
|     |       |          | 600   | 389 | 112 | 99  |   |         |       |

- Molecule 47 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | 3H    | 66       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 545   | 333 | 101 | 106 | 5 |         |       |
| 47  | 3S    | 66       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 545   | 333 | 101 | 106 | 5 |         |       |

- Molecule 48 is a protein called Cytochrome b-c1 complex subunit 9.

| Mol | Chain | Residues | Atoms |     |    |    |  | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|-------|
| 48  | 3J    | 56       | Total | C   | N  | O  |  | 0       | 0     |
|     |       |          | 460   | 302 | 81 | 77 |  |         |       |
| 48  | 3U    | 59       | Total | C   | N  | O  |  | 0       | 0     |
|     |       |          | 489   | 320 | 85 | 84 |  |         |       |

- Molecule 49 is a protein called Cytochrome b-c1 complex subunit 10.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 49  | 3K    | 51       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 421   | 281 | 74 | 65 | 1 |         |       |
| 49  | 3V    | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 438   | 292 | 77 | 67 | 2 |         |       |

- Molecule 50 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 50  | 3T    | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 397   | 250 | 76 | 69 | 2 |         |       |

- Molecule 51 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochond-

drial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 51  | V1    | 428      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3301  | 2080 | 590 | 609 | 22 |         |       |
| 51  | v1    | 422      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3259  | 2053 | 584 | 600 | 22 |         |       |

- Molecule 52 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 52  | V2    | 209      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1630  | 1038 | 273 | 308 | 11 |         |       |
| 52  | v2    | 192      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1517  | 965  | 255 | 286 | 11 |         |       |

- Molecule 53 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 53  | S1    | 687      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5290  | 3318 | 918 | 1013 | 41 |         |       |
| 53  | s1    | 687      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5290  | 3318 | 918 | 1013 | 41 |         |       |

- Molecule 54 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 54  | S7    | 155      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1241  | 793 | 222 | 212 | 14 |         |       |
| 54  | s7    | 155      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1241  | 793 | 222 | 212 | 14 |         |       |

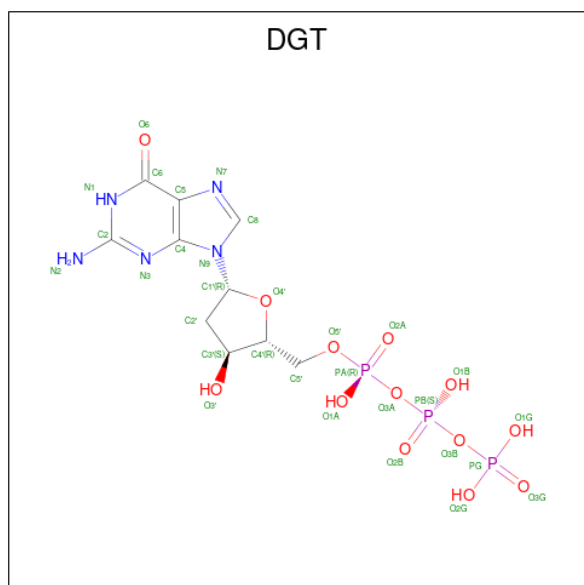
- Molecule 55 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

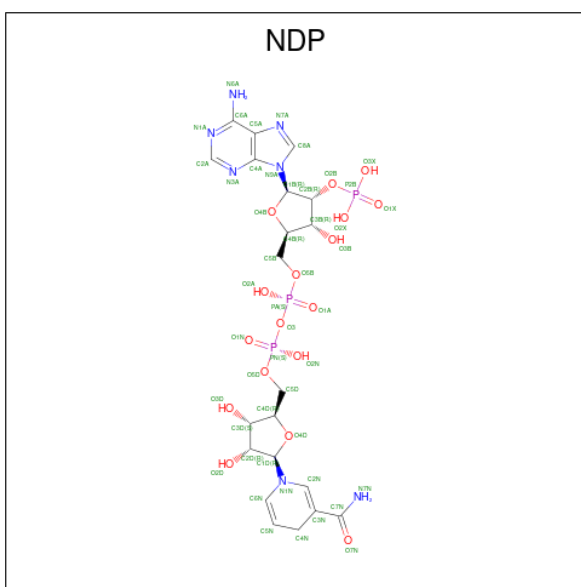
| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 55  | S8    | 178      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1408  | 885 | 243 | 268 | 12 |         |       |
| 55  | s8    | 164      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1309  | 821 | 226 | 250 | 12 |         |       |

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 56  | AL    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 56  | al    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 57 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



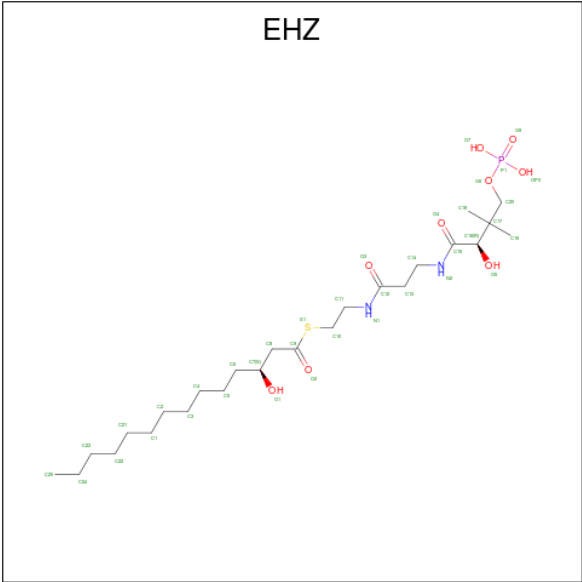


| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 58  | A9    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 58  | a9    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

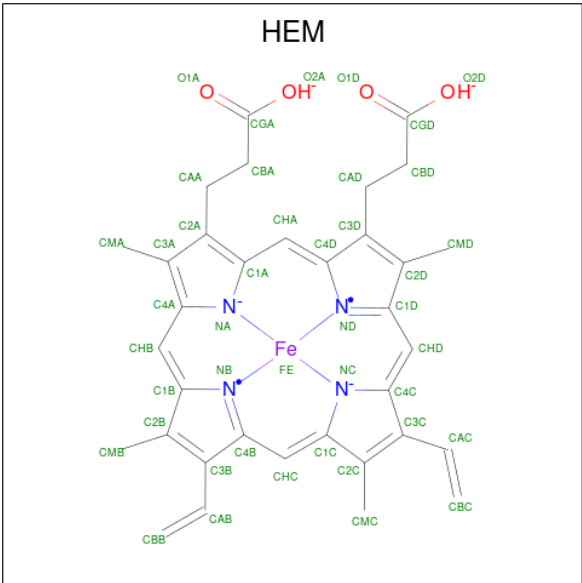
| Mol | Chain | Residues | Atoms           | AltConf |
|-----|-------|----------|-----------------|---------|
| 59  | S6    | 1        | Total Zn<br>1 1 | 0       |
| 59  | s6    | 1        | Total Zn<br>1 1 | 0       |

- Molecule 60 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C<sub>25</sub>H<sub>49</sub>N<sub>2</sub>O<sub>9</sub>PS).



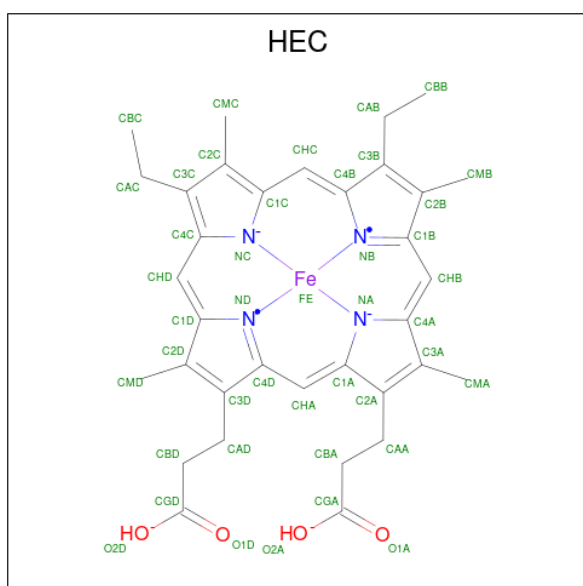
| Mol | Chain | Residues | Atoms |    |   |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---|---------|
| 60  | A6    | 1        | Total | C  | N | O | P | S | 0       |
|     |       |          | 37    | 25 | 2 | 8 | 1 | 1 |         |
| 60  | B9    | 1        | Total | C  | N | O | P | S | 0       |
|     |       |          | 37    | 25 | 2 | 8 | 1 | 1 |         |
| 60  | 5a    | 1        | Total | C  | N | O | P | S | 0       |
|     |       |          | 37    | 25 | 2 | 8 | 1 | 1 |         |
| 60  | a6    | 1        | Total | C  | N | O | P | S | 0       |
|     |       |          | 37    | 25 | 2 | 8 | 1 | 1 |         |

- Molecule 61 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



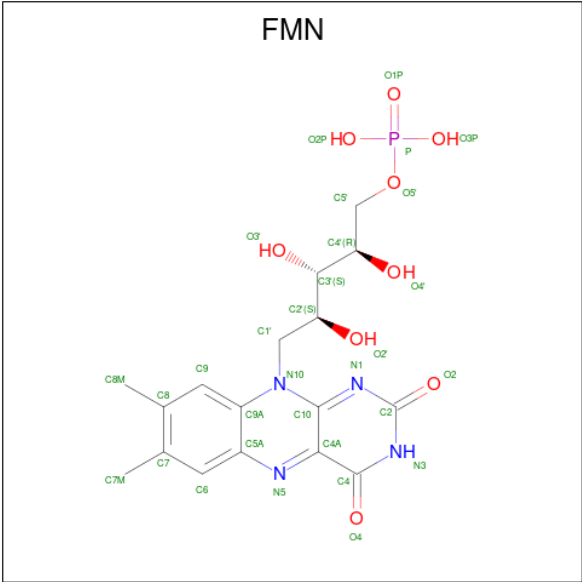
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 61  | 3C    | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 61  | 3C    | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 61  | 3N    | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 61  | 3N    | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |

- Molecule 62 is HEME C (CCD ID: HEC) (formula:  $C_{34}H_{36}FeN_4O_4$ ).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 62  | 3D    | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 62  | 3O    | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |

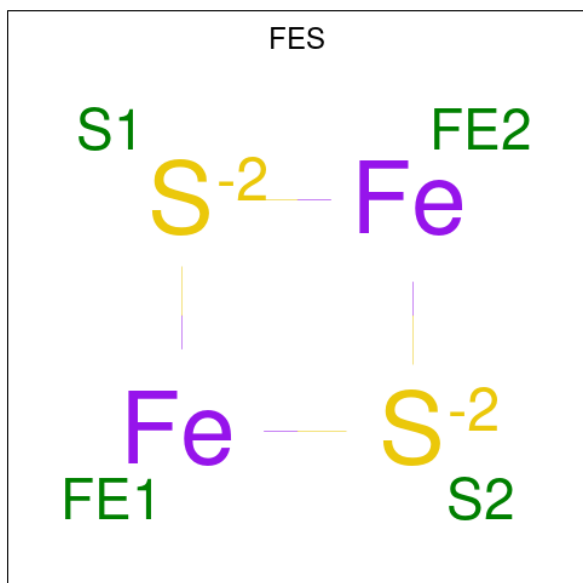
- Molecule 63 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 64  | S1    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 64  | S7    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 64  | S8    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 64  | S8    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 64  | v1    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 64  | s1    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 64  | s1    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 64  | s7    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 64  | s8    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 64  | s8    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

- Molecule 65 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 65  | V2    | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |

*Continued on next page...*

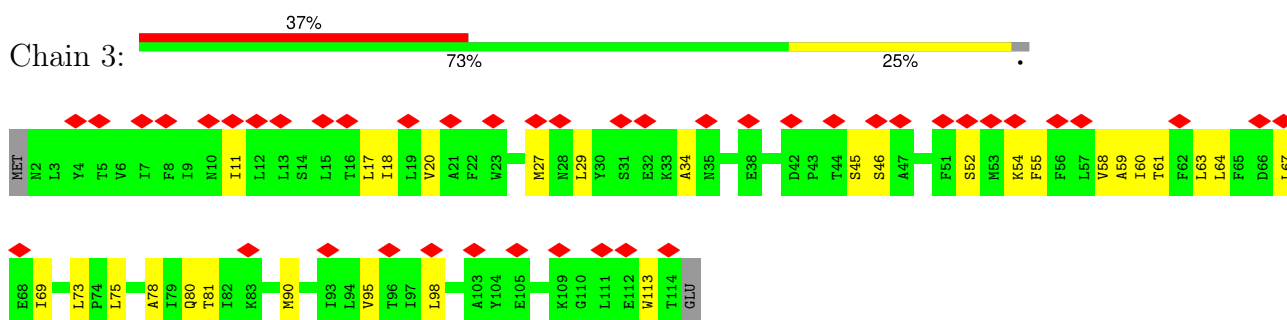
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| Mol | Chain | Residues | Atoms      |         |        | AltConf |
|-----|-------|----------|------------|---------|--------|---------|
| 65  | S1    | 1        | Total<br>4 | Fe<br>2 | S<br>2 | 0       |
| 65  | v2    | 1        | Total<br>4 | Fe<br>2 | S<br>2 | 0       |
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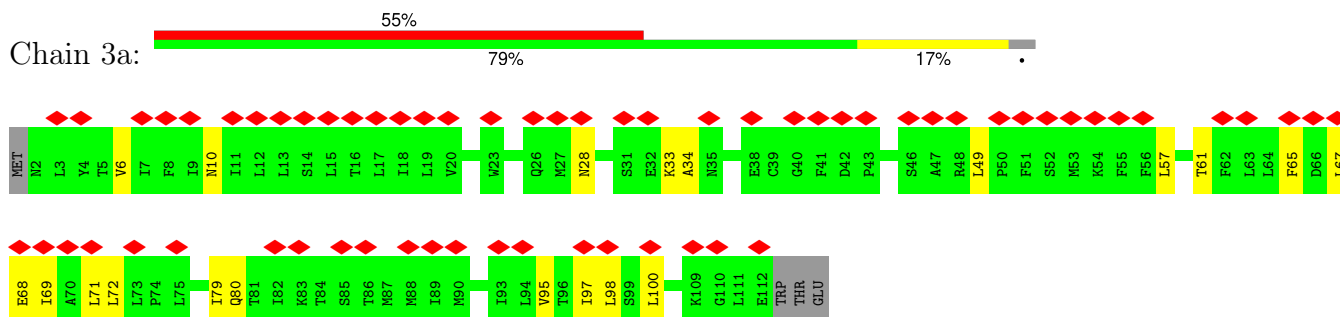
### 3 Residue-property plots [i](#)

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

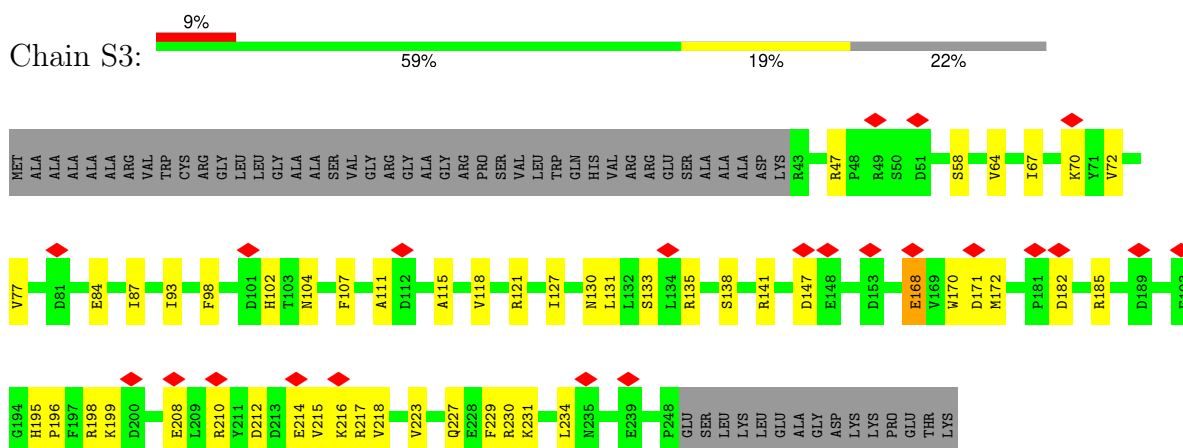
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



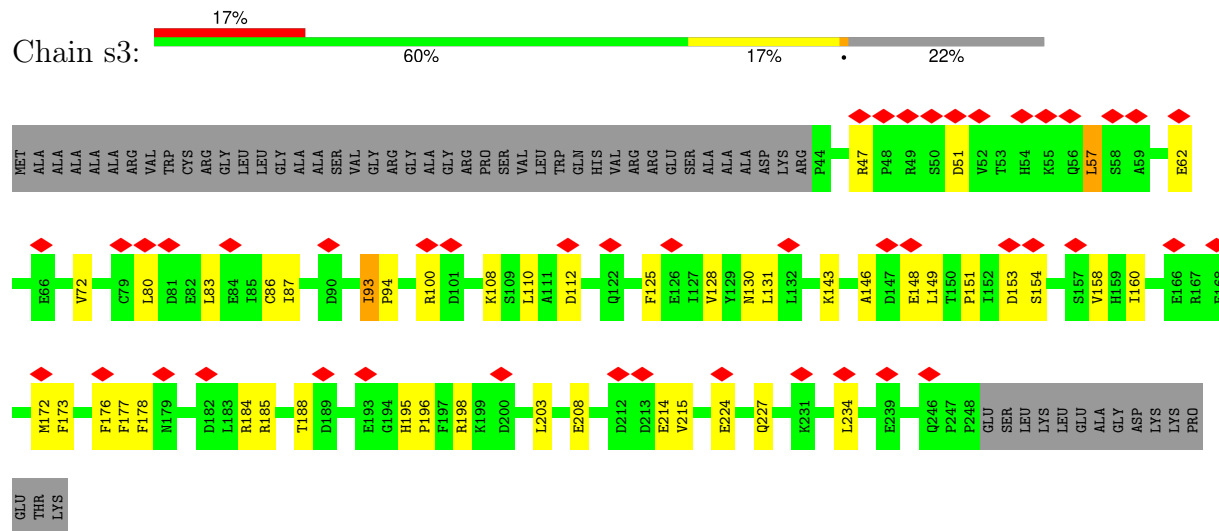
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



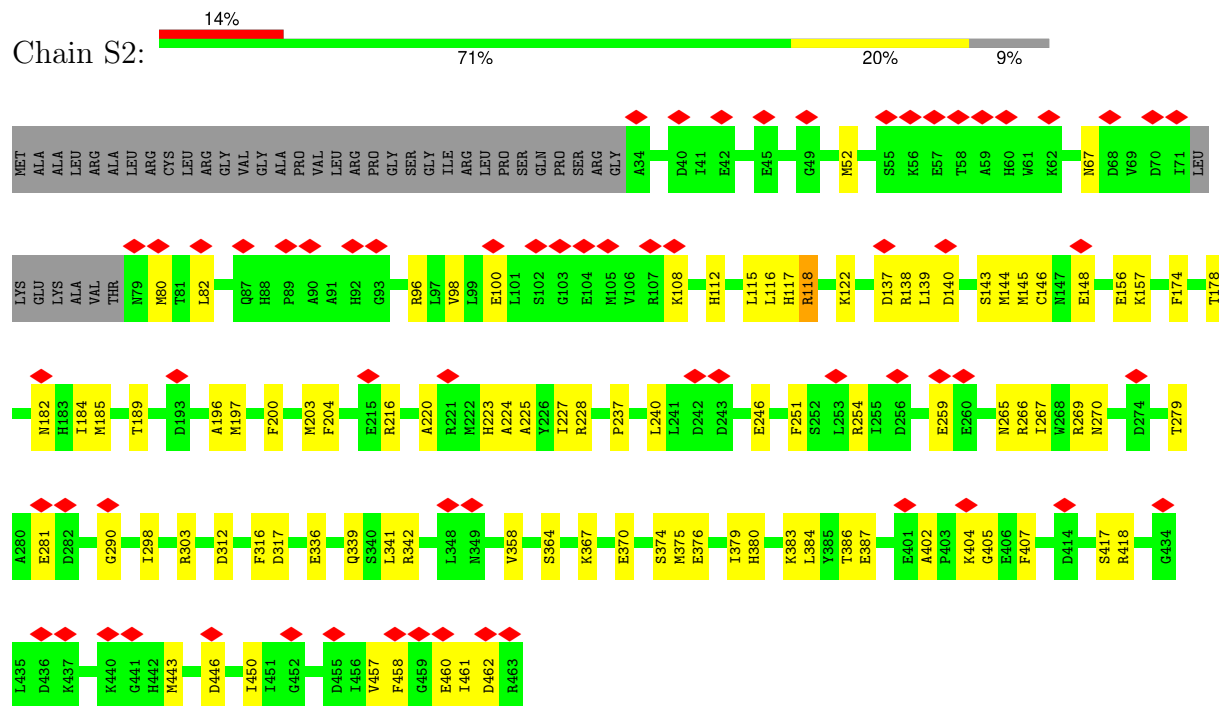
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

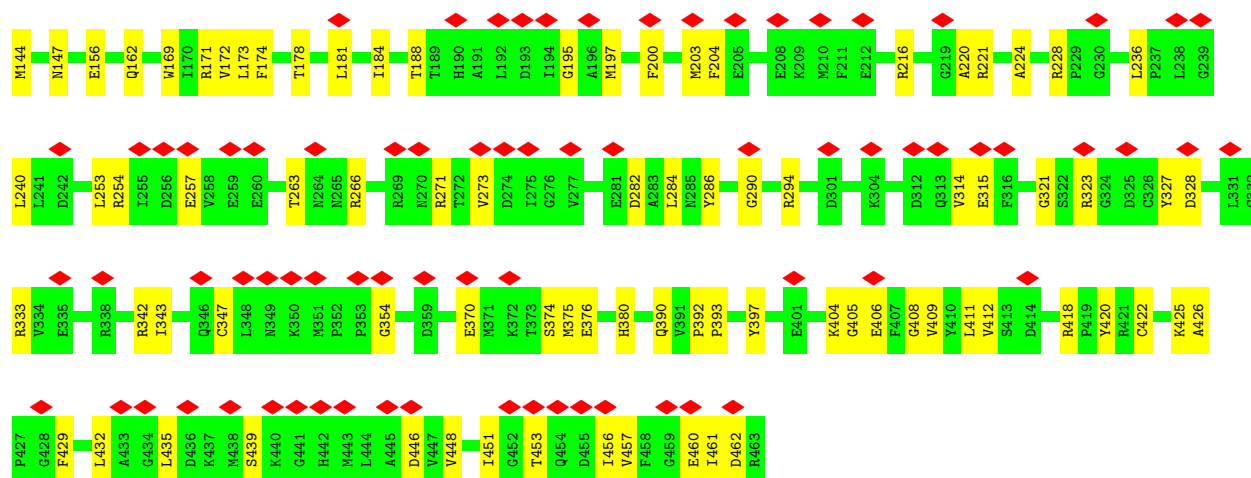


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

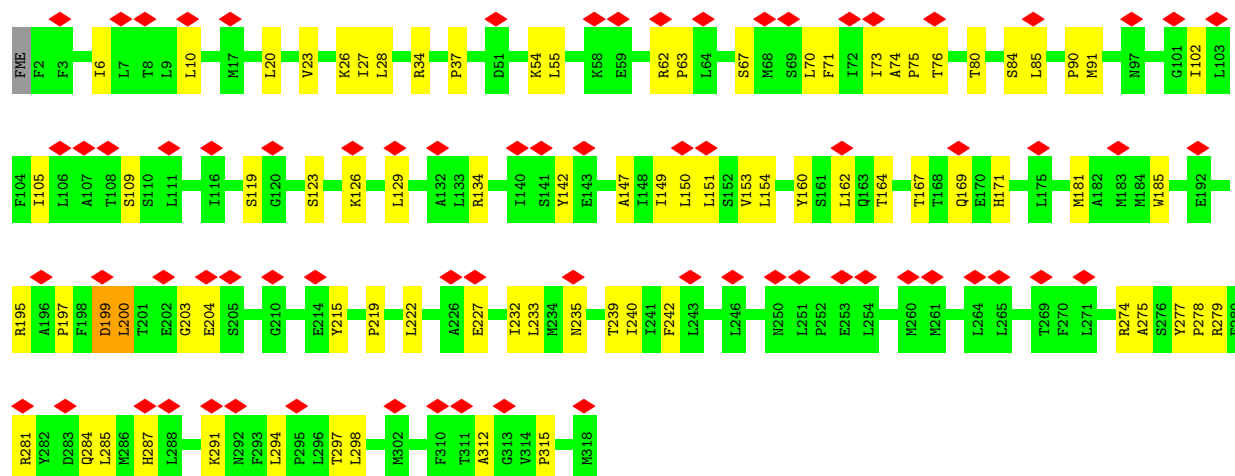
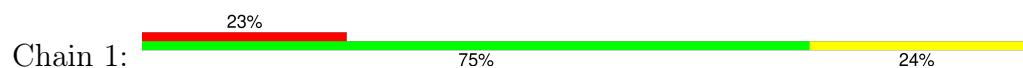


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

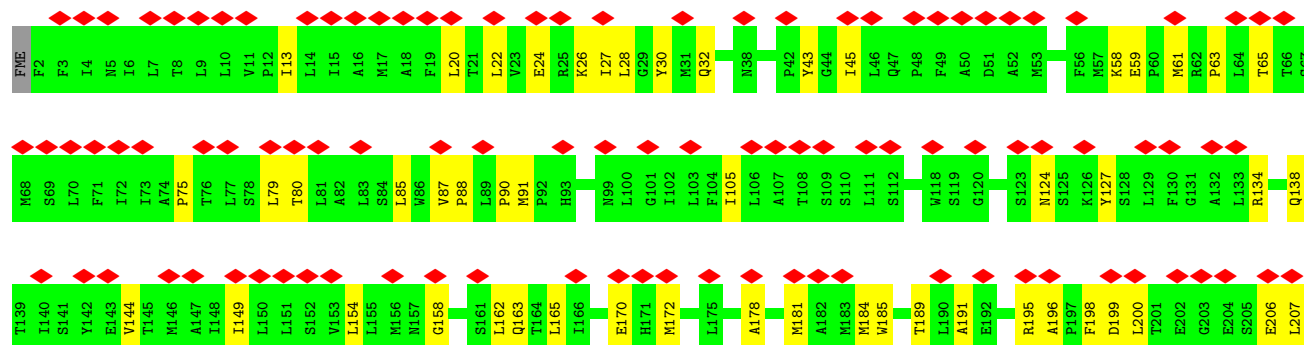
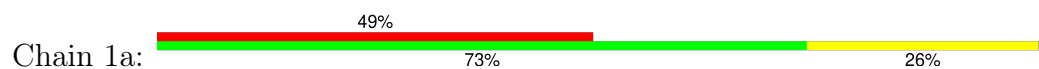


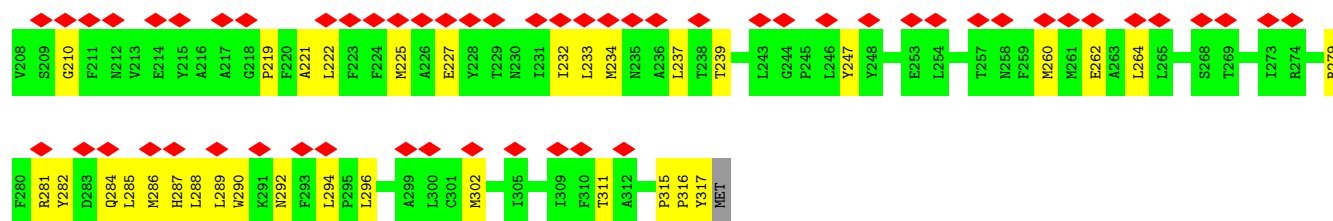


• Molecule 4: NADH-ubiquinone oxidoreductase chain 1

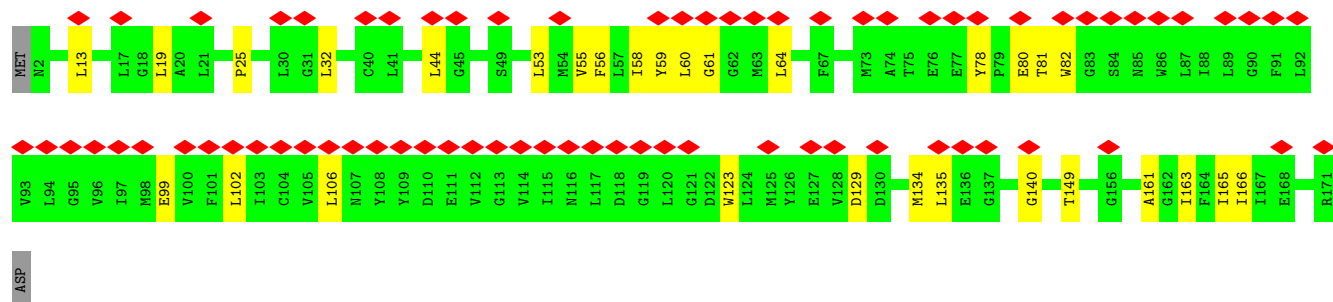
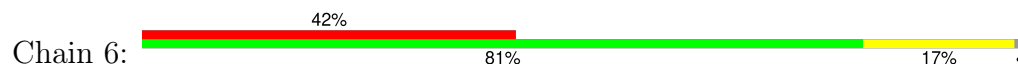


• Molecule 4: NADH-ubiquinone oxidoreductase chain 1

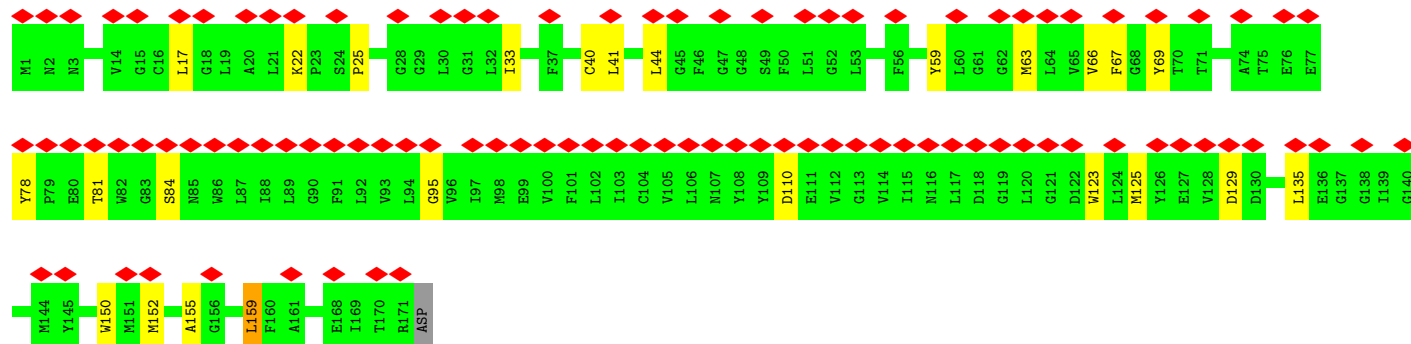
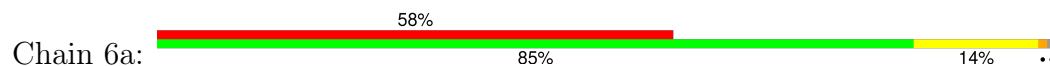




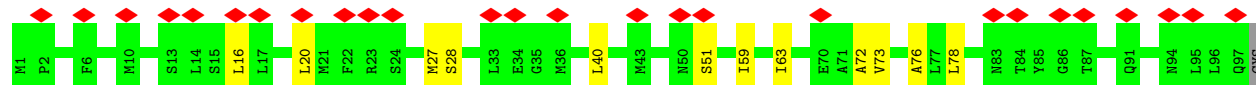
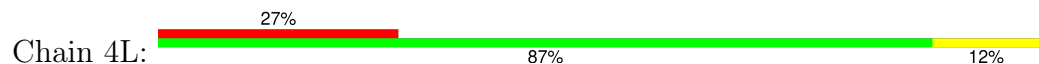
• Molecule 5: NADH-ubiquinone oxidoreductase chain 6



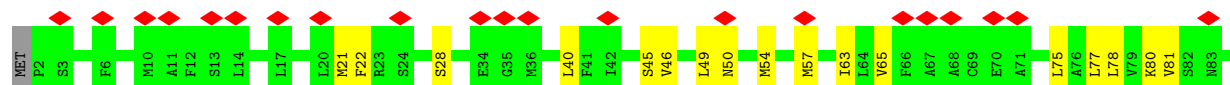
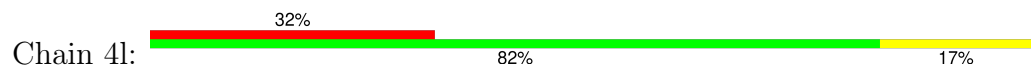
• Molecule 5: NADH-ubiquinone oxidoreductase chain 6

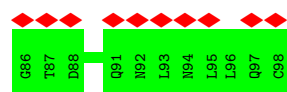


• Molecule 6: NADH-ubiquinone oxidoreductase chain 4L

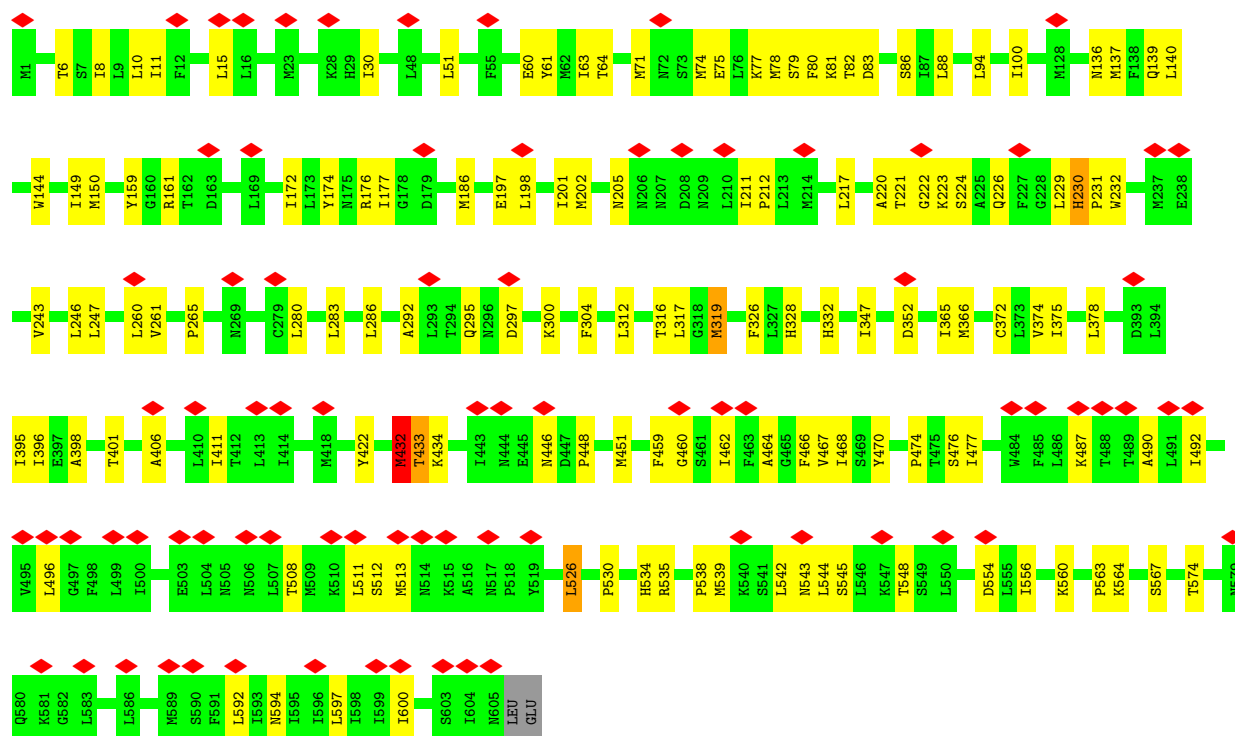
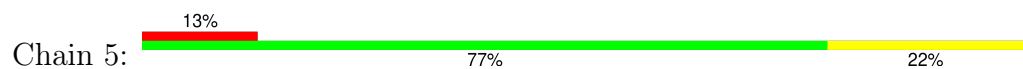


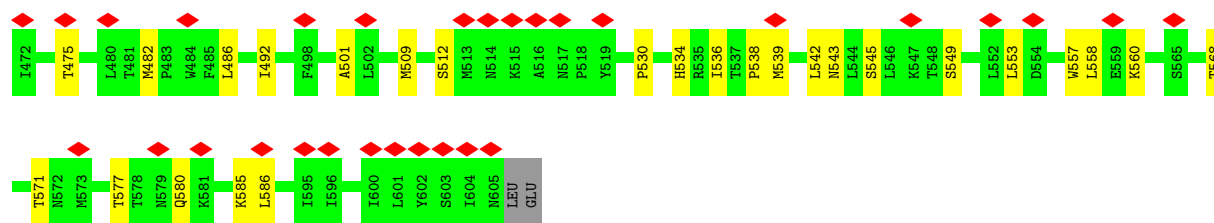
• Molecule 6: NADH-ubiquinone oxidoreductase chain 4L



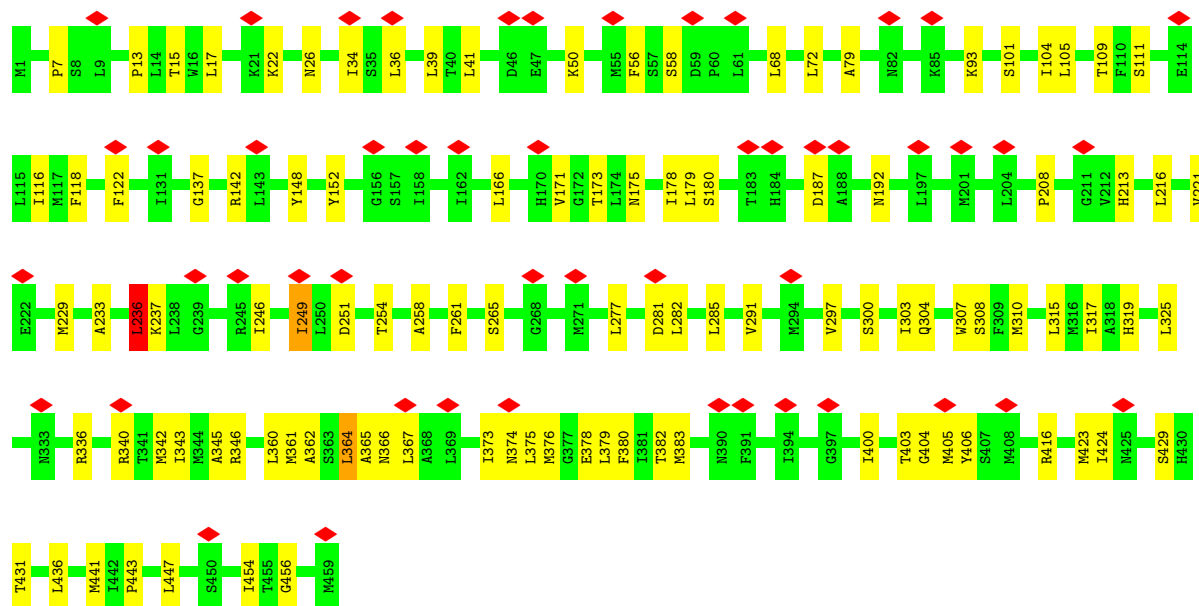
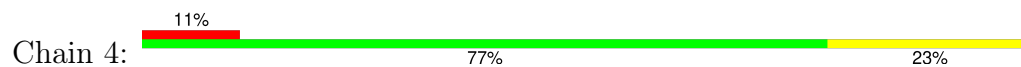


• Molecule 7: NADH-ubiquinone oxidoreductase chain 5

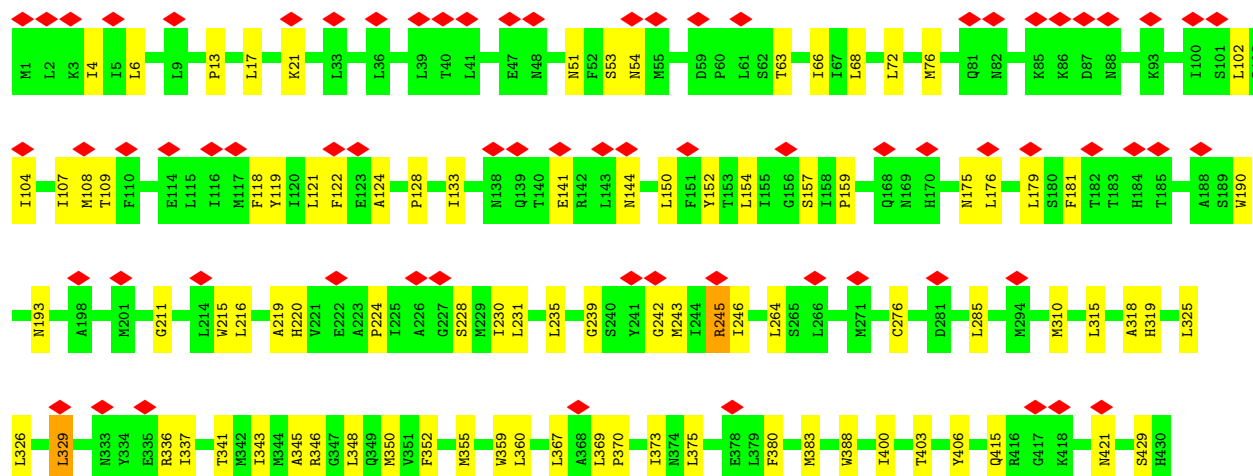
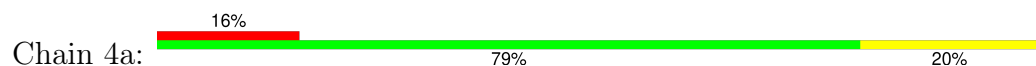


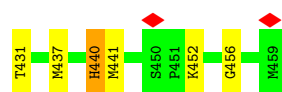


• Molecule 8: NADH-ubiquinone oxidoreductase chain 4

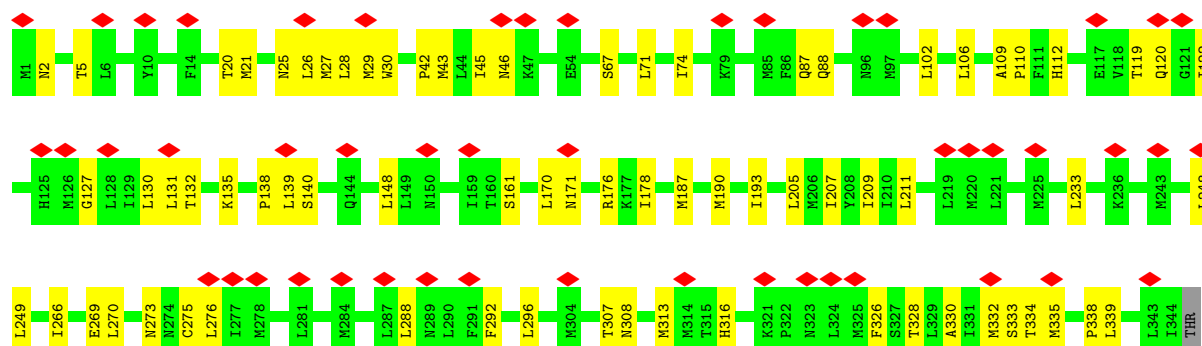
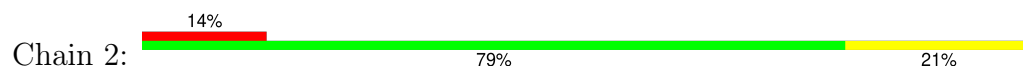


• Molecule 8: NADH-ubiquinone oxidoreductase chain 4

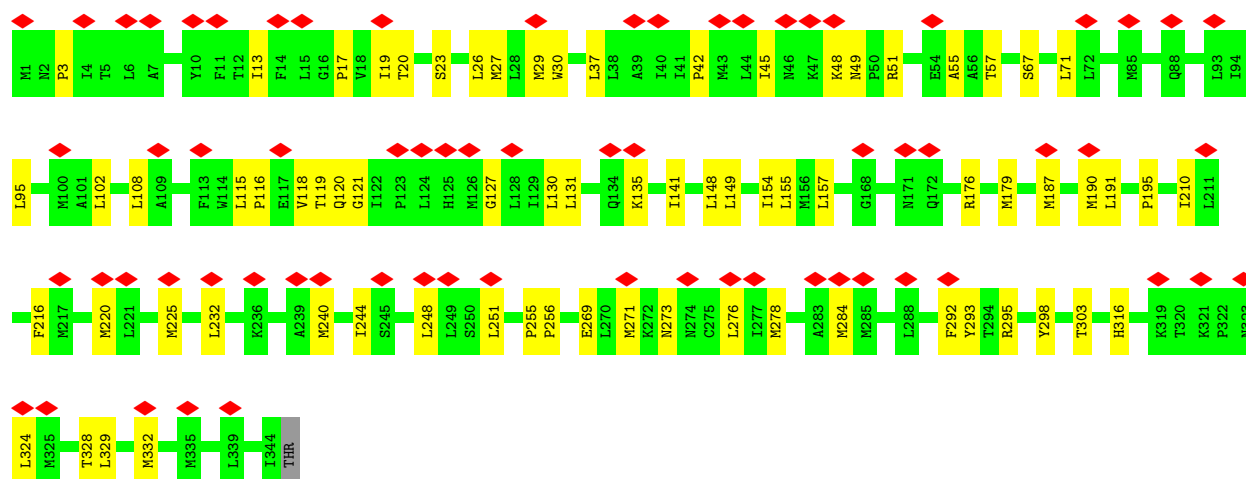
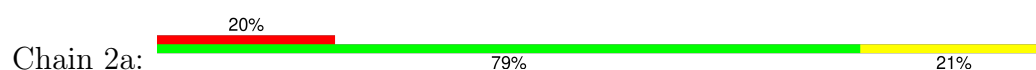




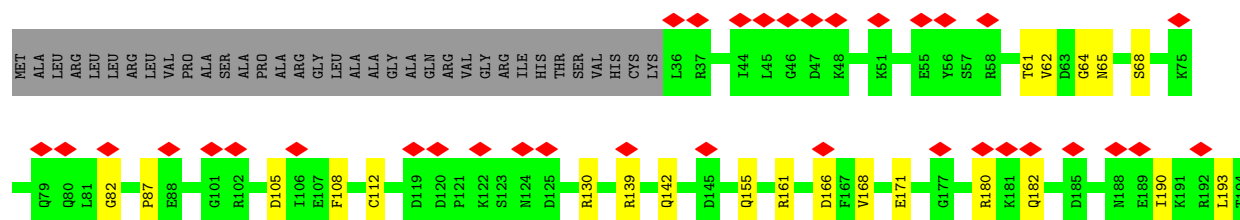
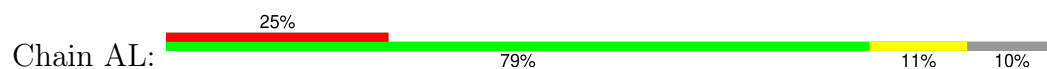
• Molecule 9: NADH-ubiquinone oxidoreductase chain 2

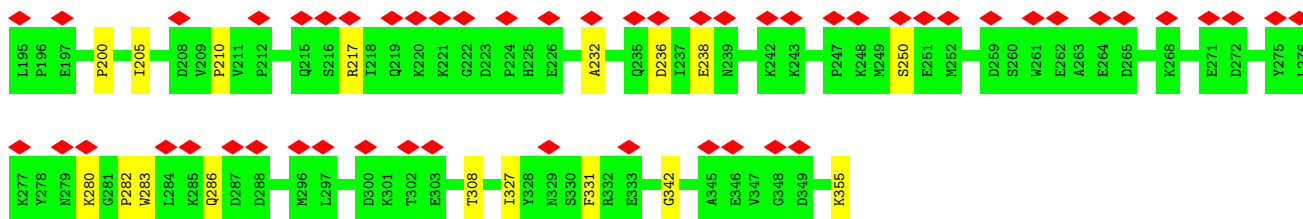


• Molecule 9: NADH-ubiquinone oxidoreductase chain 2

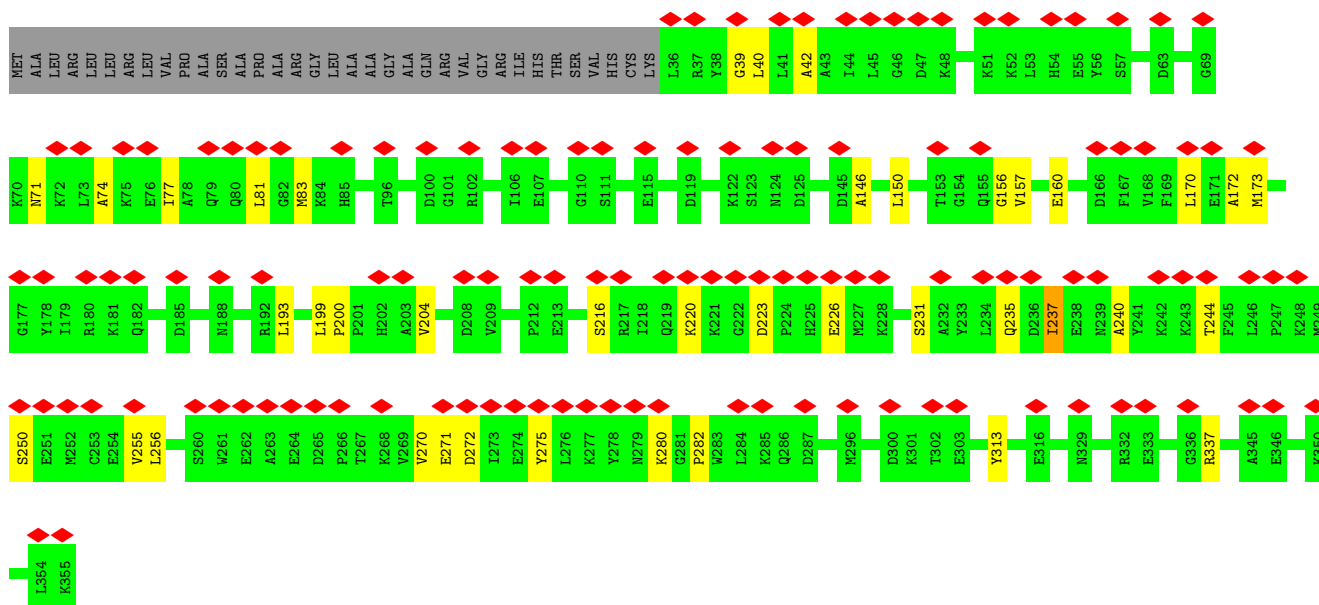
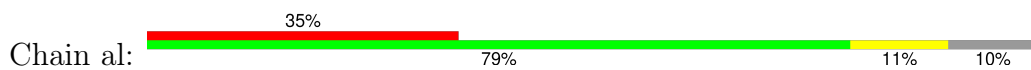


• Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

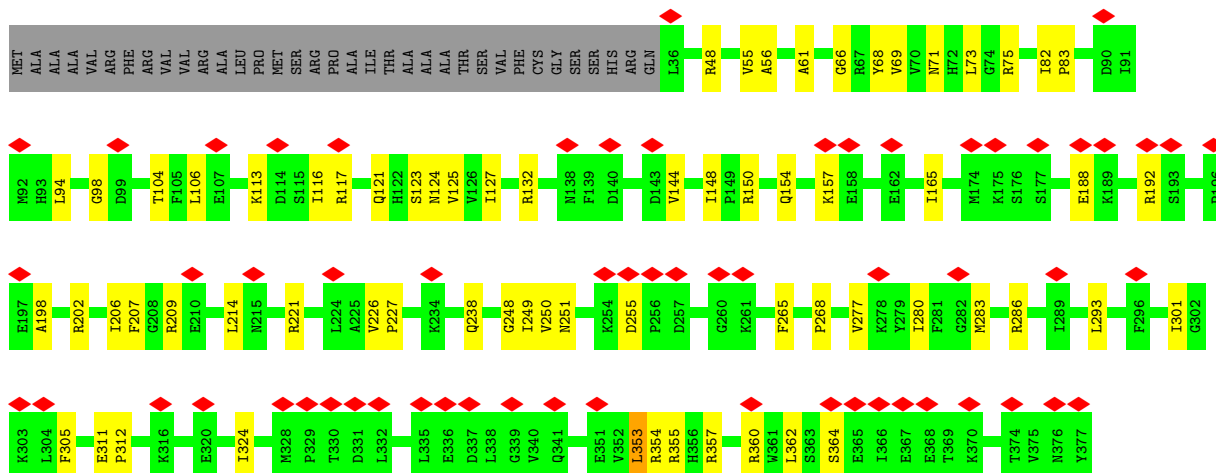
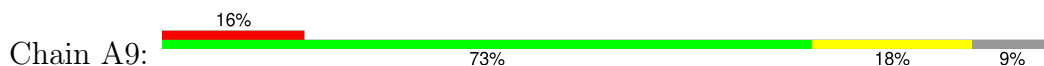




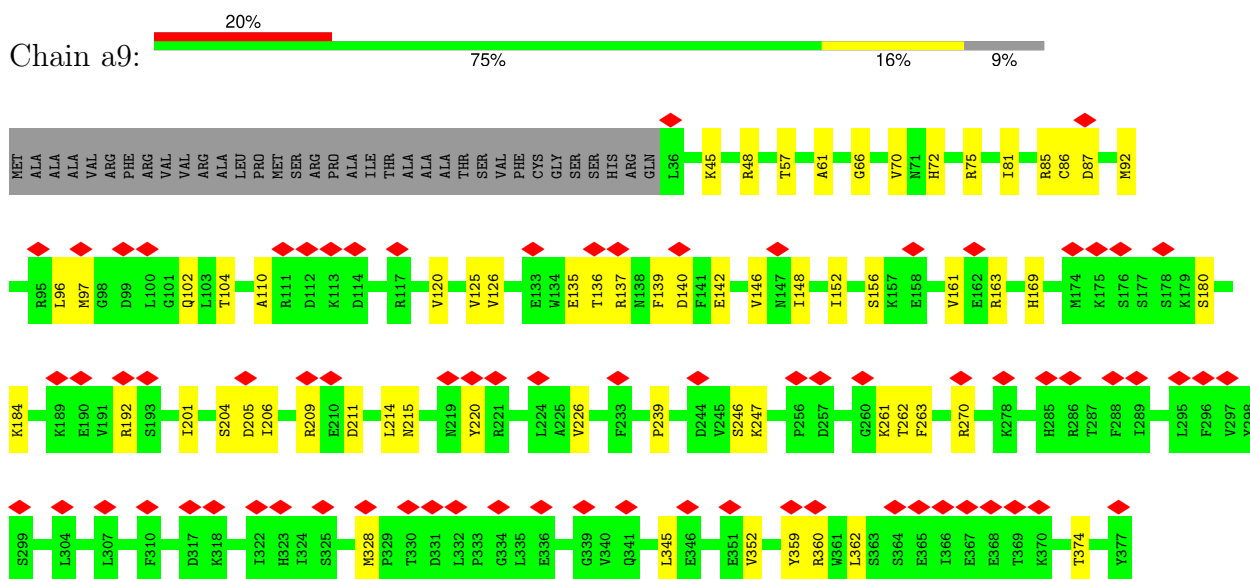
- Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



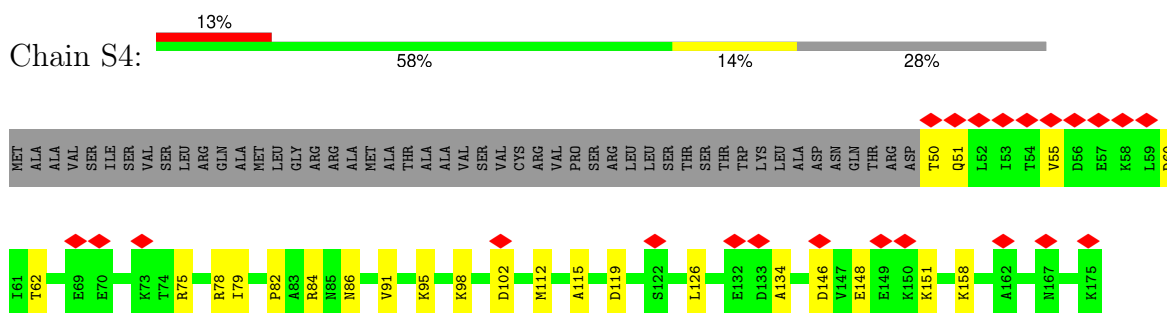
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



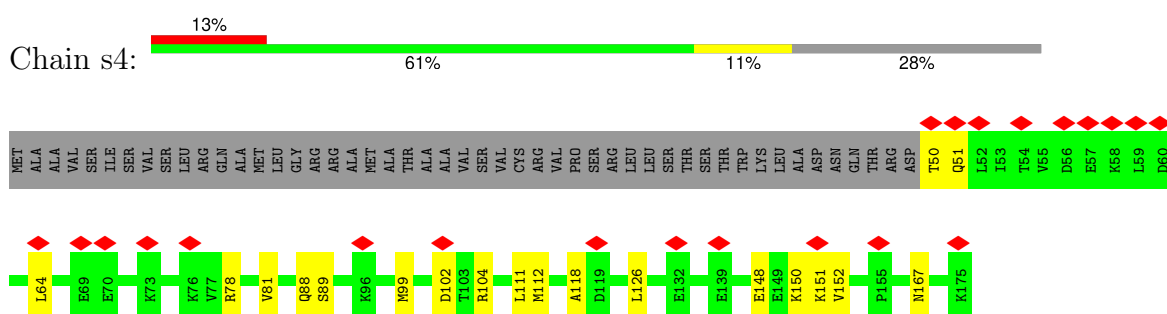
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



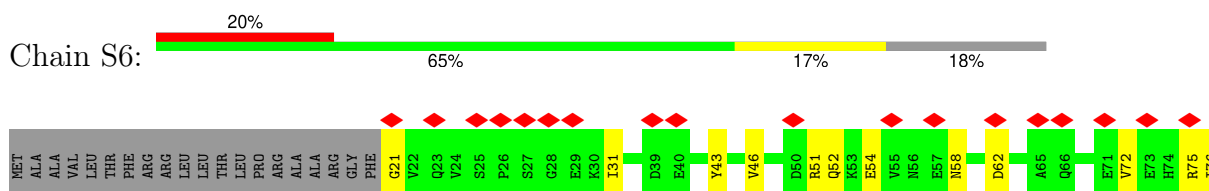
- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

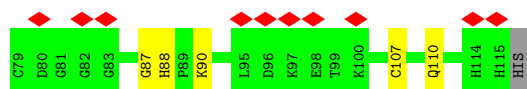
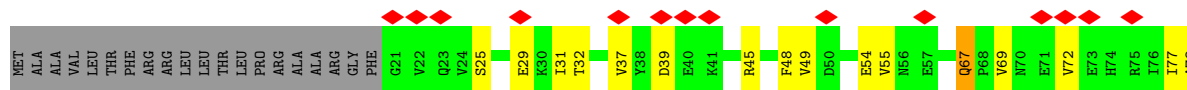


- Molecule 13: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

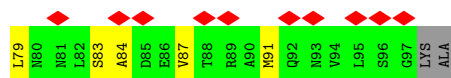
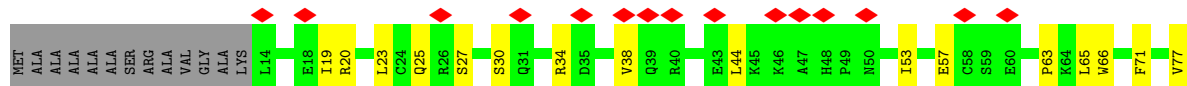




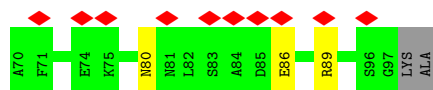
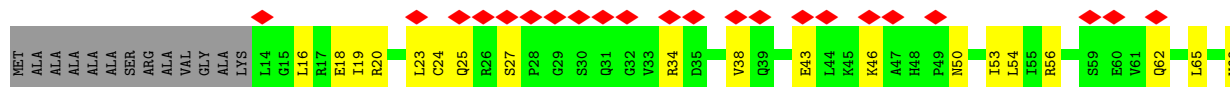
- Molecule 13: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



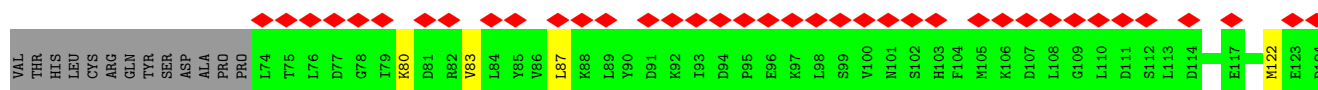
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



- Molecule 15: Acyl carrier protein, mitochondrial



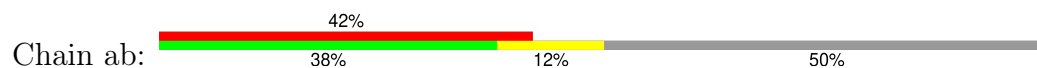
- Molecule 15: Acyl carrier protein, mitochondrial



MET ALA SER ARG VAL LEU CYS ALA CYS VAL ARG ARG LEU PRO ALA ALA PHE ALA PRO LEU PRO PRO LEU THR LEU ALA LEU ARG ALA PRO LEU SER THR THR LEU CYS PRO GLU GLY ILE ARG ARG PRO GLY ALA LEU GLN SER ALA LEU LEU ALA GLN VAL PRO GLY THR

VAL THR HIS LEU CYS ARG GLN TYR S69 D70 A71 F72 L76 D77 D81 Y85 L89 D94 P95 E96 M105 K106 Q115 V116 E117 M120 E123 D124 E125 D132 A135 E136 K137 L138 P141 Q142 E143 I144 V145 D146 D150 D153 V154 Y155 E156

- Molecule 15: Acyl carrier protein, mitochondrial



MET ALA SER ARG VAL LEU CYS ALA CYS VAL ASP ARG LEU PRO ALA ALA PHE ALA PRO LEU PRO PRO LEU THR THR LEU ALA ALA ARG PRO LEU SER THR THR LEU CYS PRO GLU GLY ILE ARG ARG PRO GLY ALA LEU GLN SER ALA LEU LEU ALA GLN VAL PRO GLY THR

VAL THR HIS LEU CYS ARG GLN TYR L74 T75 L76 D77 G78 I79 K80 D81 R82 V83 L84 Y85 V86 K87 L88 L89 Y90 D91 K92 I93 D94 P95 E96 K97 S99 V100 M101 S102 H103 F104 M105 K106 D107 L108 G109 L110 D111 S112 L113 D114 Q115 V116 E117 I118 I119 M120

A121 M122 E123 D124 E125 F126 G127 F128 E129 I130 P131 D132 I133 D134 A135 E136 K137 L138 M139 C140 P141 Q142 E143 I144 V145 D146 Y147 I148 A149 D150 K151 LYS ASP VAL TYR GLU

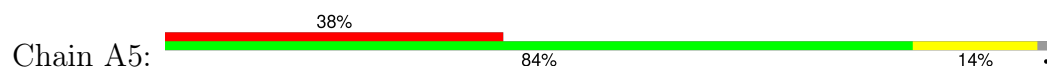
- Molecule 15: Acyl carrier protein, mitochondrial



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VAL THR HIS LEU CYS ARG GLN TYR S69 D70 A71 D77 D81 Y85 L89 Y90 D91 K92 D94 P95 E96 K97 M105 K106 D107 L108 S112 E117 E123 D124 E129 I130 P131 D132 I133 A135 E136 K137 L138 E143 D146 Y155 E156

- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

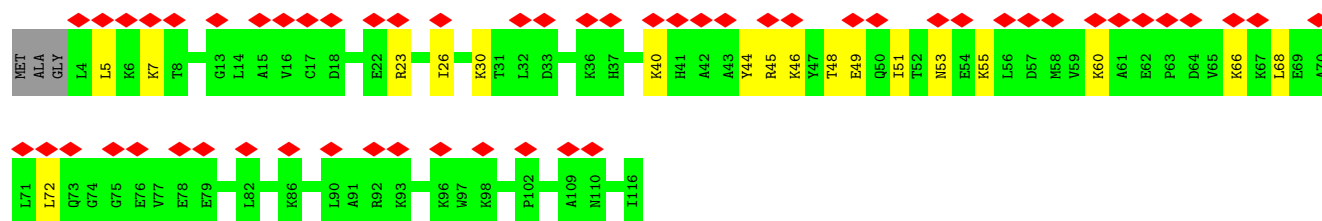


MET ALA G3 L4 L5 K6 K7 G10 G13 C17 D18 R23 L26 D33 K36 H37 F38 P39 K40 H41 A42 A43 Y44 R45 T48 E49 T52 N53 E54 K55 L56 D57 A61 E62 P63 P64 V65 K66 K67 L68 L71 L72 Q73 G74 G75 E78 L82

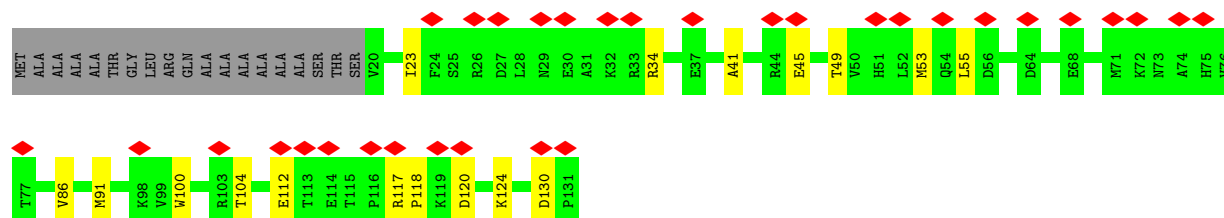
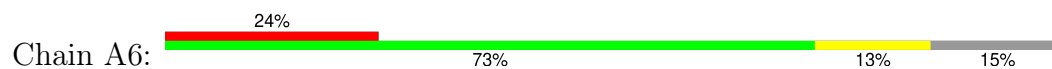
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- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

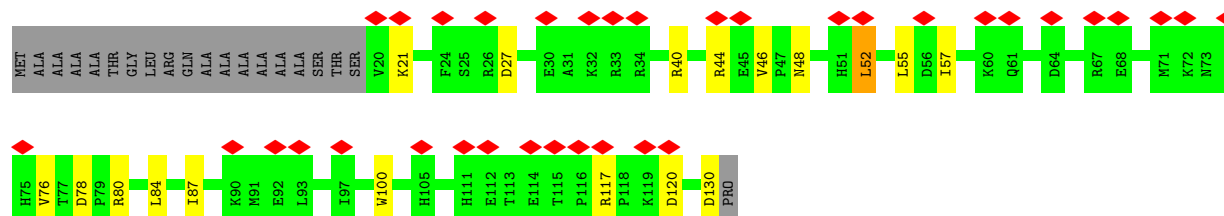
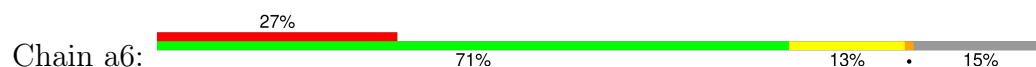




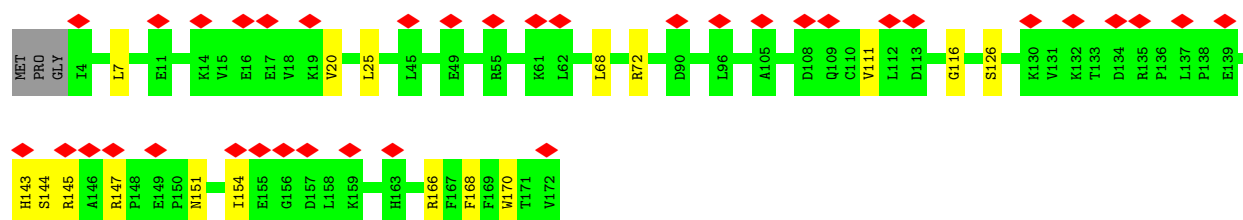
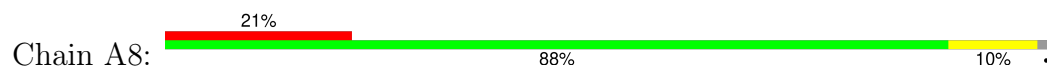
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



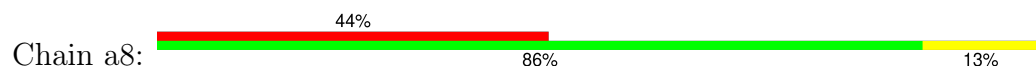
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

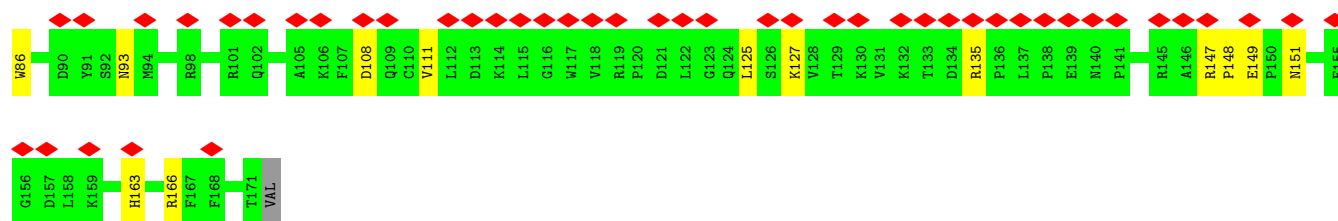


- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

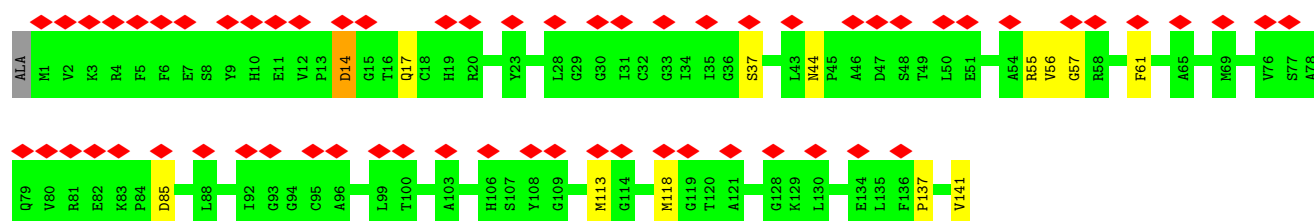
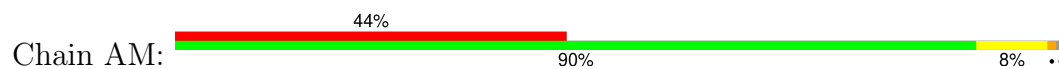


- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

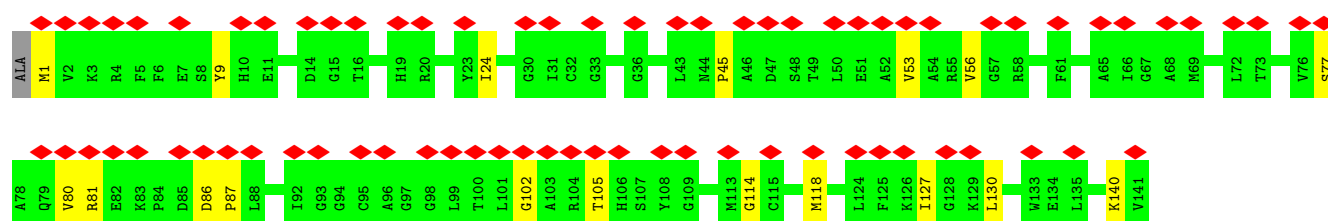
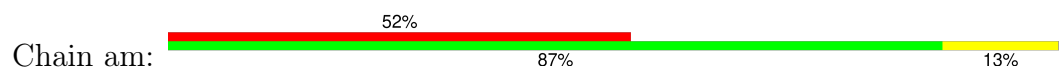




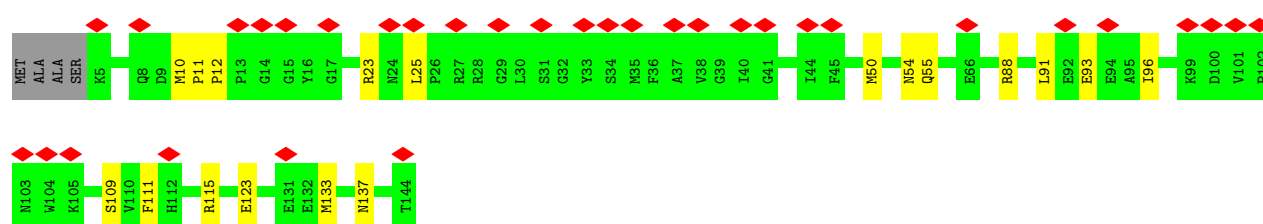
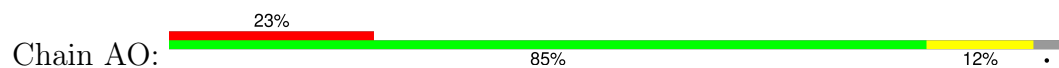
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



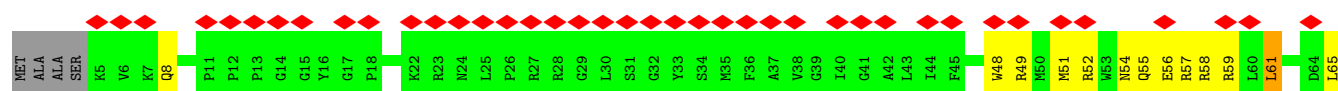
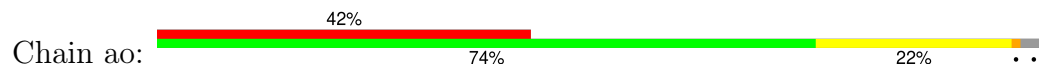
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

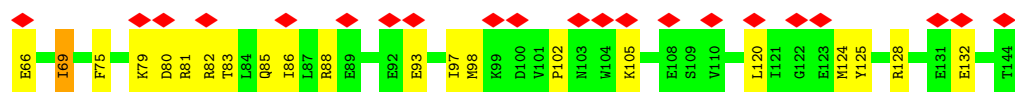


- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

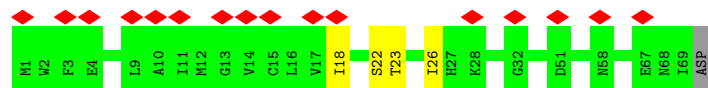


- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

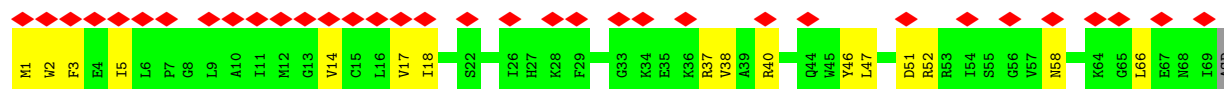
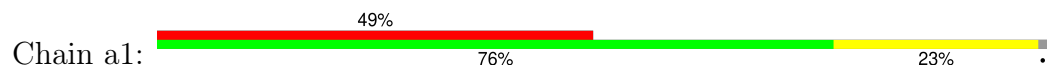




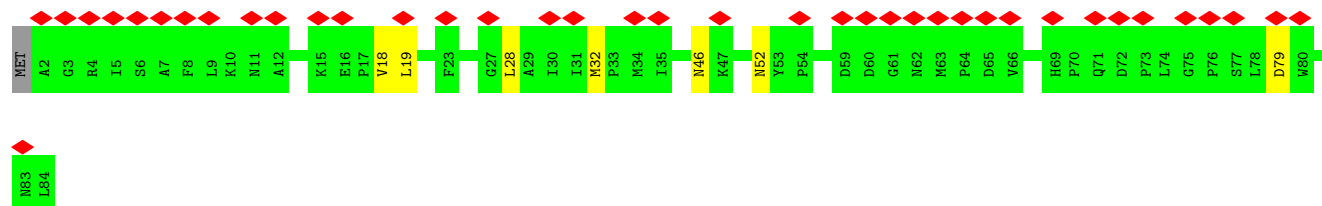
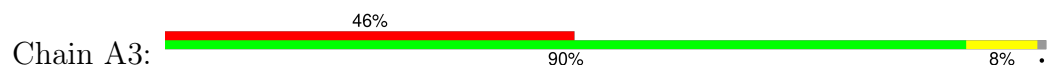
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



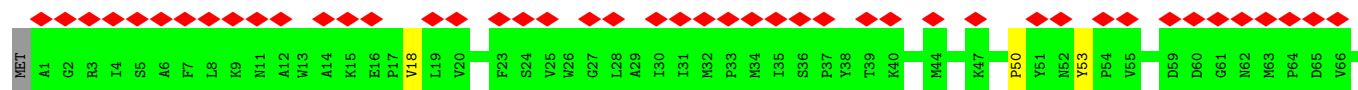
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



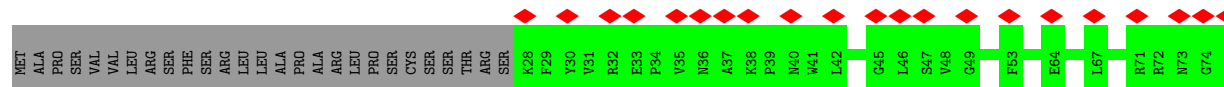
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

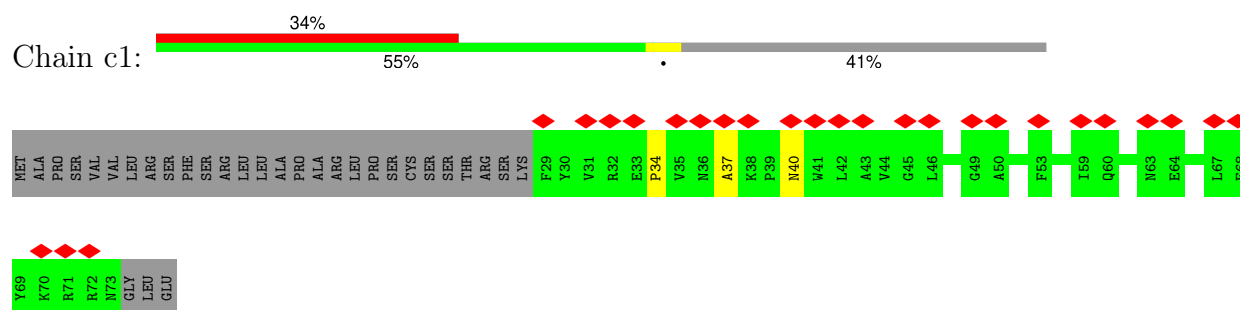


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

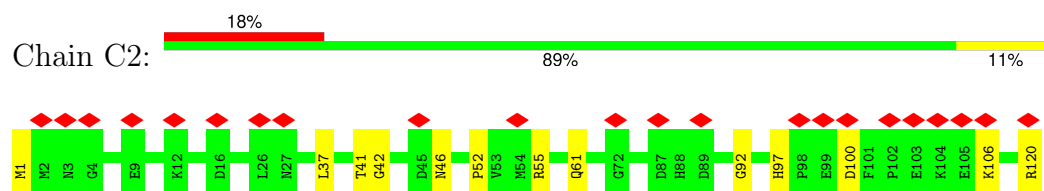




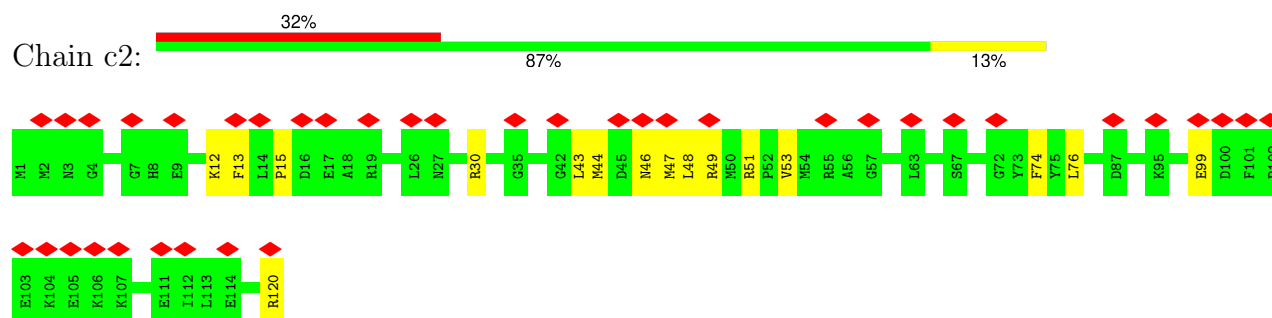
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



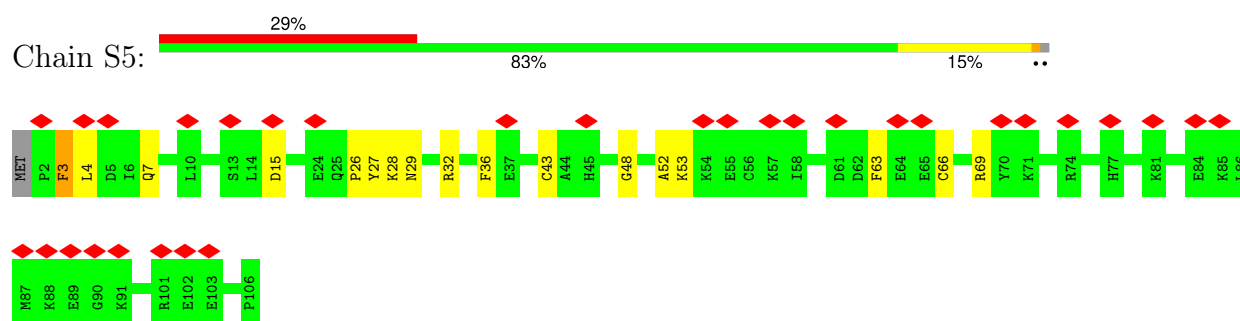
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 subunit C2



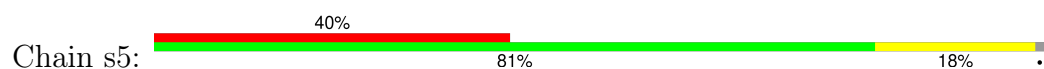
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 subunit C2

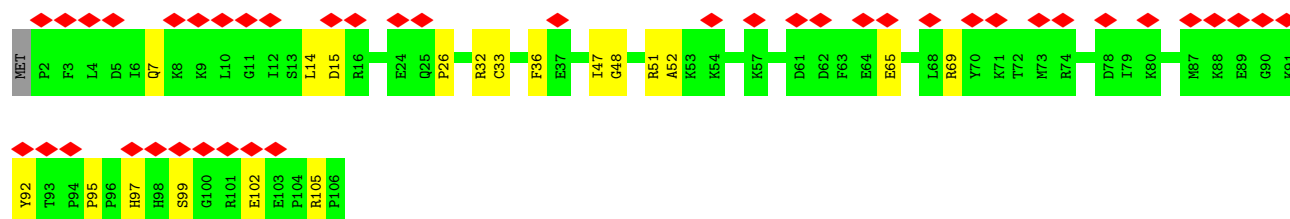


- Molecule 25: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

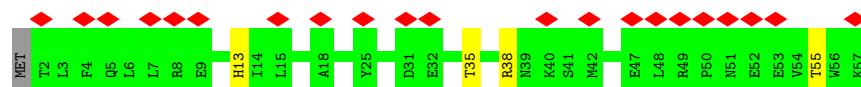
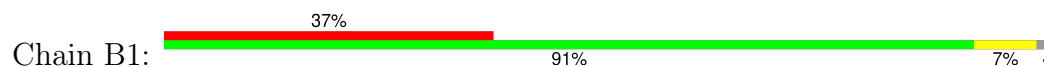


- Molecule 25: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

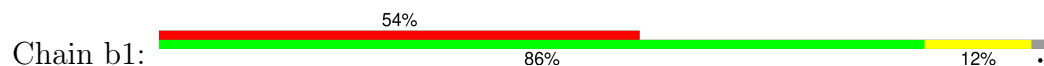




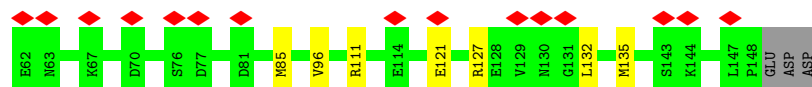
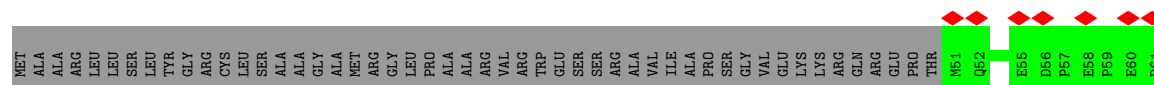
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



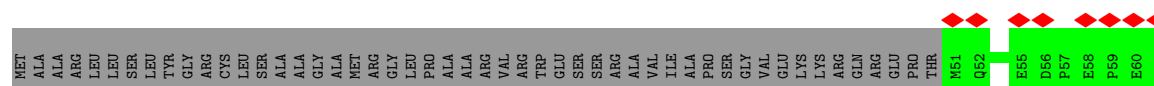
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



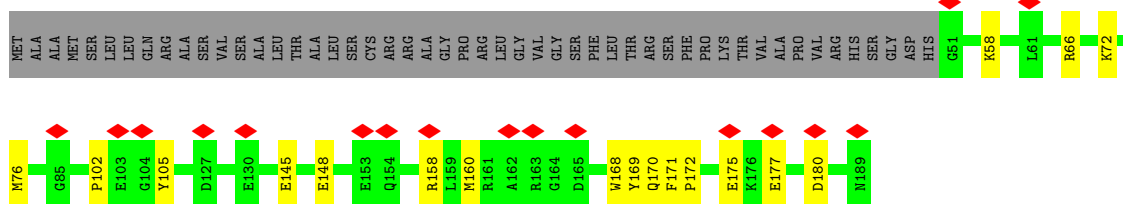
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



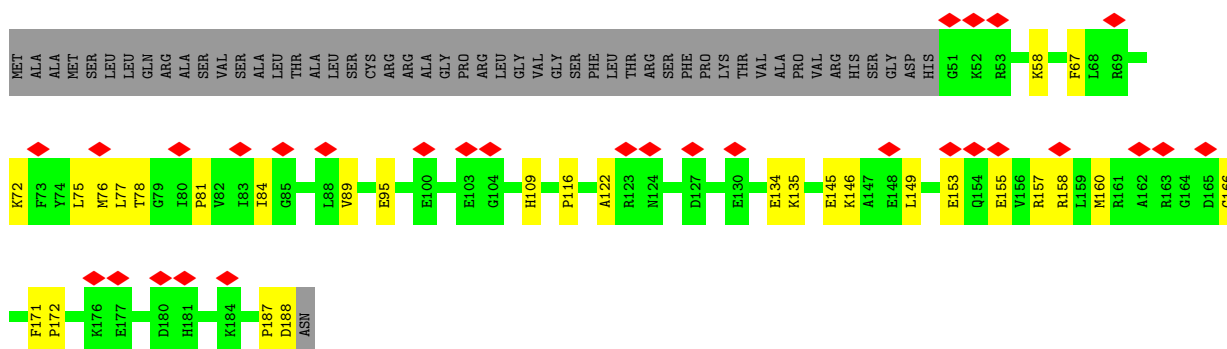
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



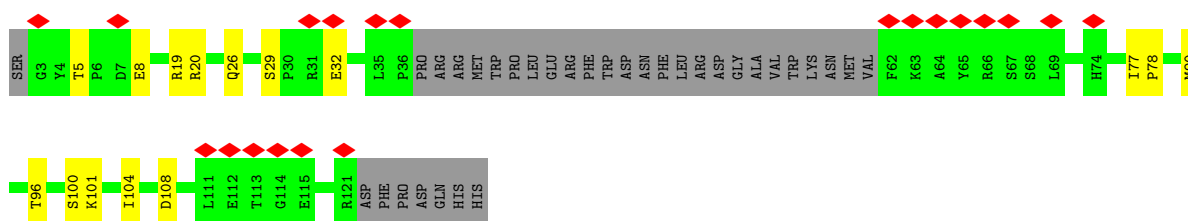
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



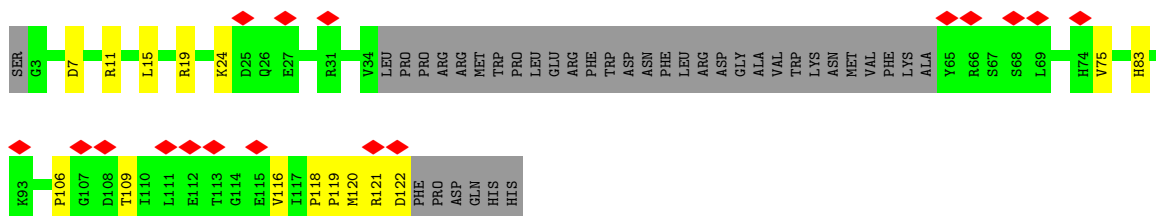
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



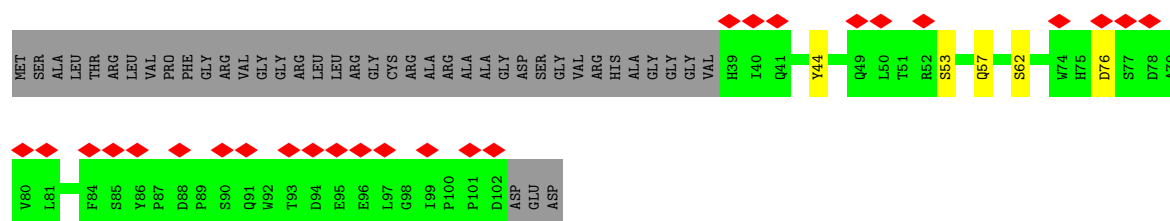
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



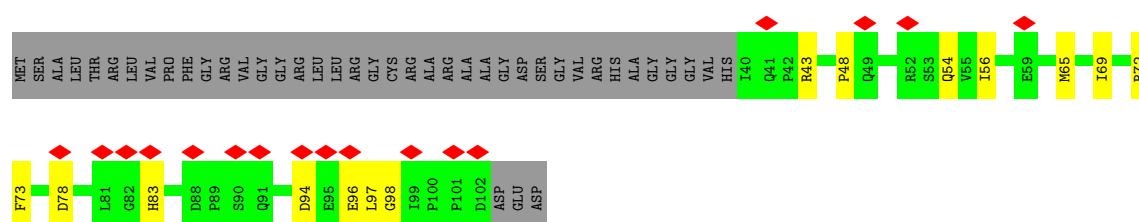
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



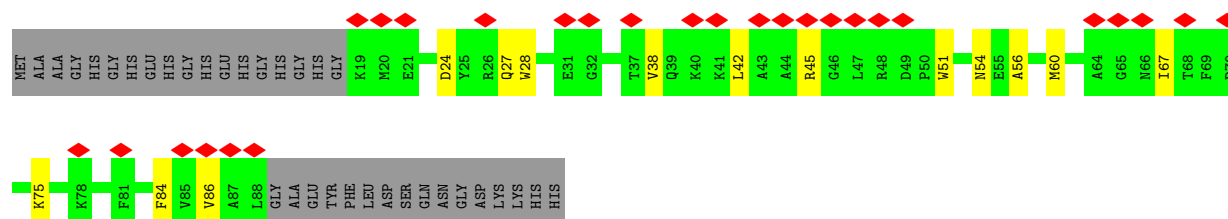
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



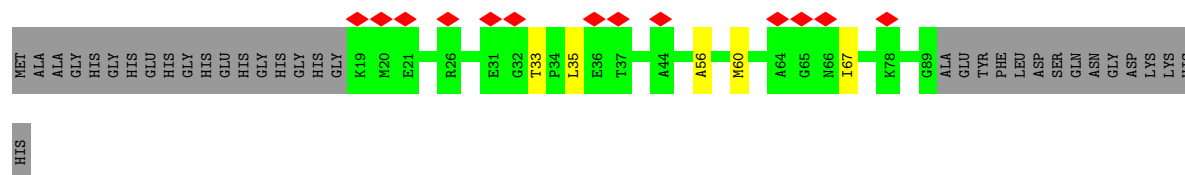
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



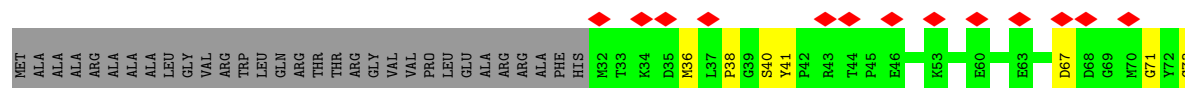
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

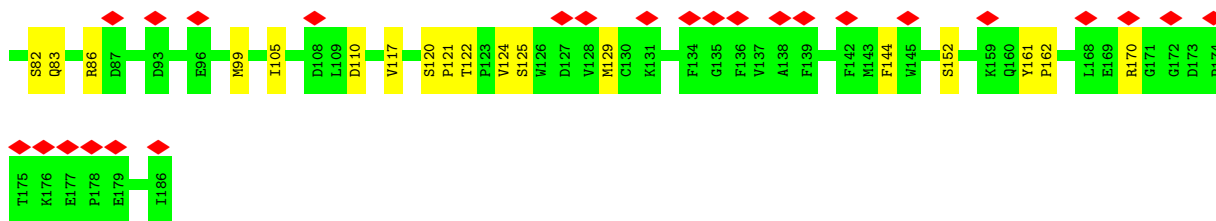


- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

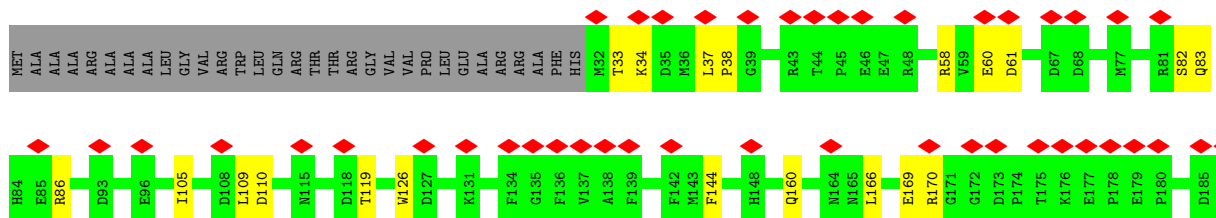
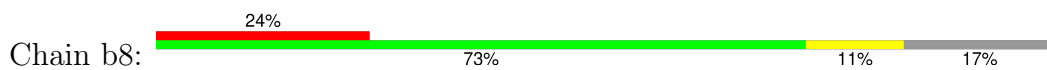


- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

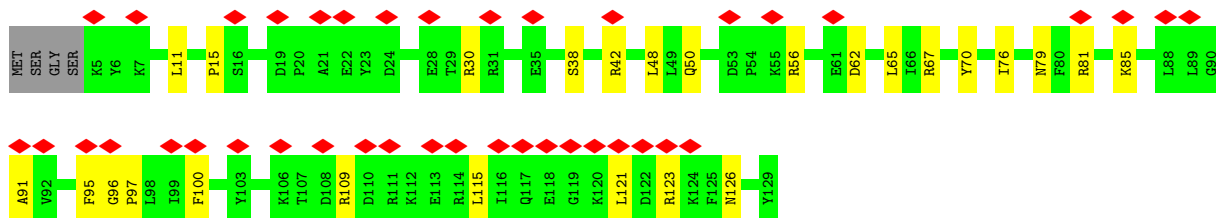
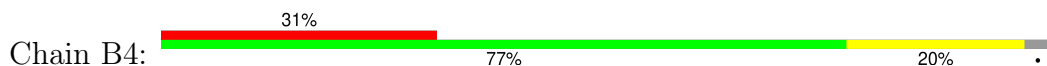




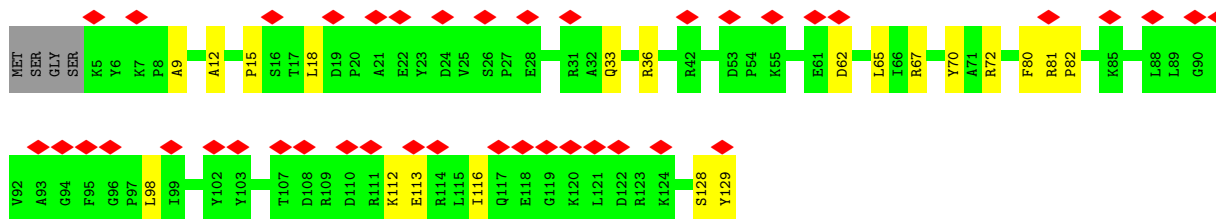
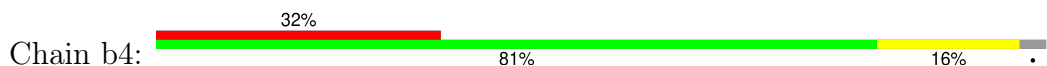
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



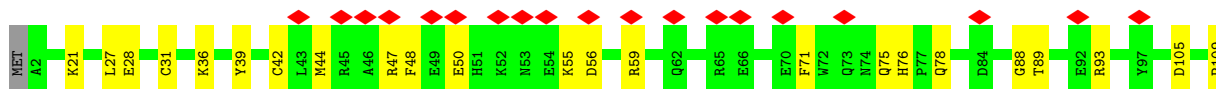
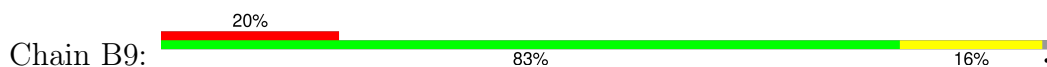
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

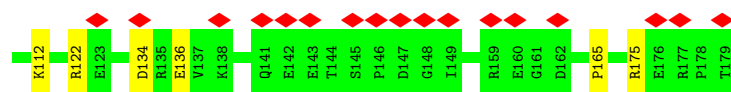


- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

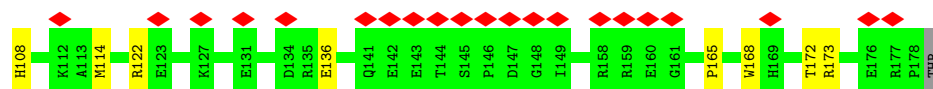
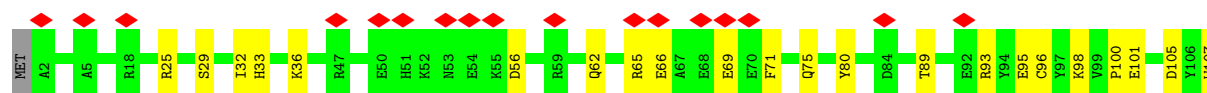
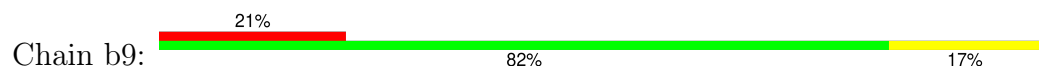


- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

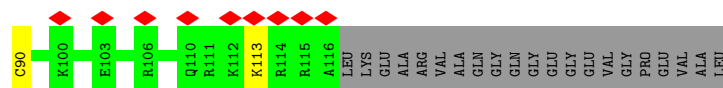
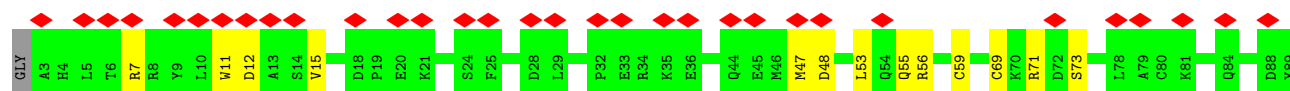
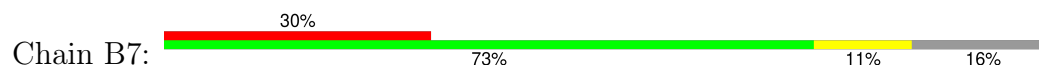




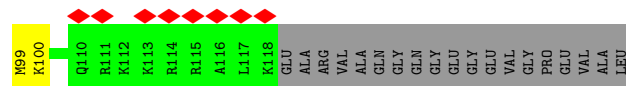
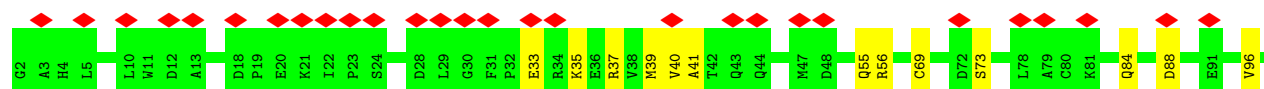
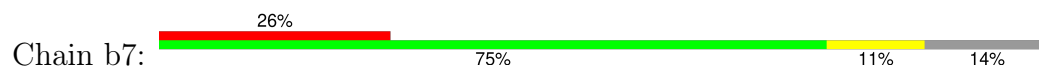
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



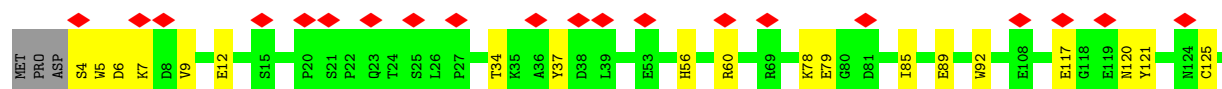
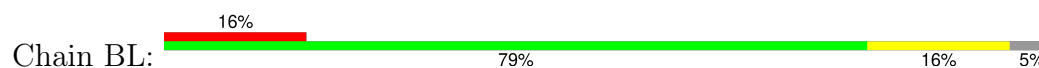
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



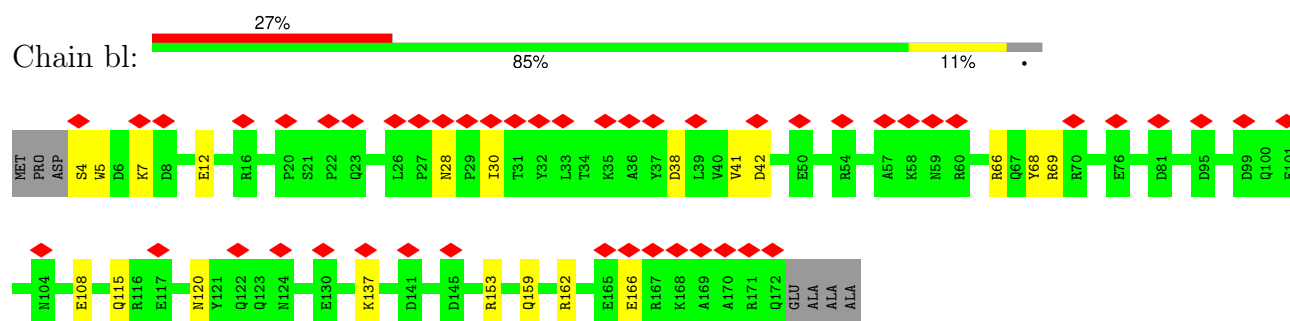
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



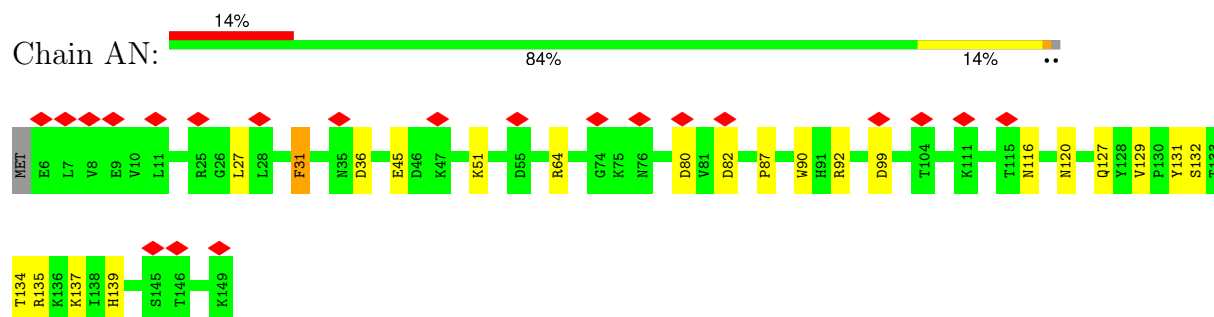
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



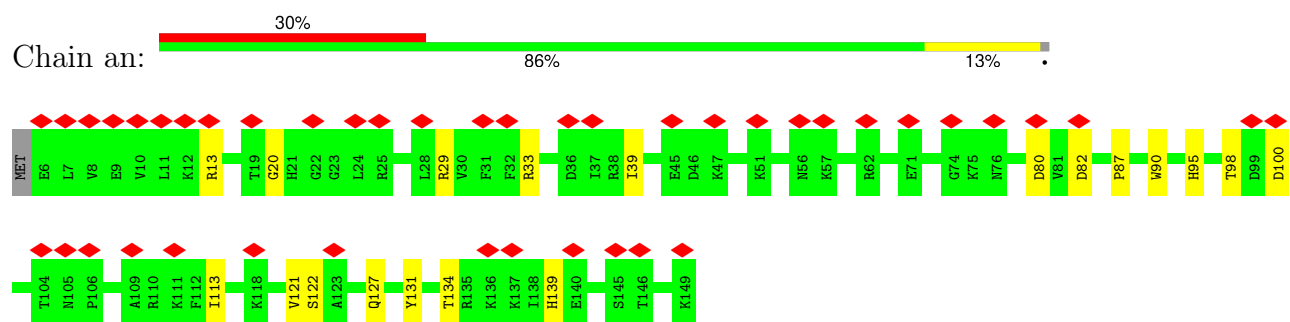
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



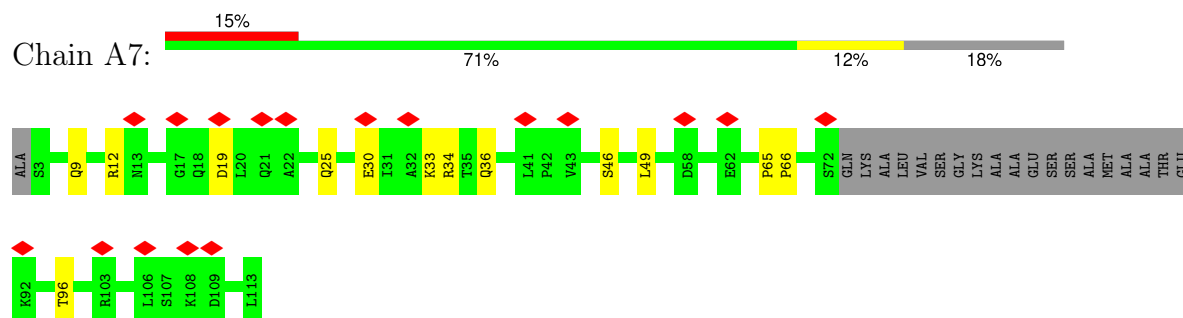
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



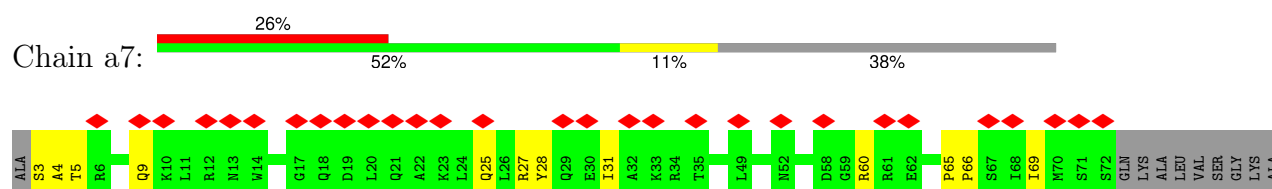
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



ALA  
GLU  
SER  
SER  
ALA  
MET  
ALA  
ALA  
THR  
GLY  
GLY  
LYS  
LYS  
VAL  
THR  
PRO  
ALA  
VAL  
PRO  
PRO  
MET  
LYS  
ARG  
THR  
GLU  
LEU  
SER  
LYS  
GLN  
PRO  
TYR  
LEU

- Molecule 39: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



MET  
ALA  
VAL  
SER  
SER  
LEU  
LEU  
LEU  
ARG  
GLY  
GLY  
ILE  
ARG  
ALA  
LEU  
LYS  
LYS  
VAL  
VAL  
LEU  
LEU  
GLU  
ALA  
ARG  
VAL  
PHE  
PRO  
GLY  
GLU  
LEU  
VAL  
SER  
VAL  
VAL  
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LEU  
SER  
THR  
GLU  
SER  
LYS  
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ALA  
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GLU  
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LEU  
LEU  
HIS  
PRO  
LYS  
THR  
GLN  
SER  
SER  
VAL  
VAL  
LYS  
GLU  
PRO  
GLU

PRO  
THR  
ASP  
THR  
T65  
T66  
L70  
L71  
H72  
H73  
L81  
L85  
D86  
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S88  
K89  
P90  
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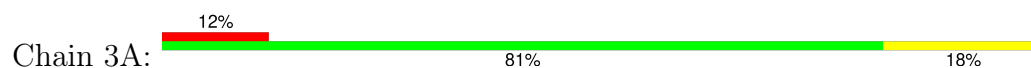
- Molecule 39: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



MET  
ALA  
VAL  
SER  
SER  
LEU  
LEU  
LEU  
ARG  
GLY  
GLY  
ILE  
ARG  
ALA  
LEU  
LYS  
LYS  
VAL  
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LEU  
LEU  
GLU  
ALA  
ARG  
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PRO  
GLY  
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HIS  
PRO  
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THR  
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VAL  
VAL  
LYS  
GLU  
PRO  
GLU

PRO  
THR  
ASP  
THR  
THR  
THR  
K68  
N69  
L70  
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L81  
D82  
L83  
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- Molecule 40: Cytochrome b-c1 complex subunit 1, mitochondrial



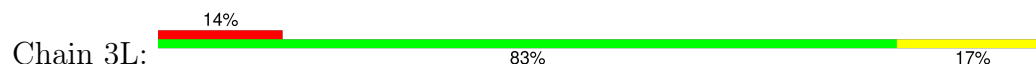
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G88  
F92  
L93  
E94  
A97  
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K99  
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V113  
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K138  
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V144  
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D158  
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R165  
D166  
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N175  
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R210  
L211  
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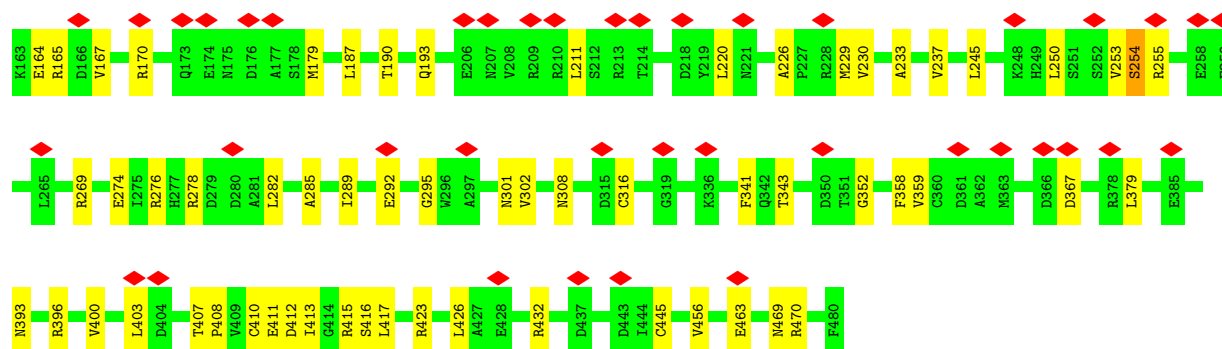
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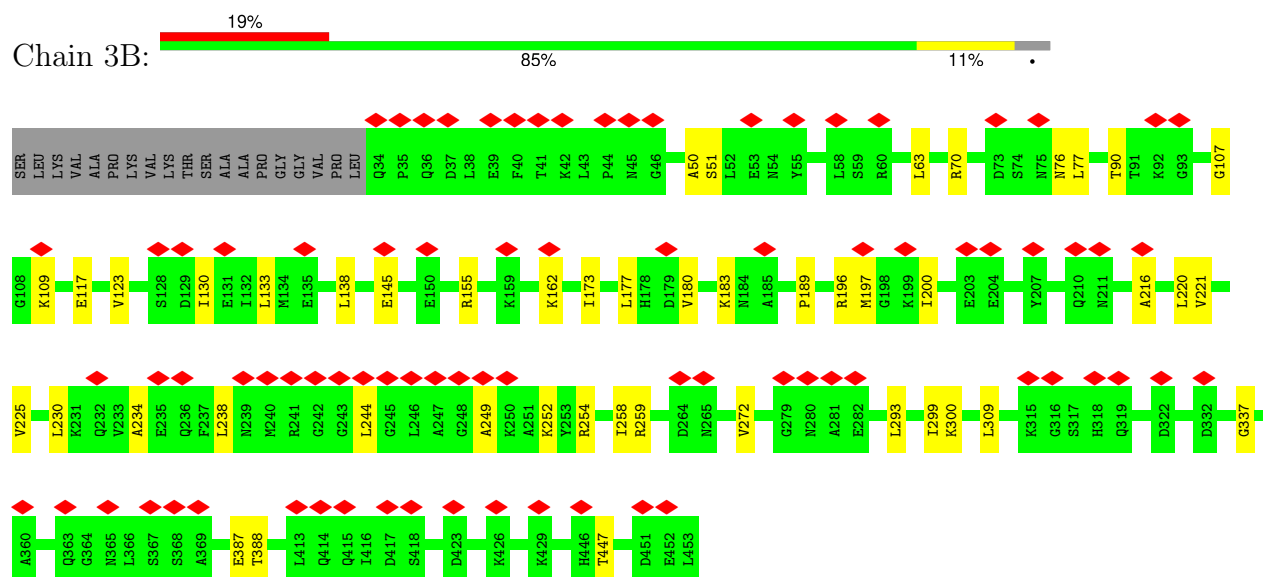
- Molecule 40: Cytochrome b-c1 complex subunit 1, mitochondrial



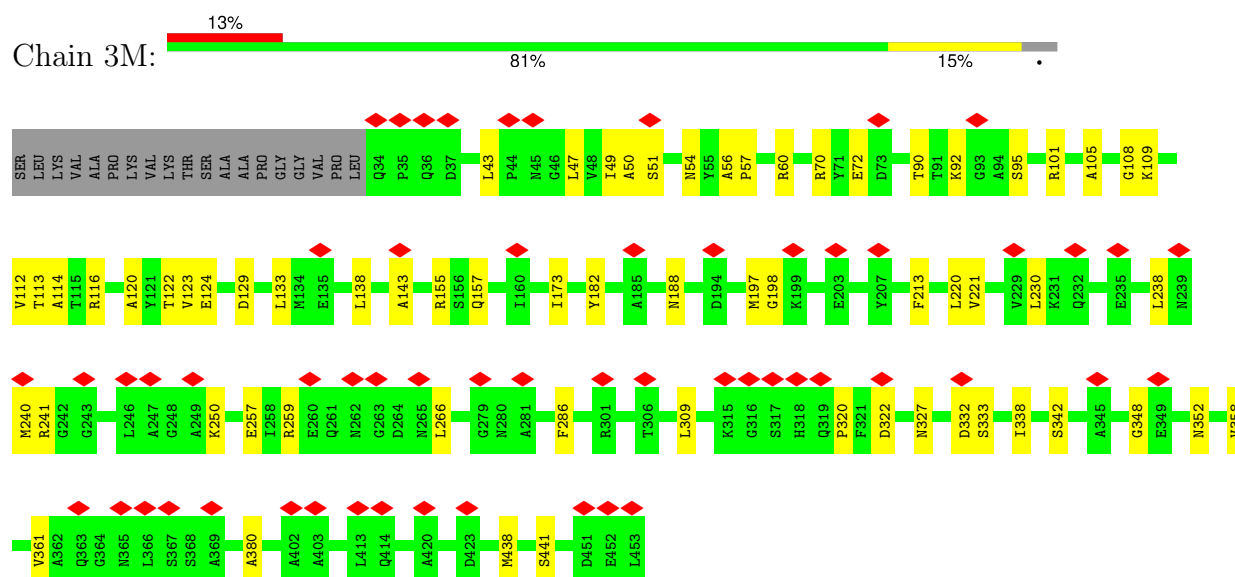
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A36  
T37  
F38  
A39  
Q40  
Q43  
S44  
E47  
T48  
D54  
N55  
R58  
E62  
S65  
T70  
D76  
T83  
E84  
K85  
L93  
E94  
K102  
M103  
M107  
E110  
E114  
A118  
I133  
K134  
A135  
L136  
S137  
K138  
D139  
L140  
P141  
K142  
V143  
D158  
S159  
E162



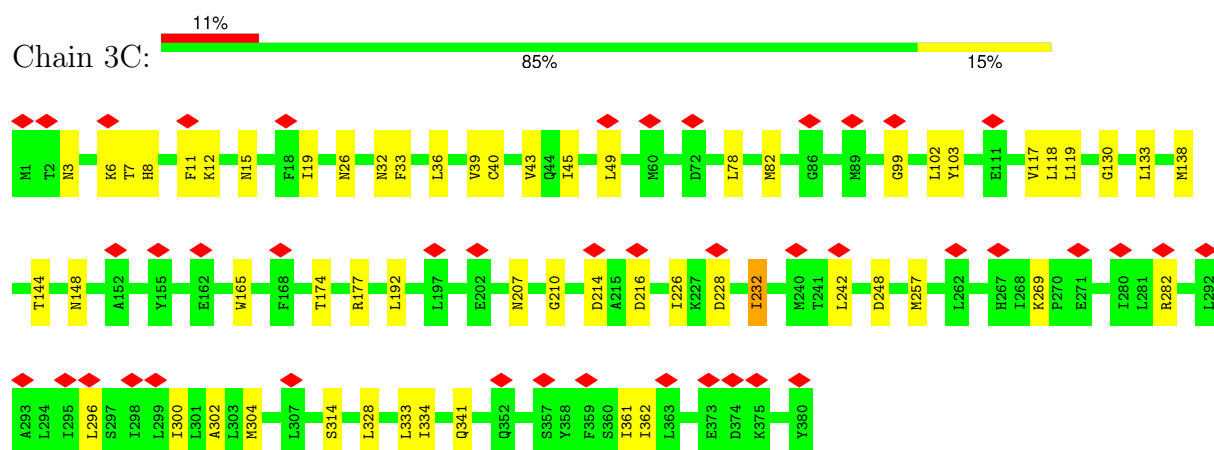
- Molecule 41: Cytochrome b-c1 complex subunit 2, mitochondrial



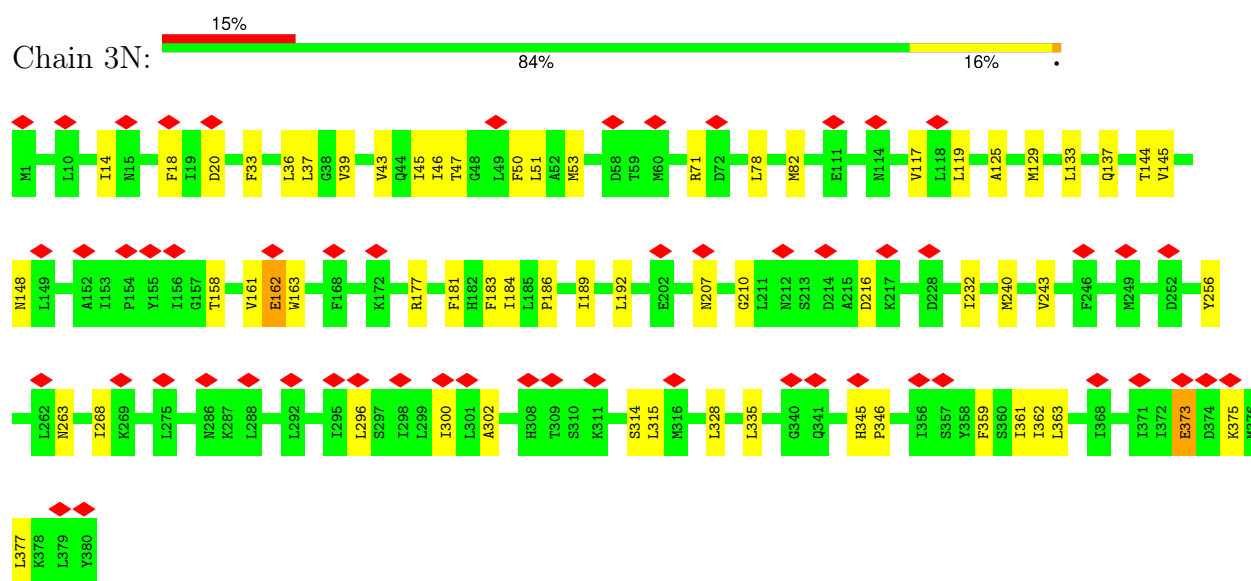
- Molecule 41: Cytochrome b-c1 complex subunit 2, mitochondrial



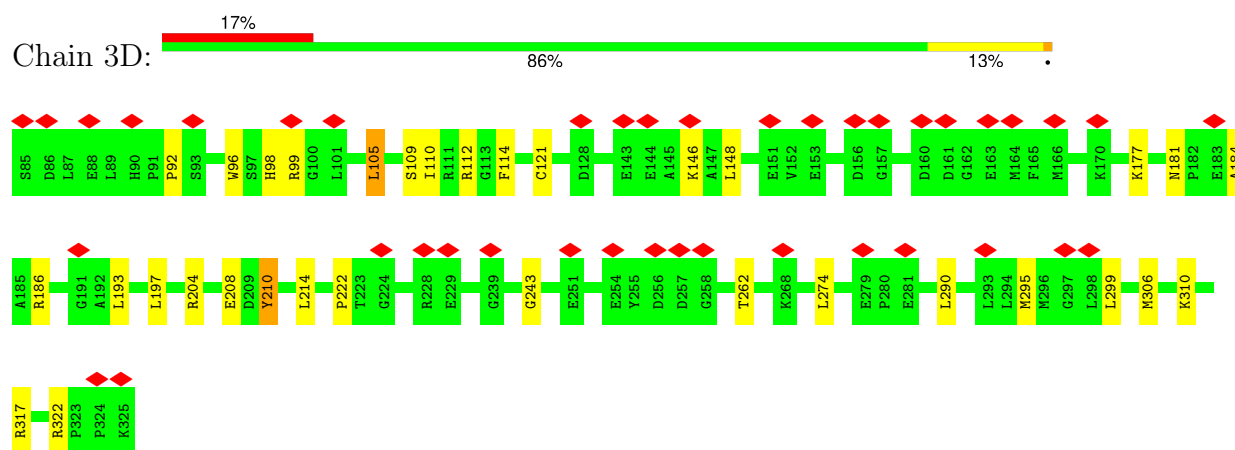
- Molecule 42: Cytochrome b



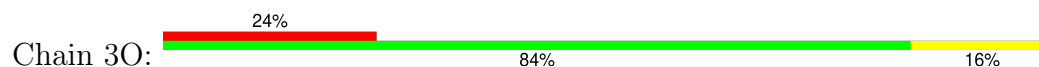
• Molecule 42: Cytochrome b

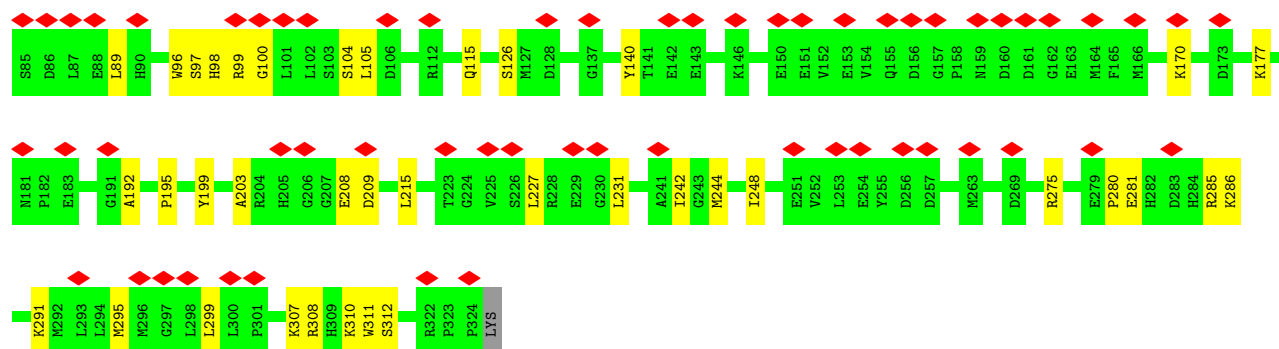


• Molecule 43: Cytochrome c1, heme protein, mitochondrial

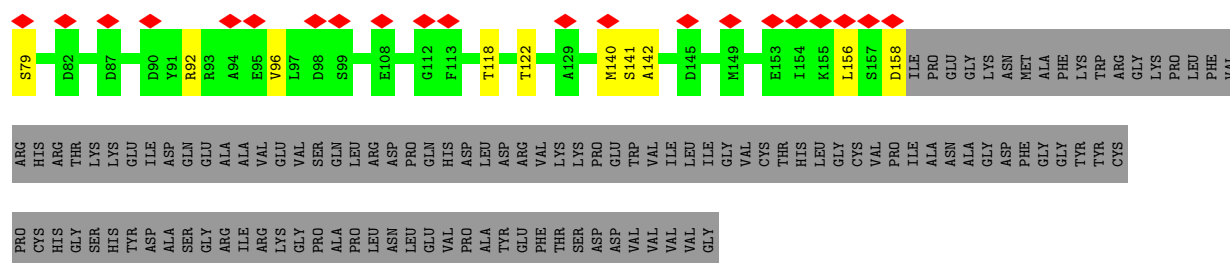
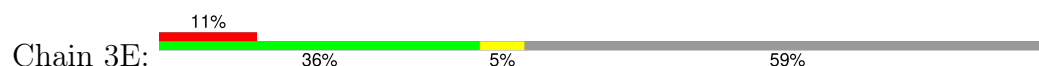


• Molecule 43: Cytochrome c1, heme protein, mitochondrial

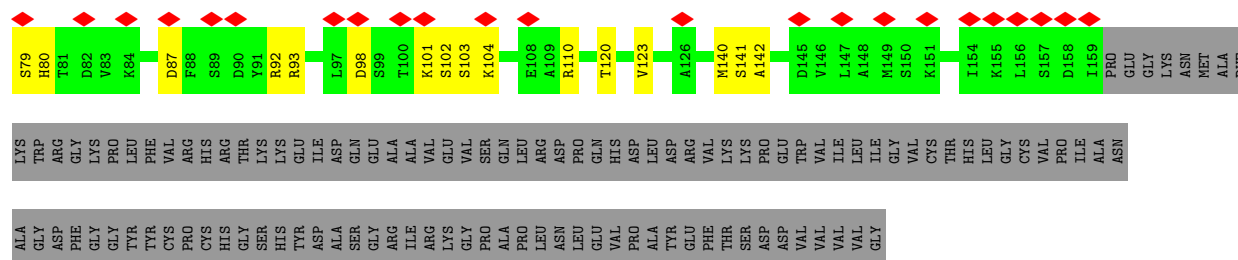
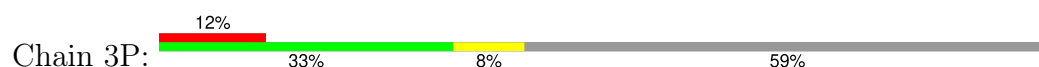




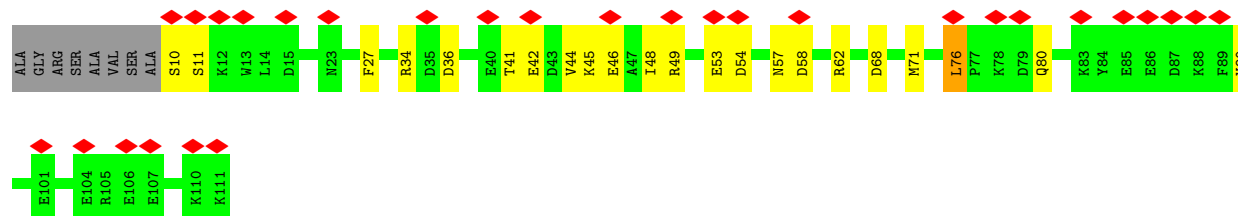
• Molecule 44: Cytochrome b-c1 complex subunit 9



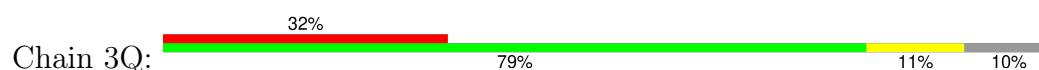
• Molecule 44: Cytochrome b-c1 complex subunit 9

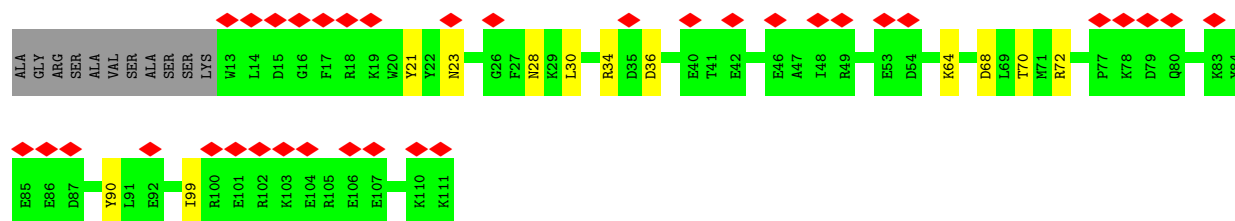


• Molecule 45: Cytochrome b-c1 complex subunit 7

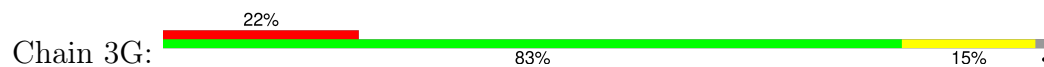


• Molecule 45: Cytochrome b-c1 complex subunit 7

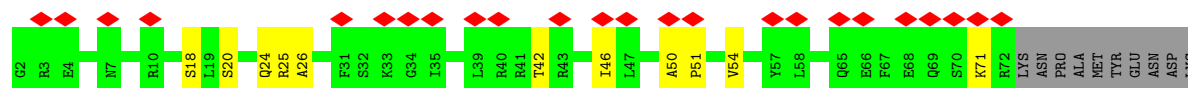
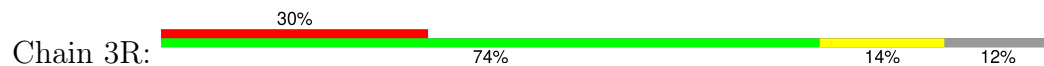




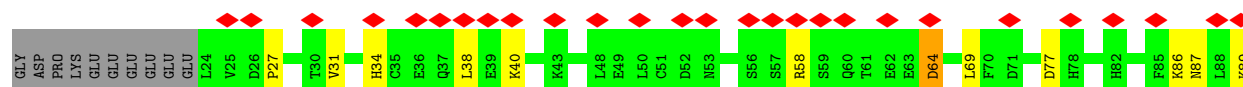
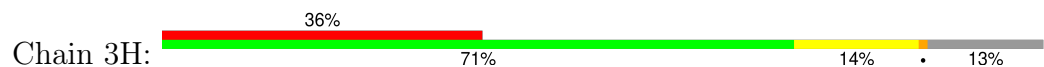
- Molecule 46: Cytochrome b-c1 complex subunit 8



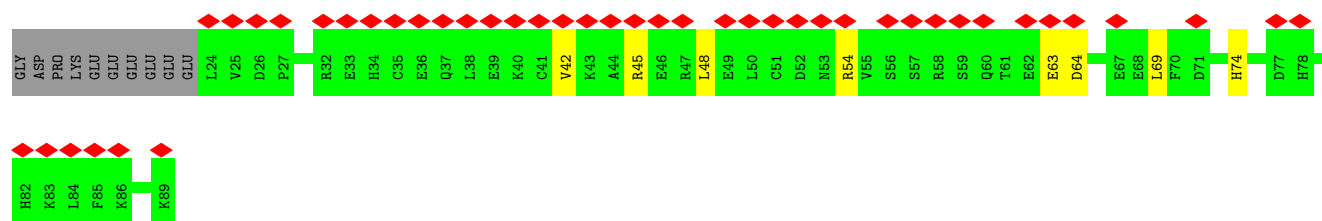
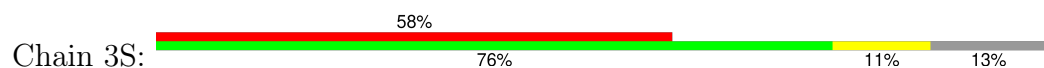
- Molecule 46: Cytochrome b-c1 complex subunit 8



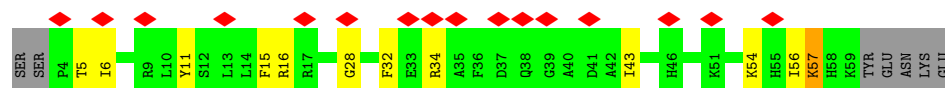
- Molecule 47: Cytochrome b-c1 complex subunit 6, mitochondrial



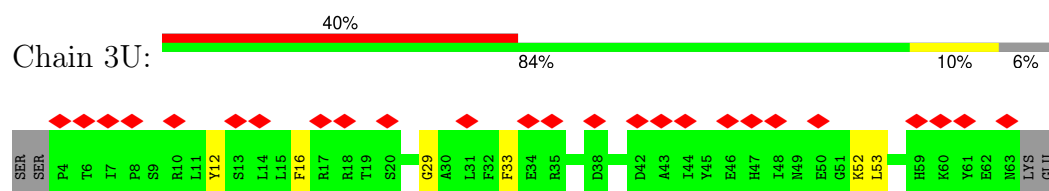
- Molecule 47: Cytochrome b-c1 complex subunit 6, mitochondrial



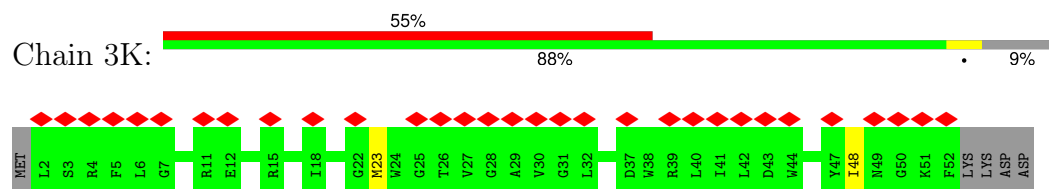
- Molecule 48: Cytochrome b-c1 complex subunit 9



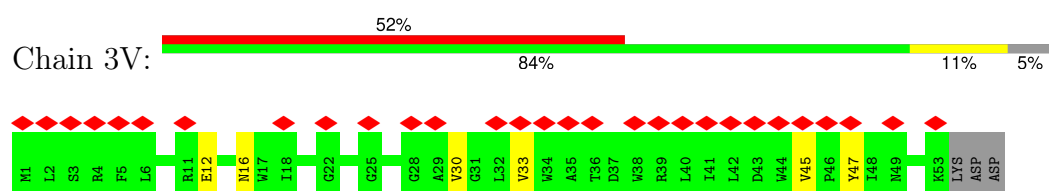
- Molecule 48: Cytochrome b-c1 complex subunit 9



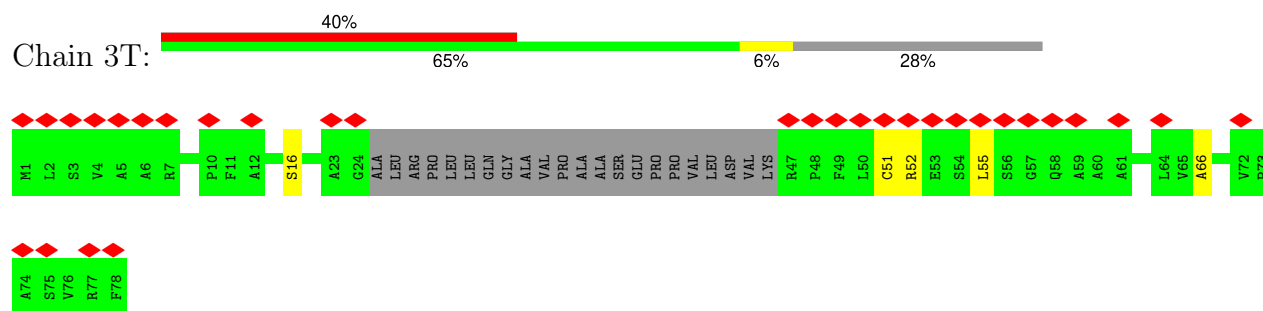
- Molecule 49: Cytochrome b-c1 complex subunit 10



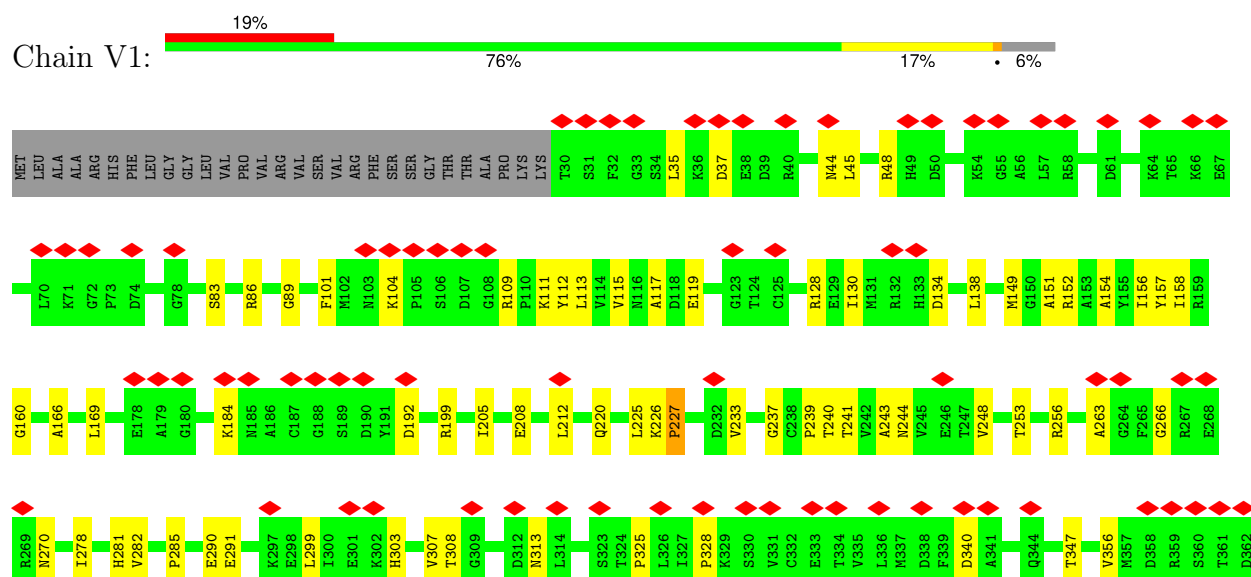
- Molecule 49: Cytochrome b-c1 complex subunit 10

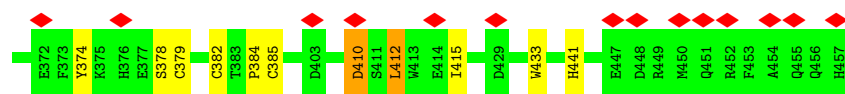


- Molecule 50: Cytochrome b-c1 complex subunit Rieske, mitochondrial



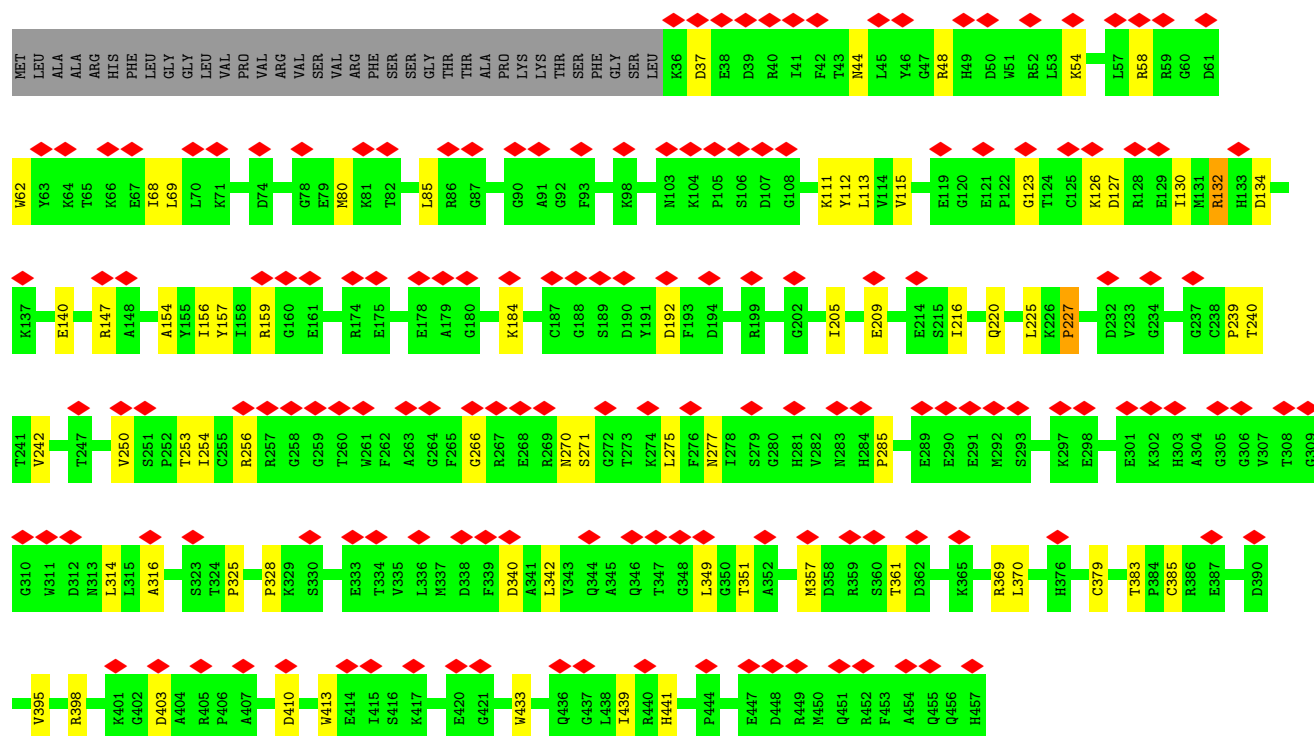
- Molecule 51: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial





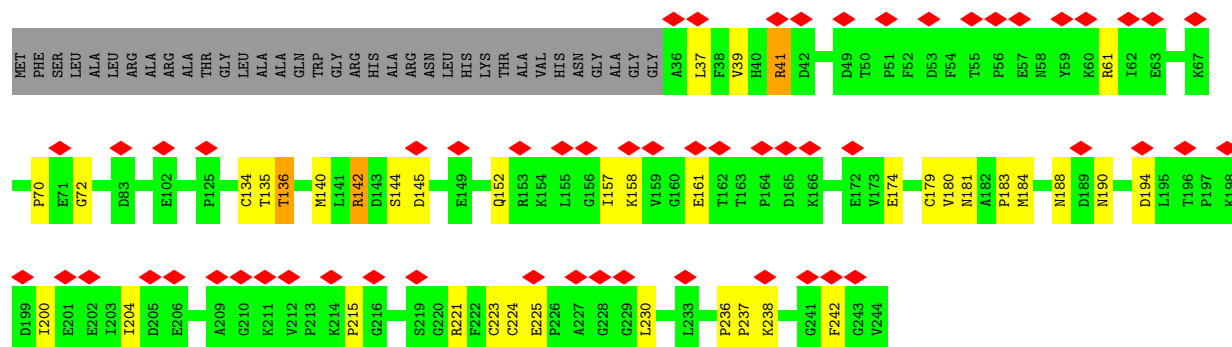
- Molecule 51: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain v1:



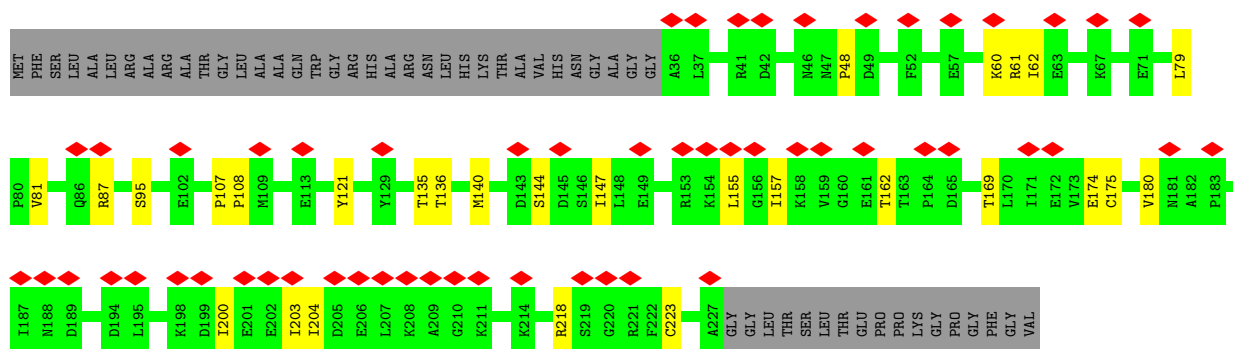
- Molecule 52: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain V2:

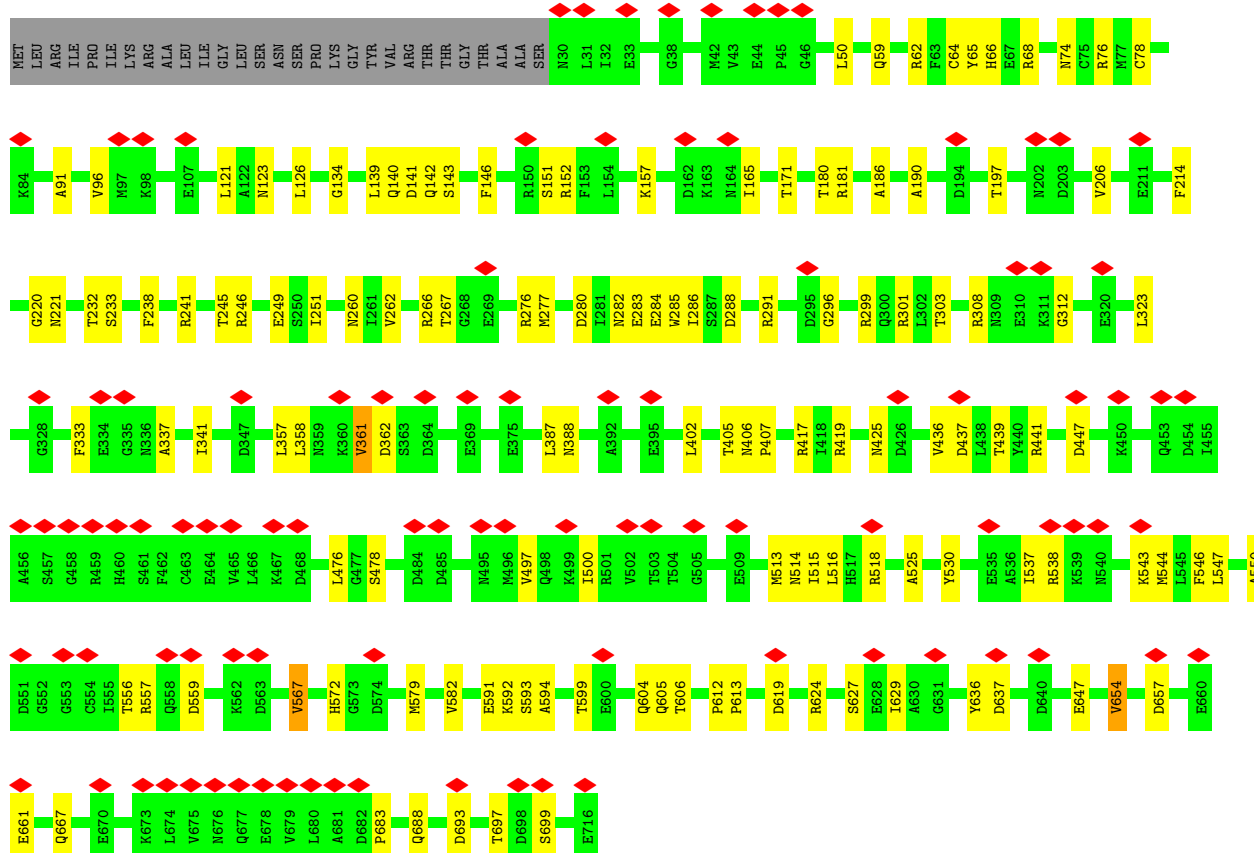
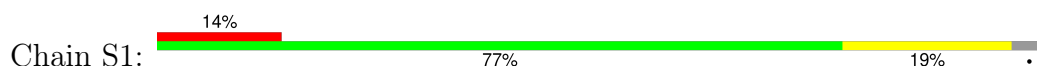


- Molecule 52: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

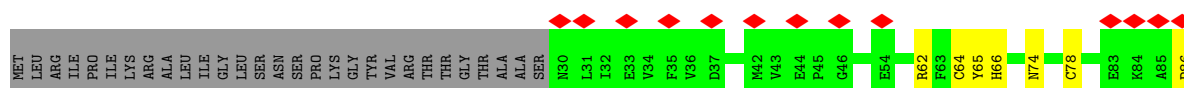
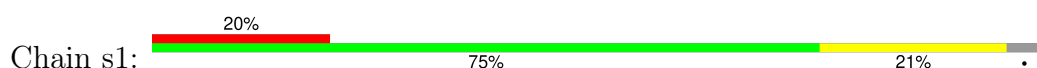
Chain v2:

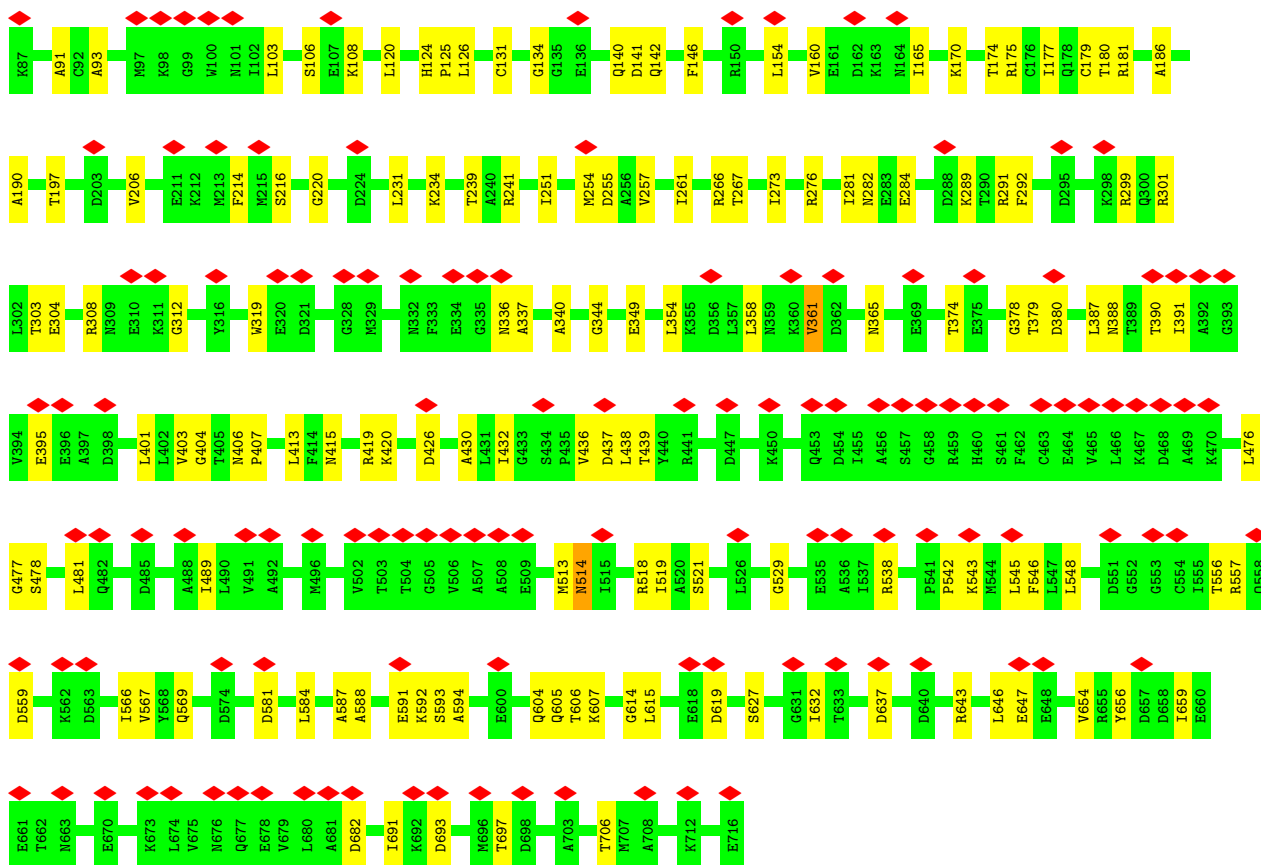


- Molecule 53: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

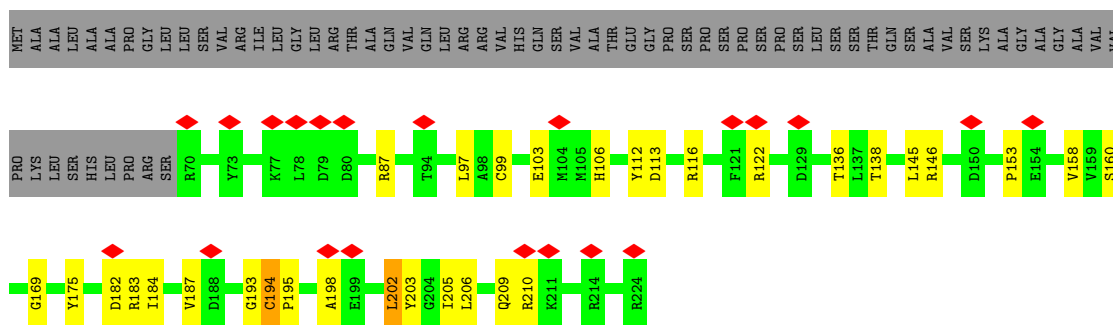


- Molecule 53: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

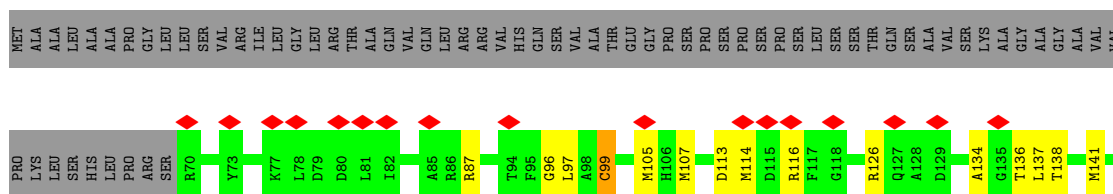


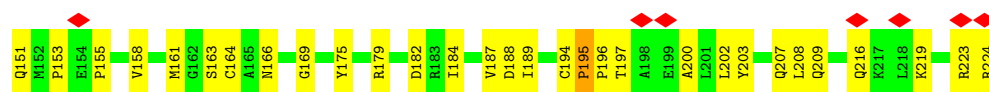


- Molecule 54: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

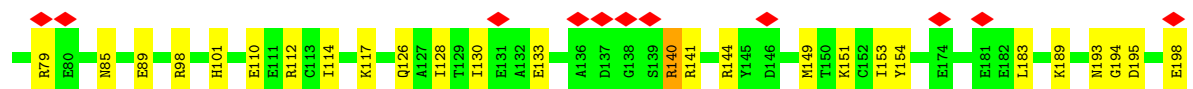
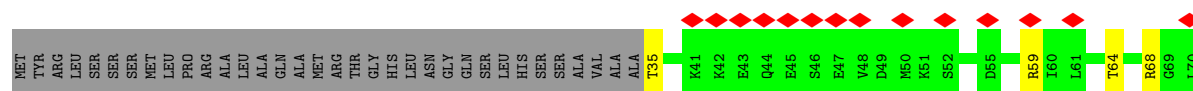


- Molecule 54: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

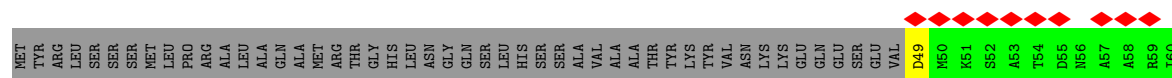




- Molecule 55: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



- Molecule 55: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 182132                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS GLACIOS                             | Depositor |
| Voltage (kV)                         | 200                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 60                                      | Depositor |
| Minimum defocus (nm)                 | 500                                     | Depositor |
| Maximum defocus (nm)                 | 3000                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 29.227                                  | Depositor |
| Minimum map value                    | -9.364                                  | Depositor |
| Average map value                    | -0.007                                  | Depositor |
| Map value standard deviation         | 1.291                                   | Depositor |
| Recommended contour level            | 3.4                                     | Depositor |
| Map size (Å)                         | 249.92, 338.8, 238.48                   | wwPDB     |
| Map dimensions                       | 271, 385, 284                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.88, 0.88, 0.88                        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, FMN, FES, DGT, NDP, SF4, ZN, 2MR, HEM, EH2, HEC

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   | 3     | 0.40         | 0/940         | 0.80        | 0/1285        |
| 1   | 3a    | 0.38         | 0/917         | 0.76        | 0/1252        |
| 2   | S3    | 0.31         | 0/1762        | 0.68        | 0/2401        |
| 2   | s3    | 0.30         | 0/1751        | 0.66        | 3/2386 (0.1%) |
| 3   | S2    | 0.33         | 0/3485        | 0.66        | 2/4720 (0.0%) |
| 3   | s2    | 0.33         | 0/3469        | 0.67        | 2/4698 (0.0%) |
| 4   | 1     | 0.42         | 1/2607 (0.0%) | 0.90        | 3/3564 (0.1%) |
| 4   | 1a    | 0.38         | 0/2599        | 0.84        | 0/3554        |
| 5   | 6     | 0.34         | 0/1322        | 0.68        | 0/1799        |
| 5   | 6a    | 0.30         | 0/1330        | 0.68        | 0/1809        |
| 6   | 4L    | 0.38         | 0/740         | 0.73        | 0/1005        |
| 6   | 4l    | 0.34         | 0/738         | 0.71        | 0/1002        |
| 7   | 5     | 0.37         | 0/4913        | 0.79        | 6/6685 (0.1%) |
| 7   | 5a    | 0.35         | 0/4913        | 0.76        | 2/6685 (0.0%) |
| 8   | 4     | 0.41         | 0/3717        | 0.82        | 3/5062 (0.1%) |
| 8   | 4a    | 0.37         | 0/3717        | 0.79        | 3/5062 (0.1%) |
| 9   | 2     | 0.41         | 0/2756        | 0.84        | 2/3751 (0.1%) |
| 9   | 2a    | 0.49         | 3/2756 (0.1%) | 1.00        | 7/3751 (0.2%) |
| 10  | AL    | 0.25         | 0/2674        | 0.59        | 2/3626 (0.1%) |
| 10  | al    | 0.26         | 0/2674        | 0.58        | 0/3626        |
| 11  | A9    | 0.27         | 0/2823        | 0.59        | 0/3828        |
| 11  | a9    | 0.25         | 0/2823        | 0.58        | 0/3828        |
| 12  | S4    | 0.21         | 0/1044        | 0.48        | 0/1409        |
| 12  | s4    | 0.21         | 0/1044        | 0.49        | 0/1409        |
| 13  | S6    | 0.22         | 0/762         | 0.50        | 0/1026        |
| 13  | s6    | 0.23         | 0/762         | 0.53        | 2/1026 (0.2%) |
| 14  | A2    | 0.29         | 0/682         | 0.69        | 0/920         |
| 14  | a2    | 0.24         | 0/682         | 0.64        | 0/920         |
| 15  | AB    | 0.30         | 0/637         | 0.63        | 0/858         |
| 15  | AC    | 0.31         | 0/718         | 0.70        | 0/970         |
| 15  | ab    | 0.24         | 0/637         | 0.58        | 0/858         |
| 15  | ac    | 0.24         | 0/718         | 0.59        | 0/970         |

| Mol | Chain | Bond lengths |              | Bond angles |               |
|-----|-------|--------------|--------------|-------------|---------------|
|     |       | RMSZ         | # Z  >5      | RMSZ        | # Z  >5       |
| 16  | A5    | 0.28         | 0/949        | 0.65        | 2/1286 (0.2%) |
| 16  | a5    | 0.30         | 0/945        | 0.64        | 0/1281        |
| 17  | A6    | 0.31         | 0/980        | 0.69        | 2/1317 (0.2%) |
| 17  | a6    | 0.30         | 0/972        | 0.63        | 1/1305 (0.1%) |
| 18  | A8    | 0.31         | 0/1422       | 0.69        | 0/1921        |
| 18  | a8    | 0.27         | 0/1427       | 0.63        | 0/1927        |
| 19  | AM    | 0.32         | 0/1069       | 0.68        | 2/1449 (0.1%) |
| 19  | am    | 0.30         | 0/1069       | 0.62        | 0/1449        |
| 20  | AO    | 0.25         | 0/1192       | 0.50        | 0/1608        |
| 20  | ao    | 0.25         | 0/1192       | 0.56        | 2/1608 (0.1%) |
| 21  | A1    | 0.36         | 0/577        | 0.68        | 0/777         |
| 21  | a1    | 0.48         | 1/577 (0.2%) | 0.72        | 0/777         |
| 22  | A3    | 0.26         | 0/671        | 0.55        | 0/921         |
| 22  | a3    | 0.26         | 0/671        | 0.58        | 0/921         |
| 23  | C1    | 0.26         | 0/418        | 0.53        | 0/567         |
| 23  | c1    | 0.26         | 0/388        | 0.51        | 0/528         |
| 24  | C2    | 0.27         | 0/1028       | 0.55        | 0/1387        |
| 24  | c2    | 0.27         | 0/1028       | 0.58        | 0/1387        |
| 25  | S5    | 0.25         | 0/900        | 0.57        | 0/1199        |
| 25  | s5    | 0.26         | 0/900        | 0.65        | 0/1199        |
| 26  | B1    | 0.26         | 0/495        | 0.56        | 0/667         |
| 26  | b1    | 0.30         | 0/495        | 0.62        | 0/667         |
| 27  | BM    | 0.26         | 0/854        | 0.57        | 0/1163        |
| 27  | bm    | 0.29         | 0/863        | 0.64        | 1/1175 (0.1%) |
| 28  | B5    | 0.28         | 0/1201       | 0.61        | 0/1626        |
| 28  | b5    | 0.28         | 0/1193       | 0.59        | 0/1615        |
| 29  | B6    | 0.32         | 0/807        | 0.67        | 0/1096        |
| 29  | b6    | 0.27         | 0/784        | 0.58        | 0/1063        |
| 30  | B2    | 0.27         | 0/580        | 0.64        | 0/794         |
| 30  | b2    | 0.23         | 0/569        | 0.53        | 0/779         |
| 31  | B3    | 0.25         | 0/587        | 0.53        | 0/793         |
| 31  | b3    | 0.25         | 0/591        | 0.51        | 0/798         |
| 32  | B8    | 0.25         | 0/1356       | 0.57        | 0/1851        |
| 32  | b8    | 0.25         | 0/1356       | 0.57        | 0/1851        |
| 33  | B4    | 0.29         | 0/1073       | 0.54        | 1/1455 (0.1%) |
| 33  | b4    | 0.29         | 0/1073       | 0.53        | 0/1455        |
| 34  | B9    | 0.28         | 0/1596       | 0.64        | 6/2162 (0.3%) |
| 34  | b9    | 0.24         | 0/1589       | 0.58        | 2/2152 (0.1%) |
| 35  | B7    | 0.23         | 0/1009       | 0.56        | 0/1355        |
| 35  | b7    | 0.27         | 0/1030       | 0.60        | 0/1382        |
| 36  | BL    | 0.27         | 0/1443       | 0.58        | 0/1951        |
| 36  | bl    | 0.28         | 0/1463       | 0.55        | 0/1977        |
| 37  | AN    | 0.26         | 0/1243       | 0.60        | 0/1692        |

| Mol | Chain | Bond lengths |                 | Bond angles |                   |
|-----|-------|--------------|-----------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5           |
| 37  | an    | 0.24         | 0/1243          | 0.57        | 0/1692            |
| 38  | A7    | 0.20         | 0/759           | 0.46        | 0/1027            |
| 38  | a7    | 0.23         | 0/572           | 0.53        | 0/774             |
| 39  | V3    | 0.24         | 0/349           | 0.62        | 0/473             |
| 39  | v3    | 0.31         | 0/311           | 0.65        | 0/420             |
| 40  | 3A    | 0.30         | 0/3529          | 0.70        | 7/4793 (0.1%)     |
| 40  | 3L    | 0.33         | 0/3530          | 0.74        | 4/4793 (0.1%)     |
| 41  | 3B    | 0.27         | 0/3205          | 0.62        | 0/4332            |
| 41  | 3M    | 0.26         | 0/3205          | 0.59        | 0/4332            |
| 42  | 3C    | 0.31         | 0/3147          | 0.66        | 0/4297            |
| 42  | 3N    | 0.31         | 0/3147          | 0.67        | 3/4297 (0.1%)     |
| 43  | 3D    | 0.26         | 0/1978          | 0.60        | 1/2685 (0.0%)     |
| 43  | 3O    | 0.24         | 0/1968          | 0.53        | 0/2674            |
| 44  | 3E    | 0.26         | 0/609           | 0.59        | 0/821             |
| 44  | 3P    | 0.28         | 0/617           | 0.64        | 0/832             |
| 45  | 3F    | 0.25         | 0/922           | 0.53        | 0/1234            |
| 45  | 3Q    | 0.26         | 0/901           | 0.57        | 0/1207            |
| 46  | 3G    | 0.37         | 0/689           | 0.78        | 1/931 (0.1%)      |
| 46  | 3R    | 0.36         | 0/617           | 0.68        | 0/833             |
| 47  | 3H    | 0.31         | 0/552           | 0.70        | 2/739 (0.3%)      |
| 47  | 3S    | 0.26         | 0/552           | 0.67        | 0/739             |
| 48  | 3J    | 0.54         | 1/473 (0.2%)    | 0.85        | 1/637 (0.2%)      |
| 48  | 3U    | 0.28         | 0/503           | 0.56        | 0/678             |
| 49  | 3K    | 0.32         | 0/437           | 0.63        | 0/598             |
| 49  | 3V    | 0.33         | 0/454           | 0.58        | 0/619             |
| 50  | 3T    | 0.25         | 0/403           | 0.51        | 0/546             |
| 51  | V1    | 0.34         | 0/3376          | 0.78        | 2/4561 (0.0%)     |
| 51  | v1    | 0.35         | 0/3333          | 0.76        | 6/4503 (0.1%)     |
| 52  | V2    | 0.40         | 0/1670          | 0.83        | 3/2276 (0.1%)     |
| 52  | v2    | 0.39         | 0/1553          | 0.89        | 0/2116            |
| 53  | S1    | 0.30         | 0/5377          | 0.73        | 9/7285 (0.1%)     |
| 53  | s1    | 0.29         | 0/5377          | 0.70        | 6/7285 (0.1%)     |
| 54  | S7    | 0.41         | 0/1272          | 0.87        | 0/1722            |
| 54  | s7    | 0.36         | 0/1272          | 0.84        | 0/1722            |
| 55  | S8    | 0.36         | 0/1438          | 0.81        | 1/1946 (0.1%)     |
| 55  | s8    | 0.36         | 0/1337          | 0.79        | 2/1808 (0.1%)     |
| All | All   | 0.32         | 6/165414 (0.0%) | 0.69        | 104/224305 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | S3    | 0                   | 1                   |
| 4   | 1     | 0                   | 2                   |
| 7   | 5a    | 0                   | 1                   |
| 8   | 4     | 0                   | 2                   |
| 18  | A8    | 0                   | 1                   |
| 37  | AN    | 0                   | 1                   |
| 41  | 3B    | 0                   | 1                   |
| 42  | 3C    | 0                   | 1                   |
| 51  | V1    | 0                   | 1                   |
| 51  | v1    | 0                   | 2                   |
| 52  | V2    | 0                   | 4                   |
| 52  | v2    | 0                   | 1                   |
| 54  | S7    | 0                   | 4                   |
| 54  | s7    | 0                   | 3                   |
| All | All   | 0                   | 25                  |

The worst 5 of 6 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 9   | 2a    | 255 | PRO  | CB-CG | -11.20 | 0.93        | 1.49     |
| 21  | a1    | 18  | ILE  | C-N   | 9.06   | 1.45        | 1.34     |
| 9   | 2a    | 255 | PRO  | CG-CD | -7.88  | 1.24        | 1.50     |
| 48  | 3J    | 57  | LYS  | CA-C  | 6.53   | 1.61        | 1.52     |
| 9   | 2a    | 255 | PRO  | N-CA  | 5.90   | 1.58        | 1.46     |

The worst 5 of 104 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 9   | 2a    | 255 | PRO  | CB-CG-CD | 18.22  | 164.40      | 106.10   |
| 9   | 2a    | 255 | PRO  | N-CD-CG  | -17.40 | 77.11       | 103.20   |
| 9   | 2a    | 255 | PRO  | CA-CB-CG | -16.77 | 72.64       | 104.50   |
| 10  | AL    | 210 | PRO  | CA-C-N   | 10.80  | 127.05      | 120.24   |
| 10  | AL    | 210 | PRO  | C-N-CA   | 10.80  | 127.05      | 120.24   |

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 4   | 1     | 154 | LEU  | Peptide |
| 4   | 1     | 199 | ASP  | Peptide |
| 8   | 4     | 249 | ILE  | Peptide |
| 8   | 4     | 366 | ASN  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 2   | S3    | 70  | LYS  | Peptide |

## 5.2 Too-close contacts ⓘ

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   | 3     | 914   | 0        | 952      | 25      | 0            |
| 1   | 3a    | 893   | 0        | 935      | 17      | 0            |
| 2   | S3    | 1712  | 0        | 1667     | 37      | 0            |
| 2   | s3    | 1701  | 0        | 1655     | 31      | 0            |
| 3   | S2    | 3410  | 0        | 3348     | 71      | 0            |
| 3   | s2    | 3386  | 0        | 3319     | 69      | 0            |
| 4   | 1     | 2530  | 0        | 2615     | 49      | 0            |
| 4   | 1a    | 2522  | 0        | 2606     | 62      | 0            |
| 5   | 6     | 1290  | 0        | 1304     | 21      | 0            |
| 5   | 6a    | 1298  | 0        | 1316     | 20      | 0            |
| 6   | 4L    | 729   | 0        | 764      | 12      | 0            |
| 6   | 4l    | 727   | 0        | 758      | 16      | 0            |
| 7   | 5     | 4790  | 0        | 4975     | 100     | 0            |
| 7   | 5a    | 4790  | 0        | 4973     | 73      | 0            |
| 8   | 4     | 3630  | 0        | 3854     | 70      | 0            |
| 8   | 4a    | 3630  | 0        | 3854     | 64      | 0            |
| 9   | 2     | 2694  | 0        | 2896     | 48      | 0            |
| 9   | 2a    | 2694  | 0        | 2896     | 48      | 0            |
| 10  | AL    | 2607  | 0        | 2562     | 22      | 0            |
| 10  | al    | 2607  | 0        | 2563     | 23      | 0            |
| 11  | A9    | 2748  | 0        | 2765     | 44      | 0            |
| 11  | a9    | 2748  | 0        | 2765     | 38      | 0            |
| 12  | S4    | 1021  | 0        | 1022     | 19      | 0            |
| 12  | s4    | 1021  | 0        | 1022     | 15      | 0            |
| 13  | S6    | 748   | 0        | 721      | 16      | 0            |
| 13  | s6    | 748   | 0        | 721      | 14      | 0            |
| 14  | A2    | 671   | 0        | 688      | 14      | 0            |
| 14  | a2    | 671   | 0        | 688      | 12      | 0            |
| 15  | AB    | 628   | 0        | 627      | 4       | 0            |
| 15  | AC    | 706   | 0        | 696      | 13      | 0            |
| 15  | ab    | 628   | 0        | 627      | 12      | 0            |
| 15  | ac    | 706   | 0        | 696      | 7       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 16  | A5    | 927   | 0        | 968      | 11      | 0            |
| 16  | a5    | 923   | 0        | 965      | 12      | 0            |
| 17  | A6    | 957   | 0        | 979      | 12      | 0            |
| 17  | a6    | 950   | 0        | 972      | 16      | 0            |
| 18  | A8    | 1385  | 0        | 1370     | 14      | 0            |
| 18  | a8    | 1389  | 0        | 1374     | 17      | 0            |
| 19  | AM    | 1045  | 0        | 1034     | 9       | 0            |
| 19  | am    | 1045  | 0        | 1034     | 11      | 0            |
| 20  | AO    | 1161  | 0        | 1161     | 14      | 0            |
| 20  | ao    | 1161  | 0        | 1161     | 31      | 0            |
| 21  | A1    | 564   | 0        | 579      | 2       | 0            |
| 21  | a1    | 564   | 0        | 579      | 11      | 0            |
| 22  | A3    | 648   | 0        | 649      | 6       | 0            |
| 22  | a3    | 648   | 0        | 652      | 5       | 0            |
| 23  | C1    | 407   | 0        | 404      | 0       | 0            |
| 23  | c1    | 377   | 0        | 371      | 2       | 0            |
| 24  | C2    | 996   | 0        | 1001     | 10      | 0            |
| 24  | c2    | 996   | 0        | 1001     | 11      | 0            |
| 25  | S5    | 877   | 0        | 871      | 14      | 0            |
| 25  | s5    | 877   | 0        | 869      | 17      | 0            |
| 26  | B1    | 482   | 0        | 479      | 2       | 0            |
| 26  | b1    | 482   | 0        | 479      | 6       | 0            |
| 27  | BM    | 826   | 0        | 766      | 7       | 0            |
| 27  | bm    | 835   | 0        | 772      | 9       | 0            |
| 28  | B5    | 1166  | 0        | 1166     | 12      | 0            |
| 28  | b5    | 1158  | 0        | 1160     | 20      | 0            |
| 29  | B6    | 783   | 0        | 792      | 12      | 0            |
| 29  | b6    | 761   | 0        | 769      | 11      | 0            |
| 30  | B2    | 555   | 0        | 506      | 5       | 0            |
| 30  | b2    | 545   | 0        | 499      | 10      | 0            |
| 31  | B3    | 569   | 0        | 573      | 12      | 0            |
| 31  | b3    | 573   | 0        | 576      | 3       | 0            |
| 32  | B8    | 1302  | 0        | 1197     | 19      | 0            |
| 32  | b8    | 1302  | 0        | 1197     | 15      | 0            |
| 33  | B4    | 1044  | 0        | 1056     | 21      | 0            |
| 33  | b4    | 1044  | 0        | 1056     | 15      | 0            |
| 34  | B9    | 1541  | 0        | 1470     | 18      | 0            |
| 34  | b9    | 1534  | 0        | 1463     | 19      | 0            |
| 35  | B7    | 984   | 0        | 970      | 11      | 0            |
| 35  | b7    | 1005  | 0        | 995      | 12      | 0            |
| 36  | BL    | 1410  | 0        | 1379     | 21      | 0            |
| 36  | bl    | 1430  | 0        | 1400     | 16      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 37  | AN    | 1201  | 0        | 1158     | 17      | 0            |
| 37  | an    | 1201  | 0        | 1158     | 14      | 0            |
| 38  | A7    | 741   | 0        | 770      | 11      | 0            |
| 38  | a7    | 560   | 0        | 579      | 8       | 0            |
| 39  | V3    | 339   | 0        | 320      | 7       | 0            |
| 39  | v3    | 303   | 0        | 290      | 6       | 0            |
| 40  | 3A    | 3459  | 0        | 3365     | 52      | 0            |
| 40  | 3L    | 3460  | 0        | 3365     | 46      | 0            |
| 41  | 3B    | 3154  | 0        | 3158     | 30      | 0            |
| 41  | 3M    | 3154  | 0        | 3158     | 41      | 0            |
| 42  | 3C    | 3046  | 0        | 3110     | 36      | 0            |
| 42  | 3N    | 3046  | 0        | 3111     | 36      | 0            |
| 43  | 3D    | 1919  | 0        | 1864     | 24      | 0            |
| 43  | 3O    | 1909  | 0        | 1849     | 28      | 0            |
| 44  | 3E    | 602   | 0        | 601      | 6       | 0            |
| 44  | 3P    | 610   | 0        | 612      | 10      | 0            |
| 45  | 3F    | 900   | 0        | 887      | 12      | 0            |
| 45  | 3Q    | 879   | 0        | 864      | 8       | 0            |
| 46  | 3G    | 670   | 0        | 666      | 9       | 0            |
| 46  | 3R    | 600   | 0        | 604      | 7       | 0            |
| 47  | 3H    | 545   | 0        | 529      | 8       | 0            |
| 47  | 3S    | 545   | 0        | 531      | 5       | 0            |
| 48  | 3J    | 460   | 0        | 464      | 8       | 0            |
| 48  | 3U    | 489   | 0        | 485      | 4       | 0            |
| 49  | 3K    | 421   | 0        | 418      | 2       | 0            |
| 49  | 3V    | 438   | 0        | 443      | 3       | 0            |
| 50  | 3T    | 397   | 0        | 418      | 5       | 0            |
| 51  | V1    | 3301  | 0        | 3248     | 50      | 0            |
| 51  | v1    | 3259  | 0        | 3212     | 44      | 0            |
| 52  | V2    | 1630  | 0        | 1623     | 24      | 0            |
| 52  | v2    | 1517  | 0        | 1509     | 19      | 0            |
| 53  | S1    | 5290  | 0        | 5317     | 90      | 0            |
| 53  | s1    | 5290  | 0        | 5317     | 93      | 0            |
| 54  | S7    | 1241  | 0        | 1250     | 25      | 0            |
| 54  | s7    | 1241  | 0        | 1248     | 37      | 0            |
| 55  | S8    | 1408  | 0        | 1341     | 29      | 0            |
| 55  | s8    | 1309  | 0        | 1261     | 36      | 0            |
| 56  | AL    | 1     | 0        | 0        | 0       | 0            |
| 56  | al    | 1     | 0        | 0        | 0       | 0            |
| 57  | AL    | 31    | 0        | 12       | 1       | 0            |
| 57  | al    | 31    | 0        | 12       | 0       | 0            |
| 58  | A9    | 48    | 0        | 26       | 3       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 58  | a9    | 48     | 0        | 25       | 1       | 0            |
| 59  | S6    | 1      | 0        | 0        | 0       | 0            |
| 59  | s6    | 1      | 0        | 0        | 0       | 0            |
| 60  | 5a    | 37     | 0        | 0        | 0       | 0            |
| 60  | A6    | 37     | 0        | 0        | 0       | 0            |
| 60  | B9    | 37     | 0        | 0        | 1       | 0            |
| 60  | a6    | 37     | 0        | 0        | 0       | 0            |
| 61  | 3C    | 86     | 0        | 60       | 1       | 0            |
| 61  | 3N    | 86     | 0        | 60       | 2       | 0            |
| 62  | 3D    | 43     | 0        | 30       | 3       | 0            |
| 62  | 3O    | 43     | 0        | 30       | 2       | 0            |
| 63  | V1    | 31     | 0        | 18       | 2       | 0            |
| 63  | v1    | 31     | 0        | 19       | 0       | 0            |
| 64  | S1    | 16     | 0        | 0        | 1       | 0            |
| 64  | S7    | 8      | 0        | 0        | 3       | 0            |
| 64  | S8    | 16     | 0        | 0        | 1       | 0            |
| 64  | V1    | 8      | 0        | 0        | 1       | 0            |
| 64  | s1    | 16     | 0        | 0        | 1       | 0            |
| 64  | s7    | 8      | 0        | 0        | 2       | 0            |
| 64  | s8    | 16     | 0        | 0        | 2       | 0            |
| 64  | v1    | 8      | 0        | 0        | 1       | 0            |
| 65  | S1    | 4      | 0        | 0        | 1       | 0            |
| 65  | V2    | 4      | 0        | 0        | 1       | 0            |
| 65  | s1    | 4      | 0        | 0        | 1       | 0            |
| 65  | v2    | 4      | 0        | 0        | 1       | 0            |
| All | All   | 162102 | 0        | 161959   | 2056    | 0            |

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

The worst 5 of 2056 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) |
|------------------|-------------------|--------------------------|-------------------|
| 43:3D:121:CYS:SG | 62:3D:401:HEC:CAB | 2.02                     | 1.45              |
| 43:3D:121:CYS:SG | 62:3D:401:HEC:C3B | 2.32                     | 1.18              |
| 35:B7:7:ARG:O    | 35:B7:11:TRP:HB2  | 1.71                     | 0.91              |
| 8:4a:13:PRO:O    | 8:4a:17:LEU:HB2   | 1.75                     | 0.87              |
| 3:S2:223:HIS:CD2 | 64:S7:301:SF4:S1  | 2.69                     | 0.86              |

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   | 3     | 111/115 (96%)  | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | 3a    | 109/115 (95%)  | 102 (94%) | 7 (6%)  | 0        | 100         | 100 |
| 2   | S3    | 204/263 (78%)  | 197 (97%) | 7 (3%)  | 0        | 100         | 100 |
| 2   | s3    | 203/263 (77%)  | 188 (93%) | 15 (7%) | 0        | 100         | 100 |
| 3   | S2    | 418/463 (90%)  | 401 (96%) | 17 (4%) | 0        | 100         | 100 |
| 3   | s2    | 416/463 (90%)  | 400 (96%) | 16 (4%) | 0        | 100         | 100 |
| 4   | 1     | 315/318 (99%)  | 294 (93%) | 20 (6%) | 1 (0%)   | 36          | 65  |
| 4   | 1a    | 314/318 (99%)  | 293 (93%) | 20 (6%) | 1 (0%)   | 36          | 65  |
| 5   | 6     | 168/172 (98%)  | 160 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 5   | 6a    | 169/172 (98%)  | 163 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 6   | 4L    | 95/98 (97%)    | 90 (95%)  | 5 (5%)  | 0        | 100         | 100 |
| 6   | 4l    | 95/98 (97%)    | 93 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 7   | 5     | 603/607 (99%)  | 573 (95%) | 28 (5%) | 2 (0%)   | 36          | 65  |
| 7   | 5a    | 603/607 (99%)  | 562 (93%) | 41 (7%) | 0        | 100         | 100 |
| 8   | 4     | 457/459 (100%) | 442 (97%) | 15 (3%) | 0        | 100         | 100 |
| 8   | 4a    | 457/459 (100%) | 439 (96%) | 18 (4%) | 0        | 100         | 100 |
| 9   | 2     | 342/345 (99%)  | 331 (97%) | 11 (3%) | 0        | 100         | 100 |
| 9   | 2a    | 342/345 (99%)  | 330 (96%) | 12 (4%) | 0        | 100         | 100 |
| 10  | AL    | 318/355 (90%)  | 299 (94%) | 19 (6%) | 0        | 100         | 100 |
| 10  | al    | 318/355 (90%)  | 304 (96%) | 14 (4%) | 0        | 100         | 100 |
| 11  | A9    | 340/377 (90%)  | 321 (94%) | 19 (6%) | 0        | 100         | 100 |
| 11  | a9    | 340/377 (90%)  | 326 (96%) | 14 (4%) | 0        | 100         | 100 |
| 12  | S4    | 124/175 (71%)  | 118 (95%) | 6 (5%)  | 0        | 100         | 100 |
| 12  | s4    | 124/175 (71%)  | 122 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 13  | S6    | 93/116 (80%)   | 93 (100%) | 0       | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 13  | s6    | 93/116 (80%)  | 90 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 14  | A2    | 82/99 (83%)   | 78 (95%)  | 4 (5%)  | 0        | 100         | 100 |
| 14  | a2    | 82/99 (83%)   | 75 (92%)  | 7 (8%)  | 0        | 100         | 100 |
| 15  | AB    | 76/156 (49%)  | 73 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 15  | AC    | 86/156 (55%)  | 84 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 15  | ab    | 76/156 (49%)  | 73 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 15  | ac    | 86/156 (55%)  | 82 (95%)  | 4 (5%)  | 0        | 100         | 100 |
| 16  | A5    | 112/116 (97%) | 106 (95%) | 6 (5%)  | 0        | 100         | 100 |
| 16  | a5    | 111/116 (96%) | 108 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 17  | A6    | 110/131 (84%) | 105 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 17  | a6    | 109/131 (83%) | 103 (94%) | 6 (6%)  | 0        | 100         | 100 |
| 18  | A8    | 167/172 (97%) | 159 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 18  | a8    | 168/172 (98%) | 162 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 19  | AM    | 139/142 (98%) | 135 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 19  | am    | 139/142 (98%) | 137 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 20  | AO    | 138/144 (96%) | 135 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 20  | ao    | 138/144 (96%) | 135 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 21  | A1    | 67/70 (96%)   | 65 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 21  | a1    | 67/70 (96%)   | 65 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 22  | A3    | 81/84 (96%)   | 75 (93%)  | 6 (7%)  | 0        | 100         | 100 |
| 22  | a3    | 81/84 (96%)   | 76 (94%)  | 5 (6%)  | 0        | 100         | 100 |
| 23  | C1    | 47/76 (62%)   | 47 (100%) | 0       | 0        | 100         | 100 |
| 23  | c1    | 43/76 (57%)   | 42 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 24  | C2    | 118/120 (98%) | 117 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 24  | c2    | 118/120 (98%) | 114 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 25  | S5    | 103/106 (97%) | 98 (95%)  | 5 (5%)  | 0        | 100         | 100 |
| 25  | s5    | 103/106 (97%) | 100 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 26  | B1    | 54/57 (95%)   | 51 (94%)  | 3 (6%)  | 0        | 100         | 100 |
| 26  | b1    | 54/57 (95%)   | 52 (96%)  | 2 (4%)  | 0        | 100         | 100 |
| 27  | BM    | 96/151 (64%)  | 93 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 27  | bm    | 97/151 (64%)  | 93 (96%)  | 4 (4%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 28  | B5    | 137/189 (72%)  | 132 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 28  | b5    | 136/189 (72%)  | 132 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 29  | B6    | 90/127 (71%)   | 89 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 29  | b6    | 86/127 (68%)   | 83 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 30  | B2    | 62/105 (59%)   | 57 (92%)  | 5 (8%)  | 0        | 100         | 100 |
| 30  | b2    | 61/105 (58%)   | 61 (100%) | 0       | 0        | 100         | 100 |
| 31  | B3    | 68/104 (65%)   | 65 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 31  | b3    | 69/104 (66%)   | 66 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 32  | B8    | 153/186 (82%)  | 143 (94%) | 10 (6%) | 0        | 100         | 100 |
| 32  | b8    | 153/186 (82%)  | 149 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 33  | B4    | 123/129 (95%)  | 121 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 33  | b4    | 123/129 (95%)  | 118 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 34  | B9    | 176/179 (98%)  | 169 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 34  | b9    | 175/179 (98%)  | 168 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 35  | B7    | 112/136 (82%)  | 110 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 35  | b7    | 115/136 (85%)  | 109 (95%) | 6 (5%)  | 0        | 100         | 100 |
| 36  | BL    | 165/176 (94%)  | 159 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 36  | bl    | 167/176 (95%)  | 159 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 37  | AN    | 142/145 (98%)  | 135 (95%) | 7 (5%)  | 0        | 100         | 100 |
| 37  | an    | 142/145 (98%)  | 138 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 38  | A7    | 88/112 (79%)   | 84 (96%)  | 4 (4%)  | 0        | 100         | 100 |
| 38  | a7    | 68/112 (61%)   | 63 (93%)  | 5 (7%)  | 0        | 100         | 100 |
| 39  | V3    | 38/104 (36%)   | 38 (100%) | 0       | 0        | 100         | 100 |
| 39  | v3    | 34/104 (33%)   | 34 (100%) | 0       | 0        | 100         | 100 |
| 40  | 3A    | 443/446 (99%)  | 427 (96%) | 16 (4%) | 0        | 100         | 100 |
| 40  | 3L    | 443/446 (99%)  | 426 (96%) | 17 (4%) | 0        | 100         | 100 |
| 41  | 3B    | 418/439 (95%)  | 405 (97%) | 13 (3%) | 0        | 100         | 100 |
| 41  | 3M    | 418/439 (95%)  | 396 (95%) | 22 (5%) | 0        | 100         | 100 |
| 42  | 3C    | 378/380 (100%) | 366 (97%) | 12 (3%) | 0        | 100         | 100 |
| 42  | 3N    | 378/380 (100%) | 361 (96%) | 17 (4%) | 0        | 100         | 100 |
| 43  | 3D    | 239/241 (99%)  | 230 (96%) | 9 (4%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed   | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|-----------|----------|-------------|-----|
| 43  | 3O    | 238/241 (99%)     | 229 (96%)   | 9 (4%)    | 0        | 100         | 100 |
| 44  | 3E    | 78/196 (40%)      | 76 (97%)    | 2 (3%)    | 0        | 100         | 100 |
| 44  | 3P    | 79/196 (40%)      | 73 (92%)    | 6 (8%)    | 0        | 100         | 100 |
| 45  | 3F    | 100/110 (91%)     | 97 (97%)    | 3 (3%)    | 0        | 100         | 100 |
| 45  | 3Q    | 97/110 (88%)      | 94 (97%)    | 3 (3%)    | 0        | 100         | 100 |
| 46  | 3G    | 77/81 (95%)       | 70 (91%)    | 7 (9%)    | 0        | 100         | 100 |
| 46  | 3R    | 69/81 (85%)       | 63 (91%)    | 6 (9%)    | 0        | 100         | 100 |
| 47  | 3H    | 64/76 (84%)       | 63 (98%)    | 1 (2%)    | 0        | 100         | 100 |
| 47  | 3S    | 64/76 (84%)       | 63 (98%)    | 1 (2%)    | 0        | 100         | 100 |
| 48  | 3J    | 54/63 (86%)       | 52 (96%)    | 1 (2%)    | 1 (2%)   | 6           | 33  |
| 48  | 3U    | 57/63 (90%)       | 56 (98%)    | 1 (2%)    | 0        | 100         | 100 |
| 49  | 3K    | 49/56 (88%)       | 45 (92%)    | 4 (8%)    | 0        | 100         | 100 |
| 49  | 3V    | 51/56 (91%)       | 49 (96%)    | 2 (4%)    | 0        | 100         | 100 |
| 50  | 3T    | 52/78 (67%)       | 50 (96%)    | 2 (4%)    | 0        | 100         | 100 |
| 51  | V1    | 426/457 (93%)     | 371 (87%)   | 55 (13%)  | 0        | 100         | 100 |
| 51  | v1    | 420/457 (92%)     | 375 (89%)   | 45 (11%)  | 0        | 100         | 100 |
| 52  | V2    | 207/244 (85%)     | 178 (86%)   | 28 (14%)  | 1 (0%)   | 24          | 56  |
| 52  | v2    | 190/244 (78%)     | 176 (93%)   | 14 (7%)   | 0        | 100         | 100 |
| 53  | S1    | 685/716 (96%)     | 620 (90%)   | 65 (10%)  | 0        | 100         | 100 |
| 53  | s1    | 685/716 (96%)     | 619 (90%)   | 66 (10%)  | 0        | 100         | 100 |
| 54  | S7    | 153/224 (68%)     | 138 (90%)   | 15 (10%)  | 0        | 100         | 100 |
| 54  | s7    | 153/224 (68%)     | 138 (90%)   | 15 (10%)  | 0        | 100         | 100 |
| 55  | S8    | 176/212 (83%)     | 158 (90%)   | 18 (10%)  | 0        | 100         | 100 |
| 55  | s8    | 162/212 (76%)     | 145 (90%)   | 16 (10%)  | 1 (1%)   | 21          | 52  |
| All | All   | 19905/22630 (88%) | 18869 (95%) | 1029 (5%) | 7 (0%)   | 100         | 100 |

5 of 7 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 1     | 91  | MET  |
| 7   | 5     | 433 | THR  |
| 4   | 1a    | 91  | MET  |
| 48  | 3J    | 57  | LYS  |
| 55  | s8    | 152 | CYS  |

### 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   | 3     | 102/104 (98%)  | 101 (99%)  | 1 (1%)   | 68          | 74  |
| 1   | 3a    | 100/104 (96%)  | 100 (100%) | 0        | 100         | 100 |
| 2   | S3    | 188/227 (83%)  | 186 (99%)  | 2 (1%)   | 65          | 73  |
| 2   | s3    | 187/227 (82%)  | 185 (99%)  | 2 (1%)   | 65          | 73  |
| 3   | S2    | 364/394 (92%)  | 359 (99%)  | 5 (1%)   | 59          | 70  |
| 3   | s2    | 362/394 (92%)  | 359 (99%)  | 3 (1%)   | 73          | 76  |
| 4   | 1     | 279/279 (100%) | 278 (100%) | 1 (0%)   | 84          | 81  |
| 4   | 1a    | 278/279 (100%) | 277 (100%) | 1 (0%)   | 84          | 81  |
| 5   | 6     | 136/138 (99%)  | 136 (100%) | 0        | 100         | 100 |
| 5   | 6a    | 137/138 (99%)  | 135 (98%)  | 2 (2%)   | 57          | 68  |
| 6   | 4L    | 87/88 (99%)    | 87 (100%)  | 0        | 100         | 100 |
| 6   | 4l    | 87/88 (99%)    | 87 (100%)  | 0        | 100         | 100 |
| 7   | 5     | 548/550 (100%) | 546 (100%) | 2 (0%)   | 84          | 81  |
| 7   | 5a    | 548/550 (100%) | 543 (99%)  | 5 (1%)   | 70          | 75  |
| 8   | 4     | 415/415 (100%) | 412 (99%)  | 3 (1%)   | 76          | 77  |
| 8   | 4a    | 415/415 (100%) | 413 (100%) | 2 (0%)   | 81          | 80  |
| 9   | 2     | 307/308 (100%) | 304 (99%)  | 3 (1%)   | 68          | 74  |
| 9   | 2a    | 307/308 (100%) | 305 (99%)  | 2 (1%)   | 76          | 77  |
| 10  | AL    | 284/309 (92%)  | 283 (100%) | 1 (0%)   | 84          | 81  |
| 10  | al    | 284/309 (92%)  | 281 (99%)  | 3 (1%)   | 65          | 73  |
| 11  | A9    | 299/325 (92%)  | 298 (100%) | 1 (0%)   | 86          | 83  |
| 11  | a9    | 299/325 (92%)  | 297 (99%)  | 2 (1%)   | 76          | 77  |
| 12  | S4    | 112/153 (73%)  | 111 (99%)  | 1 (1%)   | 70          | 75  |
| 12  | s4    | 112/153 (73%)  | 112 (100%) | 0        | 100         | 100 |
| 13  | S6    | 80/96 (83%)    | 79 (99%)   | 1 (1%)   | 61          | 71  |
| 13  | s6    | 80/96 (83%)    | 79 (99%)   | 1 (1%)   | 61          | 71  |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 14  | A2    | 74/80 (92%)    | 74 (100%)  | 0        | 100         | 100 |
| 14  | a2    | 74/80 (92%)    | 72 (97%)   | 2 (3%)   | 39          | 59  |
| 15  | AB    | 72/135 (53%)   | 72 (100%)  | 0        | 100         | 100 |
| 15  | AC    | 81/135 (60%)   | 81 (100%)  | 0        | 100         | 100 |
| 15  | ab    | 72/135 (53%)   | 72 (100%)  | 0        | 100         | 100 |
| 15  | ac    | 81/135 (60%)   | 80 (99%)   | 1 (1%)   | 63          | 72  |
| 16  | A5    | 101/102 (99%)  | 101 (100%) | 0        | 100         | 100 |
| 16  | a5    | 101/102 (99%)  | 101 (100%) | 0        | 100         | 100 |
| 17  | A6    | 106/114 (93%)  | 106 (100%) | 0        | 100         | 100 |
| 17  | a6    | 105/114 (92%)  | 104 (99%)  | 1 (1%)   | 68          | 74  |
| 18  | A8    | 152/154 (99%)  | 152 (100%) | 0        | 100         | 100 |
| 18  | a8    | 152/154 (99%)  | 151 (99%)  | 1 (1%)   | 76          | 77  |
| 19  | AM    | 106/106 (100%) | 105 (99%)  | 1 (1%)   | 70          | 75  |
| 19  | am    | 106/106 (100%) | 106 (100%) | 0        | 100         | 100 |
| 20  | AO    | 121/123 (98%)  | 121 (100%) | 0        | 100         | 100 |
| 20  | ao    | 121/123 (98%)  | 119 (98%)  | 2 (2%)   | 53          | 67  |
| 21  | A1    | 59/60 (98%)    | 59 (100%)  | 0        | 100         | 100 |
| 21  | a1    | 59/60 (98%)    | 58 (98%)   | 1 (2%)   | 53          | 67  |
| 22  | A3    | 72/73 (99%)    | 72 (100%)  | 0        | 100         | 100 |
| 22  | a3    | 72/73 (99%)    | 72 (100%)  | 0        | 100         | 100 |
| 23  | C1    | 43/67 (64%)    | 43 (100%)  | 0        | 100         | 100 |
| 23  | c1    | 40/67 (60%)    | 40 (100%)  | 0        | 100         | 100 |
| 24  | C2    | 107/107 (100%) | 107 (100%) | 0        | 100         | 100 |
| 24  | c2    | 107/107 (100%) | 107 (100%) | 0        | 100         | 100 |
| 25  | S5    | 93/94 (99%)    | 92 (99%)   | 1 (1%)   | 65          | 73  |
| 25  | s5    | 93/94 (99%)    | 93 (100%)  | 0        | 100         | 100 |
| 26  | B1    | 52/53 (98%)    | 51 (98%)   | 1 (2%)   | 50          | 65  |
| 26  | b1    | 52/53 (98%)    | 52 (100%)  | 0        | 100         | 100 |
| 27  | BM    | 89/129 (69%)   | 89 (100%)  | 0        | 100         | 100 |
| 27  | bm    | 90/129 (70%)   | 90 (100%)  | 0        | 100         | 100 |
| 28  | B5    | 123/162 (76%)  | 123 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 28  | b5    | 122/162 (75%)  | 122 (100%) | 0        | 100         | 100 |
| 29  | B6    | 86/119 (72%)   | 86 (100%)  | 0        | 100         | 100 |
| 29  | b6    | 85/119 (71%)   | 84 (99%)   | 1 (1%)   | 63          | 72  |
| 30  | B2    | 60/87 (69%)    | 60 (100%)  | 0        | 100         | 100 |
| 30  | b2    | 59/87 (68%)    | 59 (100%)  | 0        | 100         | 100 |
| 31  | B3    | 55/78 (70%)    | 55 (100%)  | 0        | 100         | 100 |
| 31  | b3    | 55/78 (70%)    | 55 (100%)  | 0        | 100         | 100 |
| 32  | B8    | 140/161 (87%)  | 139 (99%)  | 1 (1%)   | 76          | 77  |
| 32  | b8    | 140/161 (87%)  | 140 (100%) | 0        | 100         | 100 |
| 33  | B4    | 111/114 (97%)  | 111 (100%) | 0        | 100         | 100 |
| 33  | b4    | 111/114 (97%)  | 111 (100%) | 0        | 100         | 100 |
| 34  | B9    | 163/164 (99%)  | 162 (99%)  | 1 (1%)   | 78          | 79  |
| 34  | b9    | 162/164 (99%)  | 161 (99%)  | 1 (1%)   | 78          | 79  |
| 35  | B7    | 106/120 (88%)  | 106 (100%) | 0        | 100         | 100 |
| 35  | b7    | 108/120 (90%)  | 108 (100%) | 0        | 100         | 100 |
| 36  | BL    | 152/158 (96%)  | 152 (100%) | 0        | 100         | 100 |
| 36  | bl    | 154/158 (98%)  | 154 (100%) | 0        | 100         | 100 |
| 37  | AN    | 130/131 (99%)  | 129 (99%)  | 1 (1%)   | 73          | 76  |
| 37  | an    | 130/131 (99%)  | 130 (100%) | 0        | 100         | 100 |
| 38  | A7    | 83/95 (87%)    | 83 (100%)  | 0        | 100         | 100 |
| 38  | a7    | 63/95 (66%)    | 63 (100%)  | 0        | 100         | 100 |
| 39  | V3    | 39/95 (41%)    | 39 (100%)  | 0        | 100         | 100 |
| 39  | v3    | 35/95 (37%)    | 35 (100%)  | 0        | 100         | 100 |
| 40  | 3A    | 372/373 (100%) | 371 (100%) | 1 (0%)   | 86          | 83  |
| 40  | 3L    | 372/373 (100%) | 371 (100%) | 1 (0%)   | 86          | 83  |
| 41  | 3B    | 330/344 (96%)  | 329 (100%) | 1 (0%)   | 86          | 83  |
| 41  | 3M    | 330/344 (96%)  | 330 (100%) | 0        | 100         | 100 |
| 42  | 3C    | 332/332 (100%) | 329 (99%)  | 3 (1%)   | 70          | 75  |
| 42  | 3N    | 332/332 (100%) | 329 (99%)  | 3 (1%)   | 70          | 75  |
| 43  | 3D    | 206/206 (100%) | 205 (100%) | 1 (0%)   | 81          | 80  |
| 43  | 3O    | 205/206 (100%) | 205 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Rotameric    | Outliers | Percentiles |     |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 44  | 3E    | 69/166 (42%)      | 68 (99%)     | 1 (1%)   | 59          | 70  |
| 44  | 3P    | 70/166 (42%)      | 70 (100%)    | 0        | 100         | 100 |
| 45  | 3F    | 94/98 (96%)       | 93 (99%)     | 1 (1%)   | 65          | 73  |
| 45  | 3Q    | 91/98 (93%)       | 91 (100%)    | 0        | 100         | 100 |
| 46  | 3G    | 72/73 (99%)       | 72 (100%)    | 0        | 100         | 100 |
| 46  | 3R    | 64/73 (88%)       | 64 (100%)    | 0        | 100         | 100 |
| 47  | 3H    | 63/72 (88%)       | 62 (98%)     | 1 (2%)   | 55          | 68  |
| 47  | 3S    | 63/72 (88%)       | 63 (100%)    | 0        | 100         | 100 |
| 48  | 3J    | 47/54 (87%)       | 47 (100%)    | 0        | 100         | 100 |
| 48  | 3U    | 50/54 (93%)       | 49 (98%)     | 1 (2%)   | 48          | 64  |
| 49  | 3K    | 41/46 (89%)       | 41 (100%)    | 0        | 100         | 100 |
| 49  | 3V    | 43/46 (94%)       | 43 (100%)    | 0        | 100         | 100 |
| 50  | 3T    | 41/58 (71%)       | 41 (100%)    | 0        | 100         | 100 |
| 51  | V1    | 343/366 (94%)     | 338 (98%)    | 5 (2%)   | 57          | 68  |
| 51  | v1    | 338/366 (92%)     | 338 (100%)   | 0        | 100         | 100 |
| 52  | V2    | 182/204 (89%)     | 181 (100%)   | 1 (0%)   | 81          | 80  |
| 52  | v2    | 170/204 (83%)     | 170 (100%)   | 0        | 100         | 100 |
| 53  | S1    | 579/602 (96%)     | 577 (100%)   | 2 (0%)   | 86          | 83  |
| 53  | s1    | 579/602 (96%)     | 577 (100%)   | 2 (0%)   | 86          | 83  |
| 54  | S7    | 131/185 (71%)     | 128 (98%)    | 3 (2%)   | 44          | 62  |
| 54  | s7    | 131/185 (71%)     | 130 (99%)    | 1 (1%)   | 73          | 76  |
| 55  | S8    | 145/178 (82%)     | 144 (99%)    | 1 (1%)   | 76          | 77  |
| 55  | s8    | 138/178 (78%)     | 137 (99%)    | 1 (1%)   | 76          | 77  |
| All | All   | 17545/19460 (90%) | 17455 (100%) | 90 (0%)  | 78          | 80  |

5 of 90 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | a1    | 38  | VAL  |
| 42  | 3N    | 183 | PHE  |
| 34  | b9    | 25  | ARG  |
| 43  | 3D    | 105 | LEU  |
| 51  | V1    | 233 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 213 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | ac    | 142 | GLN  |
| 40  | 3A    | 86  | ASN  |
| 51  | v1    | 303 | HIS  |
| 24  | c2    | 27  | ASN  |
| 33  | b4    | 86  | ASN  |

### 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 |
| 3   | 2MR  | s2    | 118 | 3    | 3,4,13       | 0.83 | 0        | 2,4,15      | 1.27 | 0        |
| 3   | 2MR  | S2    | 118 | 3    | 10,12,13     | 2.72 | 3 (30%)  | 5,13,15     | 7.36 | 4 (80%)  |

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 |
|-----|------|-------|-----|------|---------|------------|-------|
| 3   | 2MR  | s2    | 118 | 3    | -       | 1/1/2/15   | -     |
| 3   | 2MR  | S2    | 118 | 3    | -       | 4/10/13/15 | -     |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 3   | S2    | 118 | 2MR  | CZ-NE | 5.73 | 1.46        | 1.34     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | S2    | 118 | 2MR  | CZ-NH2  | 5.42  | 1.44        | 1.33     |
| 3   | S2    | 118 | 2MR  | CQ1-NH1 | -2.49 | 1.41        | 1.46     |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | S2    | 118 | 2MR  | NE-CZ-NH2  | 12.39 | 130.84      | 119.48   |
| 3   | S2    | 118 | 2MR  | CD-NE-CZ   | 10.13 | 142.39      | 123.36   |
| 3   | S2    | 118 | 2MR  | CQ2-NH2-CZ | 3.05  | 130.19      | 123.65   |
| 3   | S2    | 118 | 2MR  | CG-CD-NE   | -2.38 | 105.52      | 112.20   |

There are no chirality outliers.

All (5) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 3   | s2    | 118 | 2MR  | O-C-CA-CB   |
| 3   | S2    | 118 | 2MR  | CA-CB-CG-CD |
| 3   | S2    | 118 | 2MR  | C-CA-CB-CG  |
| 3   | S2    | 118 | 2MR  | N-CA-CB-CG  |
| 3   | S2    | 118 | 2MR  | NE-CD-CG-CB |

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | S2    | 118 | 2MR  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 4 are monoatomic - leaving 32 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 | $\# Z  > 2$ |
| 65  | FES  | V2    | 301 | 52    | 0,4,4        | -    | -           | -           |      |             |
| 64  | SF4  | v1    | 502 | 51    | 0,12,12      | -    | -           | -           |      |             |
| 58  | NDP  | a9    | 501 | 11,54 | 51,52,52     | 0.33 | 0           | 71,80,80    | 0.43 | 0           |
| 63  | FMN  | v1    | 501 | -     | 33,33,33     | 0.27 | 0           | 48,50,50    | 0.54 | 1 (2%)      |
| 64  | SF4  | S1    | 801 | 53    | 0,12,12      | -    | -           | -           |      |             |
| 60  | EHZ  | 5a    | 701 | 7     | 31,36,37     | 0.25 | 0           | 36,44,47    | 1.14 | 1 (2%)      |
| 61  | HEM  | 3N    | 402 | 42    | 50,50,50     | 1.37 | 7 (14%)     | 67,82,82    | 1.60 | 15 (22%)    |
| 64  | SF4  | S8    | 302 | 55    | 0,12,12      | -    | -           | -           |      |             |
| 61  | HEM  | 3N    | 401 | 42    | 50,50,50     | 1.31 | 6 (12%)     | 67,82,82    | 1.61 | 12 (17%)    |
| 57  | DGT  | al    | 502 | -     | 32,33,33     | 0.57 | 0           | 48,52,52    | 0.59 | 0           |
| 62  | HEC  | 3O    | 401 | 43    | 50,50,50     | 1.31 | 6 (12%)     | 68,82,82    | 1.51 | 14 (20%)    |
| 64  | SF4  | S1    | 802 | 53    | 0,12,12      | -    | -           | -           |      |             |
| 60  | EHZ  | A6    | 201 | -     | 31,36,37     | 0.20 | 0           | 36,44,47    | 1.26 | 1 (2%)      |
| 65  | FES  | s1    | 803 | 53    | 0,4,4        | -    | -           | -           |      |             |
| 65  | FES  | S1    | 803 | 53    | 0,4,4        | -    | -           | -           |      |             |
| 64  | SF4  | S7    | 301 | 54,3  | 0,12,12      | -    | -           | -           |      |             |
| 58  | NDP  | A9    | 501 | -     | 51,52,52     | 0.32 | 0           | 71,80,80    | 0.42 | 0           |
| 65  | FES  | v2    | 301 | 52    | 0,4,4        | -    | -           | -           |      |             |
| 64  | SF4  | s8    | 302 | 55    | 0,12,12      | -    | -           | -           |      |             |
| 63  | FMN  | V1    | 501 | 51    | 33,33,33     | 0.30 | 0           | 48,50,50    | 0.48 | 0           |
| 64  | SF4  | s1    | 801 | 53    | 0,12,12      | -    | -           | -           |      |             |
| 62  | HEC  | 3D    | 401 | 43    | 50,50,50     | 1.45 | 9 (18%)     | 68,82,82    | 1.77 | 18 (26%)    |
| 61  | HEM  | 3C    | 401 | 42    | 50,50,50     | 1.31 | 8 (16%)     | 67,82,82    | 1.62 | 12 (17%)    |
| 57  | DGT  | AL    | 502 | 56    | 32,33,33     | 0.57 | 0           | 48,52,52    | 0.58 | 0           |
| 64  | SF4  | s8    | 301 | 55    | 0,12,12      | -    | -           | -           |      |             |
| 64  | SF4  | S8    | 301 | 55    | 0,12,12      | -    | -           | -           |      |             |
| 64  | SF4  | V1    | 502 | 51    | 0,12,12      | -    | -           | -           |      |             |
| 64  | SF4  | s7    | 301 | 54    | 0,12,12      | -    | -           | -           |      |             |
| 60  | EHZ  | B9    | 201 | -     | 31,36,37     | 0.20 | 0           | 36,44,47    | 1.04 | 1 (2%)      |
| 61  | HEM  | 3C    | 402 | 42    | 50,50,50     | 1.34 | 6 (12%)     | 67,82,82    | 1.62 | 16 (23%)    |
| 64  | SF4  | s1    | 802 | 53    | 0,12,12      | -    | -           | -           |      |             |
| 60  | EHZ  | a6    | 201 | -     | 31,36,37     | 0.19 | 0           | 36,44,47    | 1.25 | 1 (2%)      |

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   |
|-----|------|-------|-----|-------|---------|-------------|---------|
| 65  | FES  | V2    | 301 | 52    | -       | -           | 0/1/1/1 |
| 64  | SF4  | v1    | 502 | 51    | -       | -           | 0/6/5/5 |
| 58  | NDP  | a9    | 501 | 11,54 | -       | 10/34/77/77 | 0/5/5/5 |
| 63  | FMN  | v1    | 501 | -     | -       | 4/18/18/18  | 0/3/3/3 |
| 64  | SF4  | S1    | 801 | 53    | -       | -           | 0/6/5/5 |
| 60  | EHZ  | 5a    | 701 | 7     | -       | 4/42/44/45  | -       |
| 61  | HEM  | 3N    | 402 | 42    | -       | 7/14/54/54  | -       |
| 64  | SF4  | S8    | 302 | 55    | -       | -           | 0/6/5/5 |
| 61  | HEM  | 3N    | 401 | 42    | -       | 9/14/54/54  | -       |
| 57  | DGT  | al    | 502 | -     | -       | 2/22/34/34  | 0/3/3/3 |
| 62  | HEC  | 3O    | 401 | 43    | 1/1/3/7 | 5/14/54/54  | -       |
| 64  | SF4  | S1    | 802 | 53    | -       | -           | 0/6/5/5 |
| 60  | EHZ  | A6    | 201 | -     | -       | 3/42/44/45  | -       |
| 65  | FES  | s1    | 803 | 53    | -       | -           | 0/1/1/1 |
| 65  | FES  | S1    | 803 | 53    | -       | -           | 0/1/1/1 |
| 64  | SF4  | S7    | 301 | 54,3  | -       | -           | 0/6/5/5 |
| 58  | NDP  | A9    | 501 | -     | -       | 9/34/77/77  | 0/5/5/5 |
| 65  | FES  | v2    | 301 | 52    | -       | -           | 0/1/1/1 |
| 64  | SF4  | s8    | 302 | 55    | -       | -           | 0/6/5/5 |
| 63  | FMN  | V1    | 501 | 51    | -       | 5/18/18/18  | 0/3/3/3 |
| 64  | SF4  | s1    | 801 | 53    | -       | -           | 0/6/5/5 |
| 61  | HEM  | 3C    | 401 | 42    | -       | 9/14/54/54  | -       |
| 62  | HEC  | 3D    | 401 | 43    | 1/1/3/7 | 7/14/54/54  | -       |
| 57  | DGT  | AL    | 502 | 56    | -       | 1/22/34/34  | 0/3/3/3 |
| 64  | SF4  | s8    | 301 | 55    | -       | -           | 0/6/5/5 |
| 64  | SF4  | S8    | 301 | 55    | -       | -           | 0/6/5/5 |
| 64  | SF4  | V1    | 502 | 51    | -       | -           | 0/6/5/5 |
| 64  | SF4  | s7    | 301 | 54    | -       | -           | 0/6/5/5 |
| 60  | EHZ  | B9    | 201 | -     | -       | 8/42/44/45  | -       |
| 61  | HEM  | 3C    | 402 | 42    | -       | 7/14/54/54  | -       |
| 64  | SF4  | s1    | 802 | 53    | -       | -           | 0/6/5/5 |
| 60  | EHZ  | a6    | 201 | -     | -       | 10/42/44/45 | -       |

The worst 5 of 42 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 61  | 3C    | 402 | HEM  | C4D-ND | -3.81 | 1.33        | 1.40     |
| 61  | 3N    | 402 | HEM  | C4D-ND | -3.62 | 1.34        | 1.40     |
| 61  | 3N    | 401 | HEM  | C4D-ND | -3.58 | 1.34        | 1.40     |
| 61  | 3C    | 401 | HEM  | C4D-ND | -3.43 | 1.34        | 1.40     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 61  | 3C    | 401 | HEM  | C1B-NB | -3.43 | 1.34        | 1.40     |

The worst 5 of 92 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 60  | a6    | 201 | EHZ  | C10-S1-C9  | 7.12 | 122.89      | 101.84   |
| 60  | A6    | 201 | EHZ  | C10-S1-C9  | 6.83 | 122.02      | 101.84   |
| 60  | 5a    | 701 | EHZ  | C10-S1-C9  | 6.03 | 119.67      | 101.84   |
| 60  | B9    | 201 | EHZ  | C10-S1-C9  | 5.84 | 119.11      | 101.84   |
| 61  | 3N    | 401 | HEM  | CHC-C4B-NB | 4.69 | 129.47      | 124.42   |

All (2) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 62  | 3D    | 401 | HEC  | NA   |
| 62  | 3O    | 401 | HEC  | NA   |

5 of 100 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 57  | al    | 502 | DGT  | PB-O3A-PA-O5'   |
| 58  | A9    | 501 | NDP  | C5B-O5B-PA-O3   |
| 58  | A9    | 501 | NDP  | C2N-C3N-C7N-O7N |
| 58  | A9    | 501 | NDP  | C2N-C3N-C7N-N7N |
| 58  | a9    | 501 | NDP  | C5D-O5D-PN-O3   |

There are no ring outliers.

22 monomers are involved in 32 short contacts:

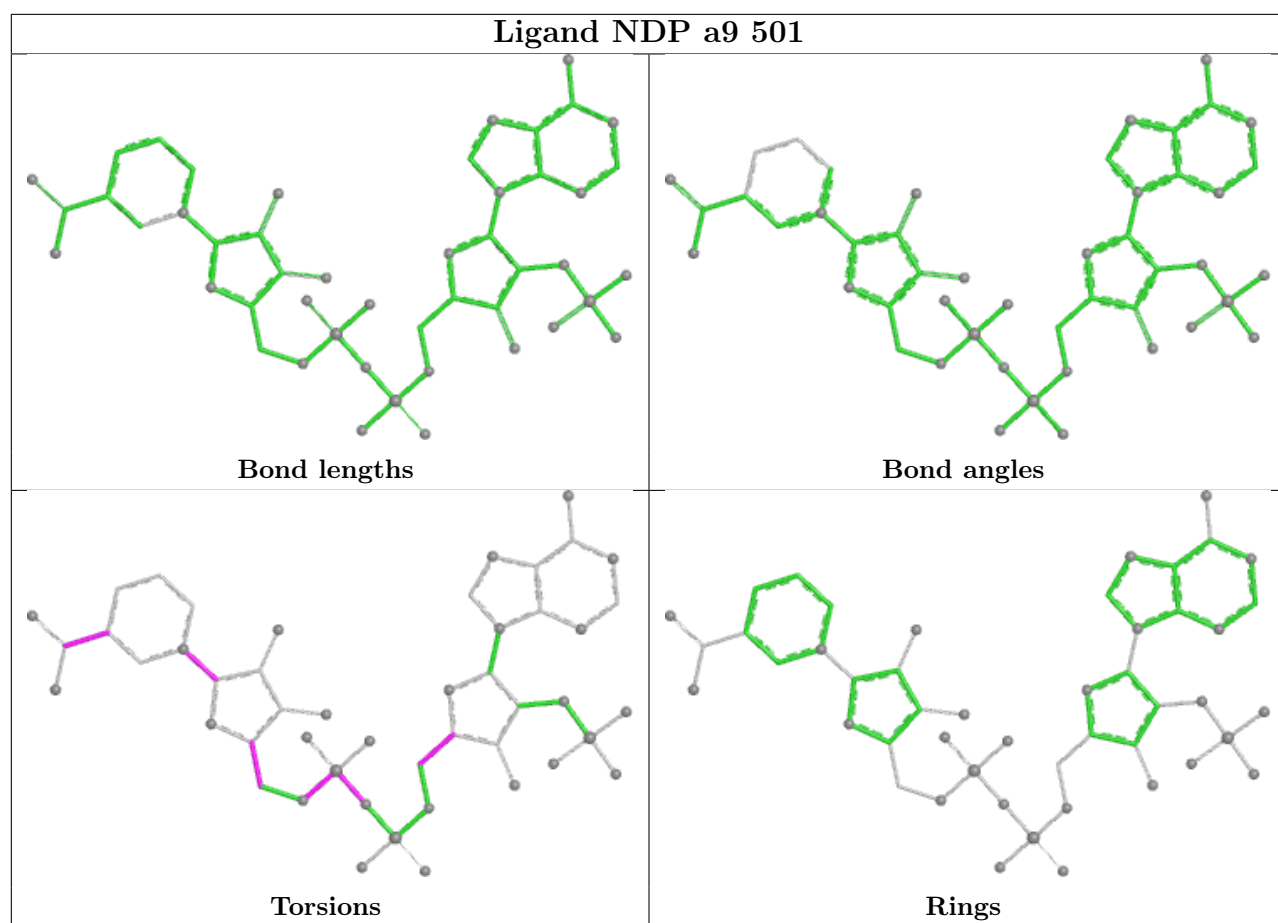
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 65  | V2    | 301 | FES  | 1       | 0            |
| 64  | v1    | 502 | SF4  | 1       | 0            |
| 58  | a9    | 501 | NDP  | 1       | 0            |
| 64  | S1    | 801 | SF4  | 1       | 0            |
| 61  | 3N    | 402 | HEM  | 1       | 0            |
| 61  | 3N    | 401 | HEM  | 1       | 0            |
| 62  | 3O    | 401 | HEC  | 2       | 0            |
| 65  | s1    | 803 | FES  | 1       | 0            |
| 65  | S1    | 803 | FES  | 1       | 0            |
| 64  | S7    | 301 | SF4  | 3       | 0            |
| 58  | A9    | 501 | NDP  | 3       | 0            |

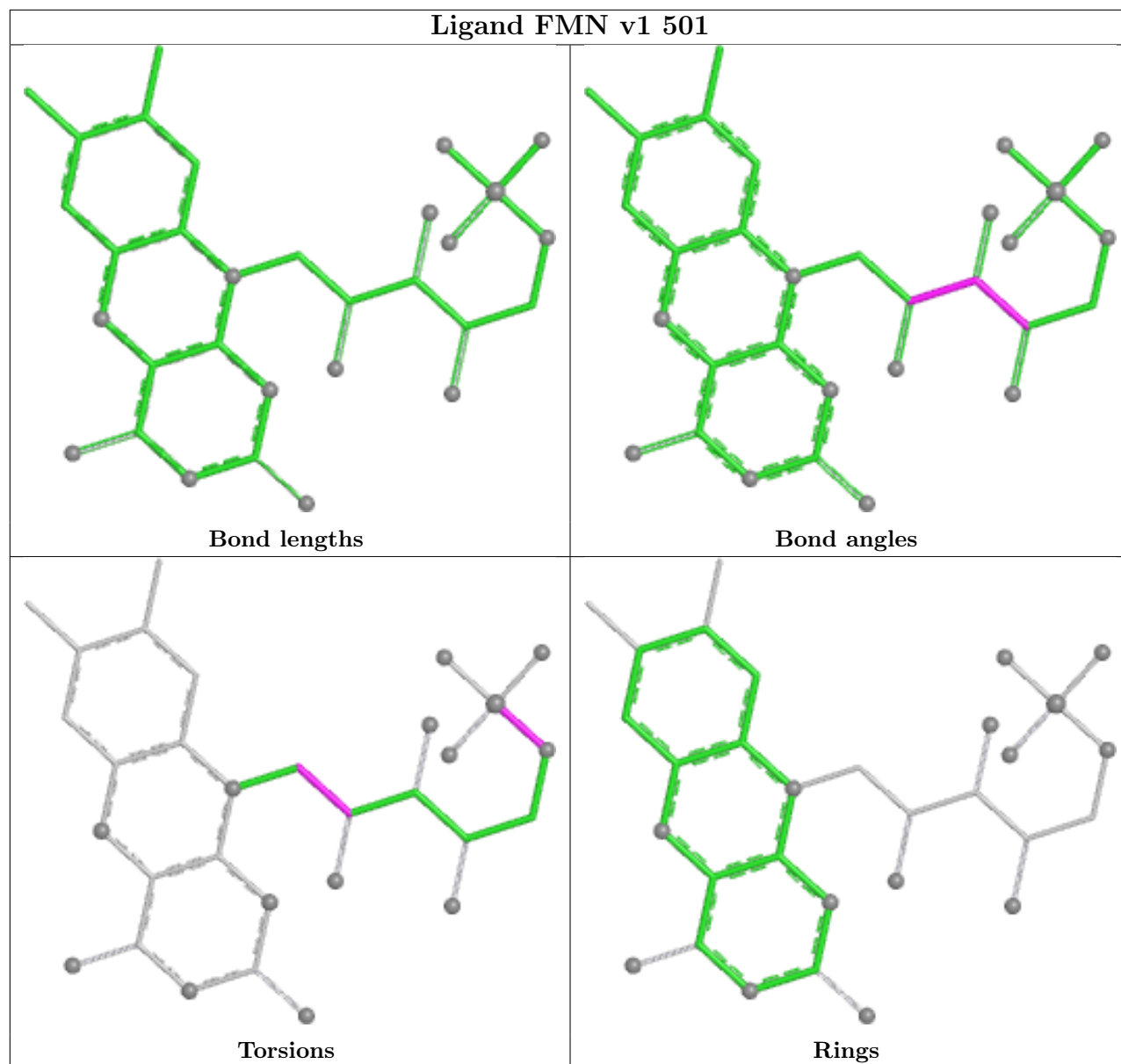
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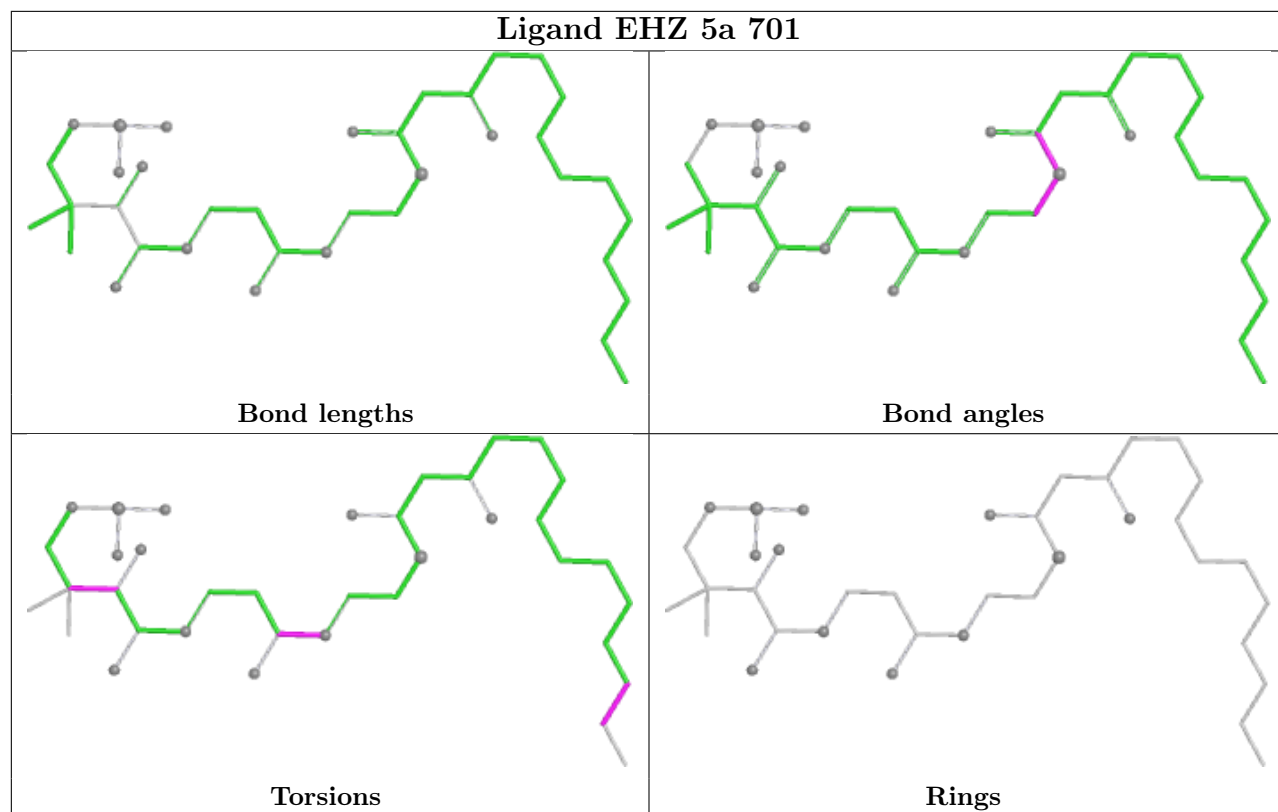
*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 65  | v2    | 301 | FES  | 1       | 0            |
| 63  | V1    | 501 | FMN  | 2       | 0            |
| 64  | s1    | 801 | SF4  | 1       | 0            |
| 62  | 3D    | 401 | HEC  | 3       | 0            |
| 61  | 3C    | 401 | HEM  | 1       | 0            |
| 57  | AL    | 502 | DGT  | 1       | 0            |
| 64  | s8    | 301 | SF4  | 2       | 0            |
| 64  | S8    | 301 | SF4  | 1       | 0            |
| 64  | V1    | 502 | SF4  | 1       | 0            |
| 64  | s7    | 301 | SF4  | 2       | 0            |
| 60  | B9    | 201 | EHZ  | 1       | 0            |

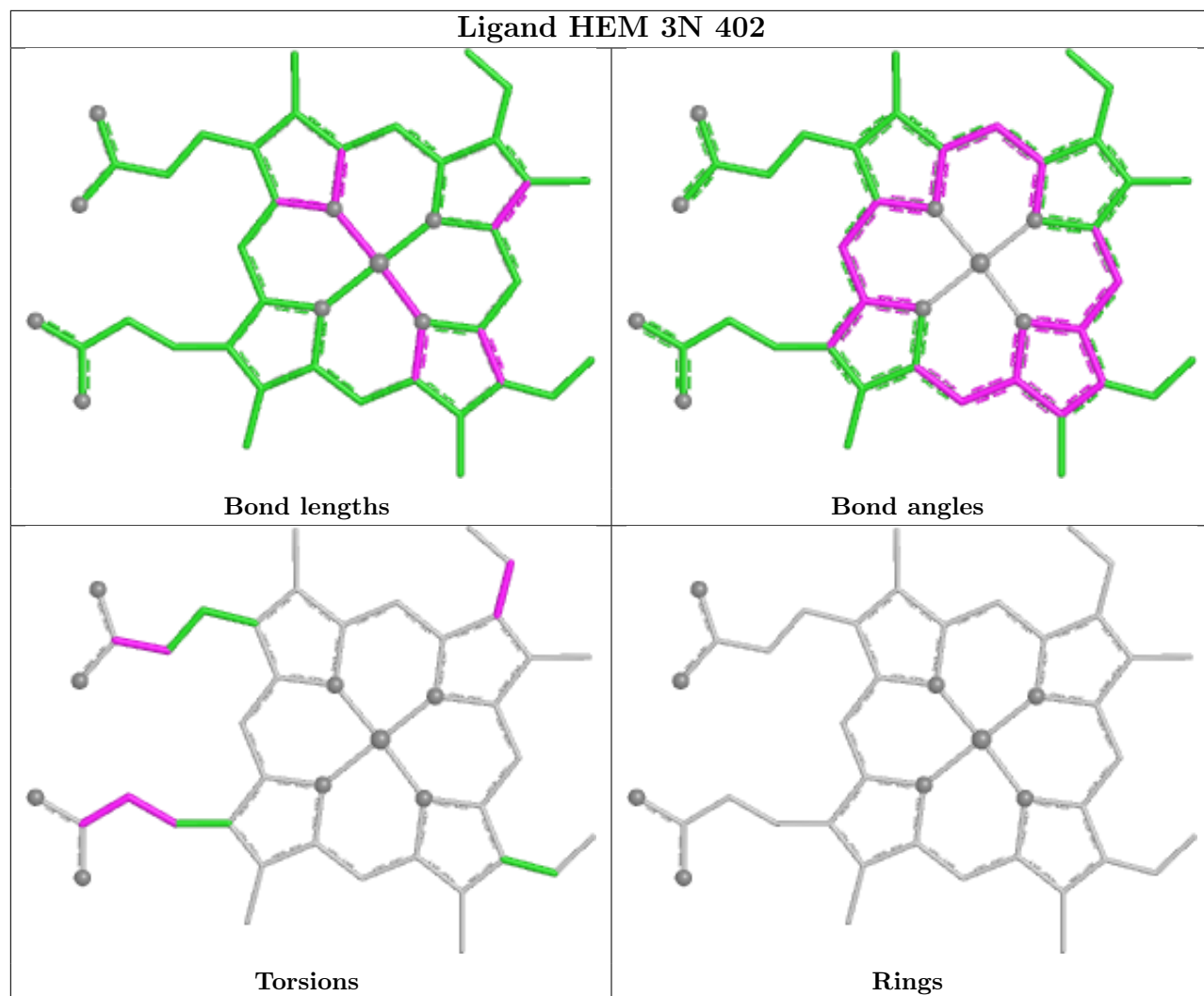
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



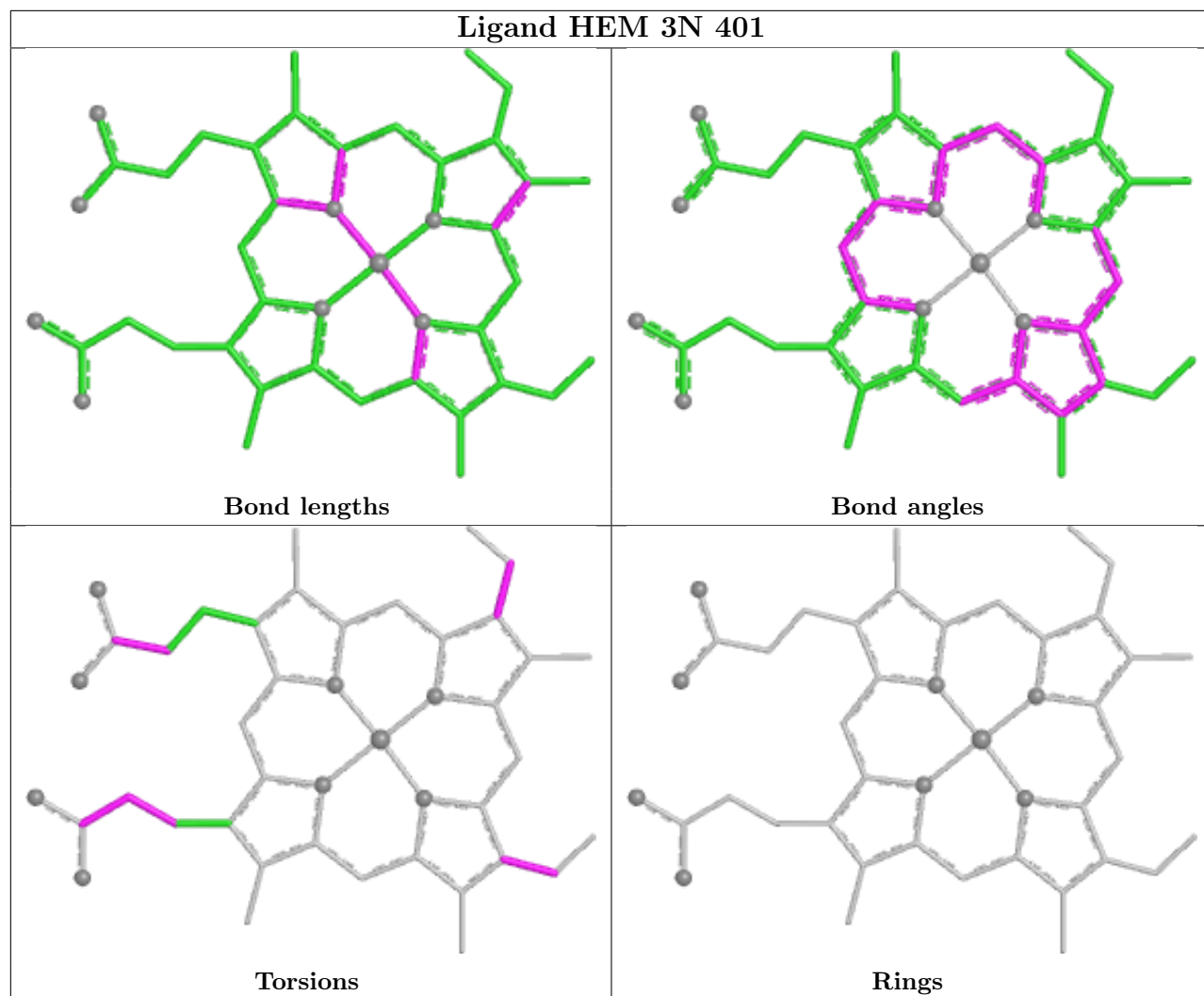


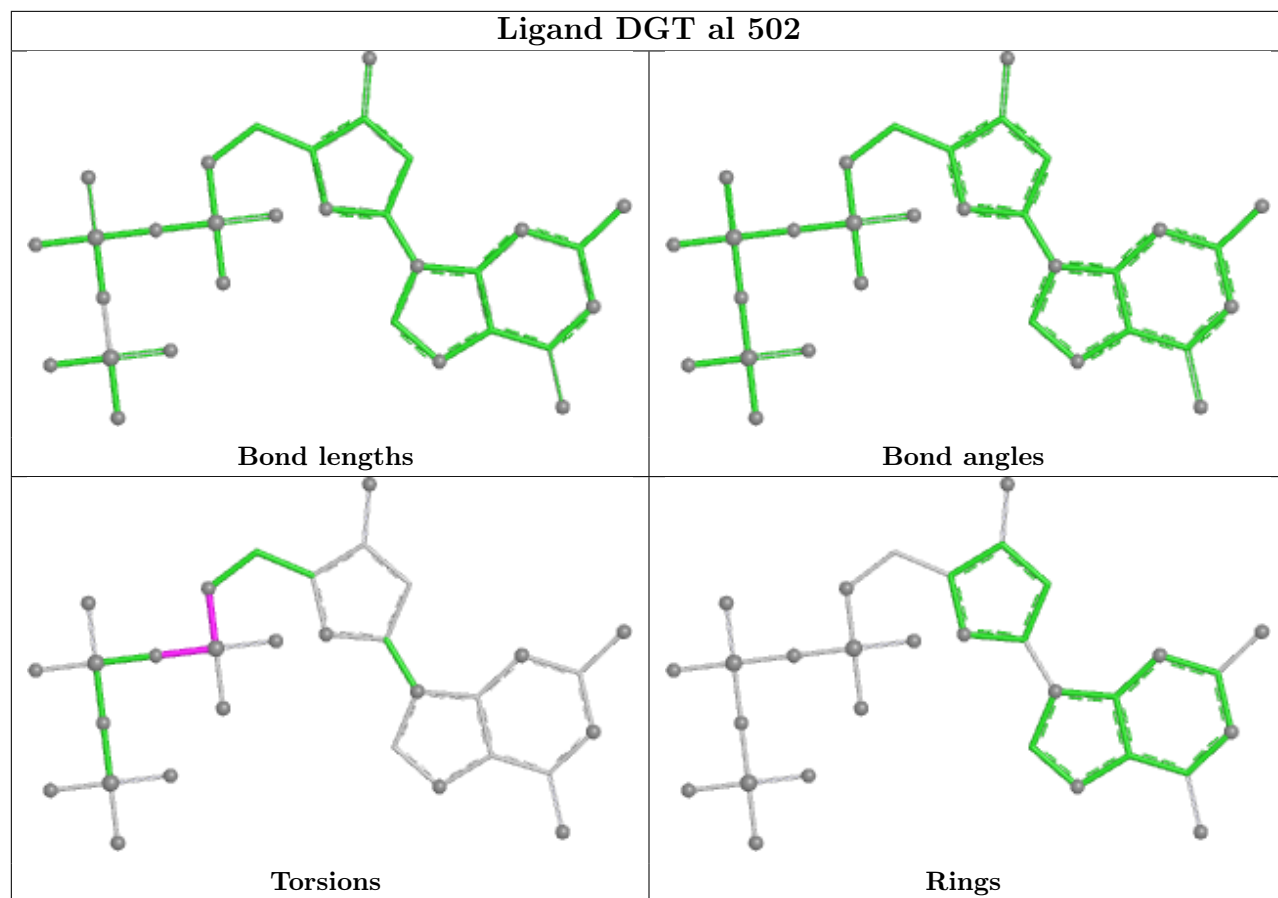


## Ligand HEM 3N 402

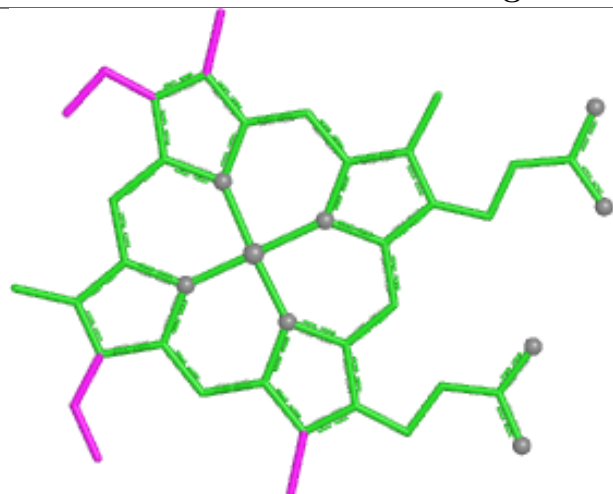


## Ligand HEM 3N 401

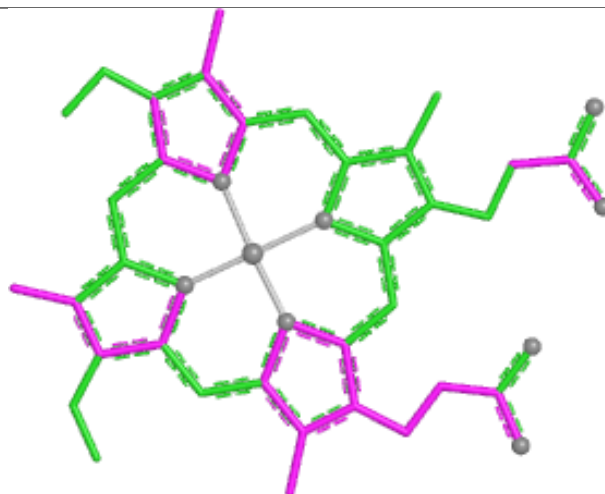




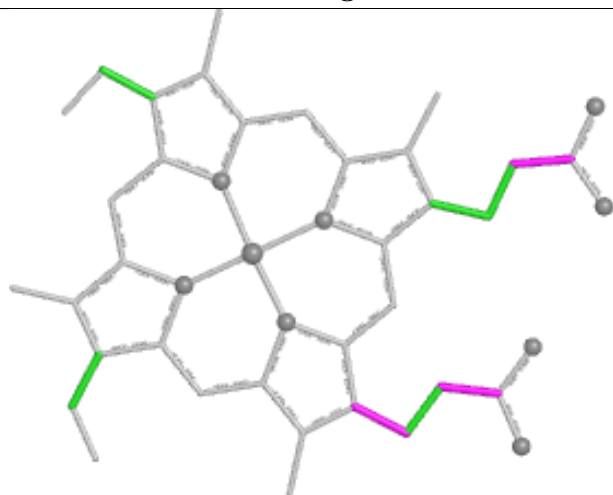
## Ligand HEC 3O 401



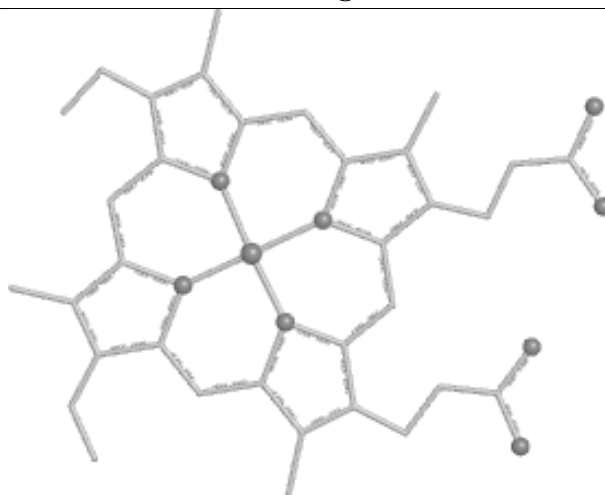
Bond lengths



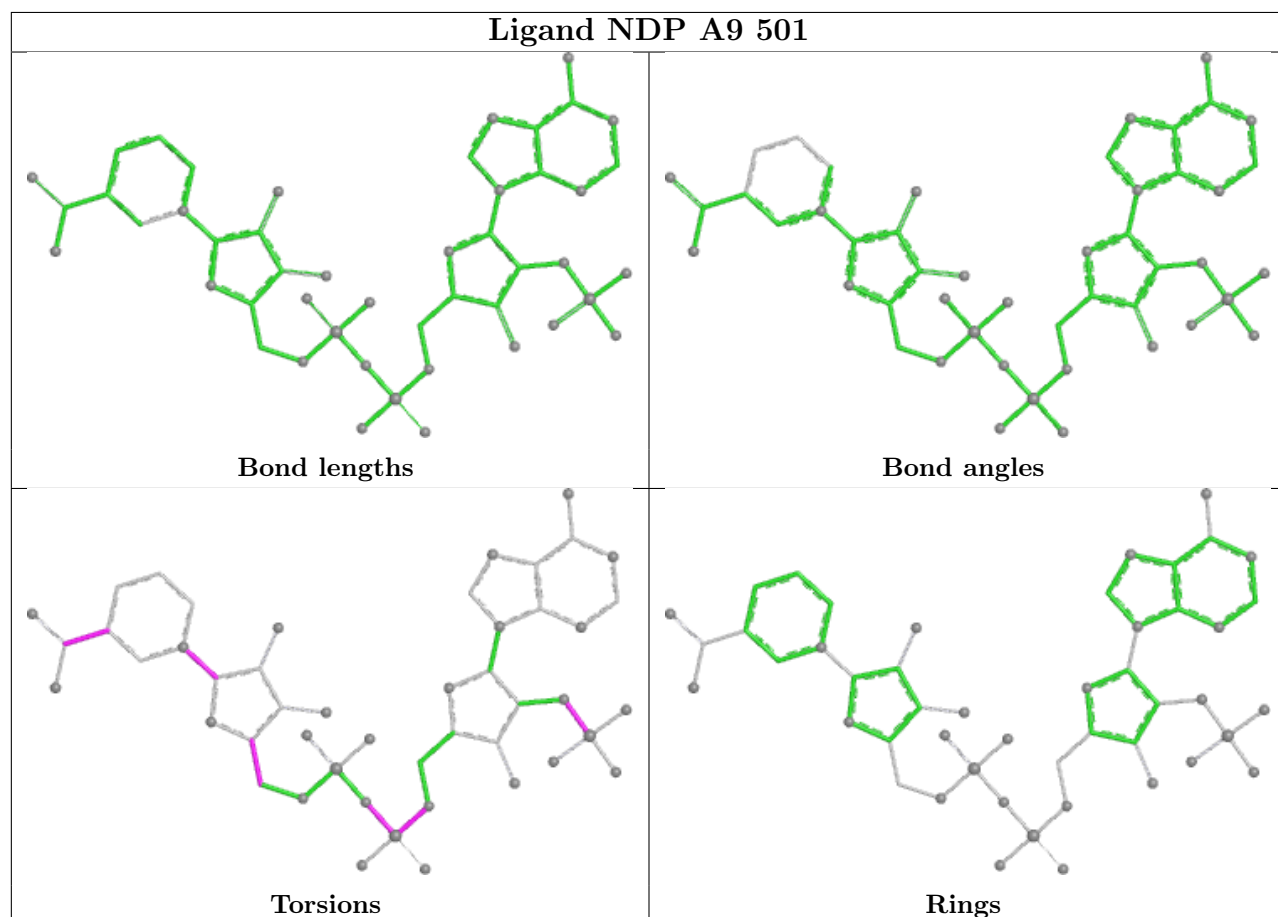
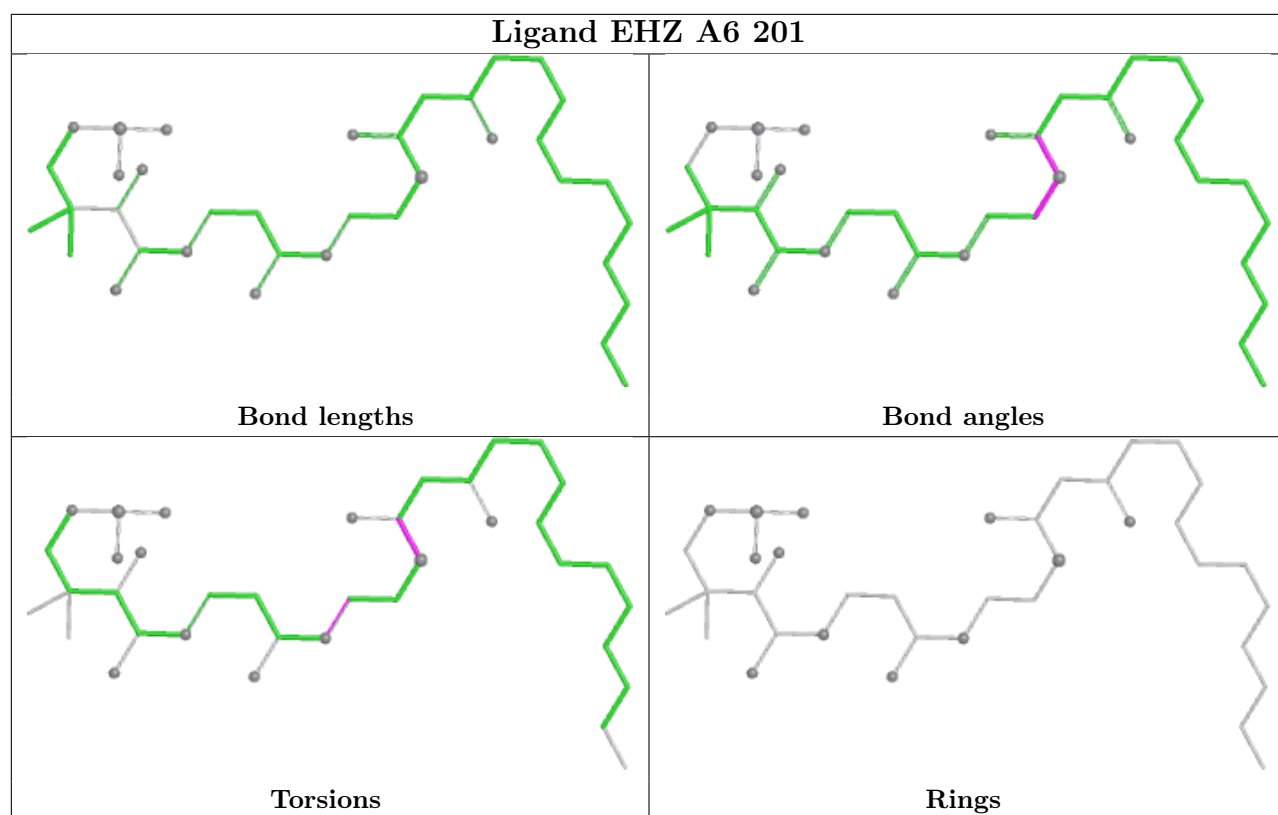
Bond angles



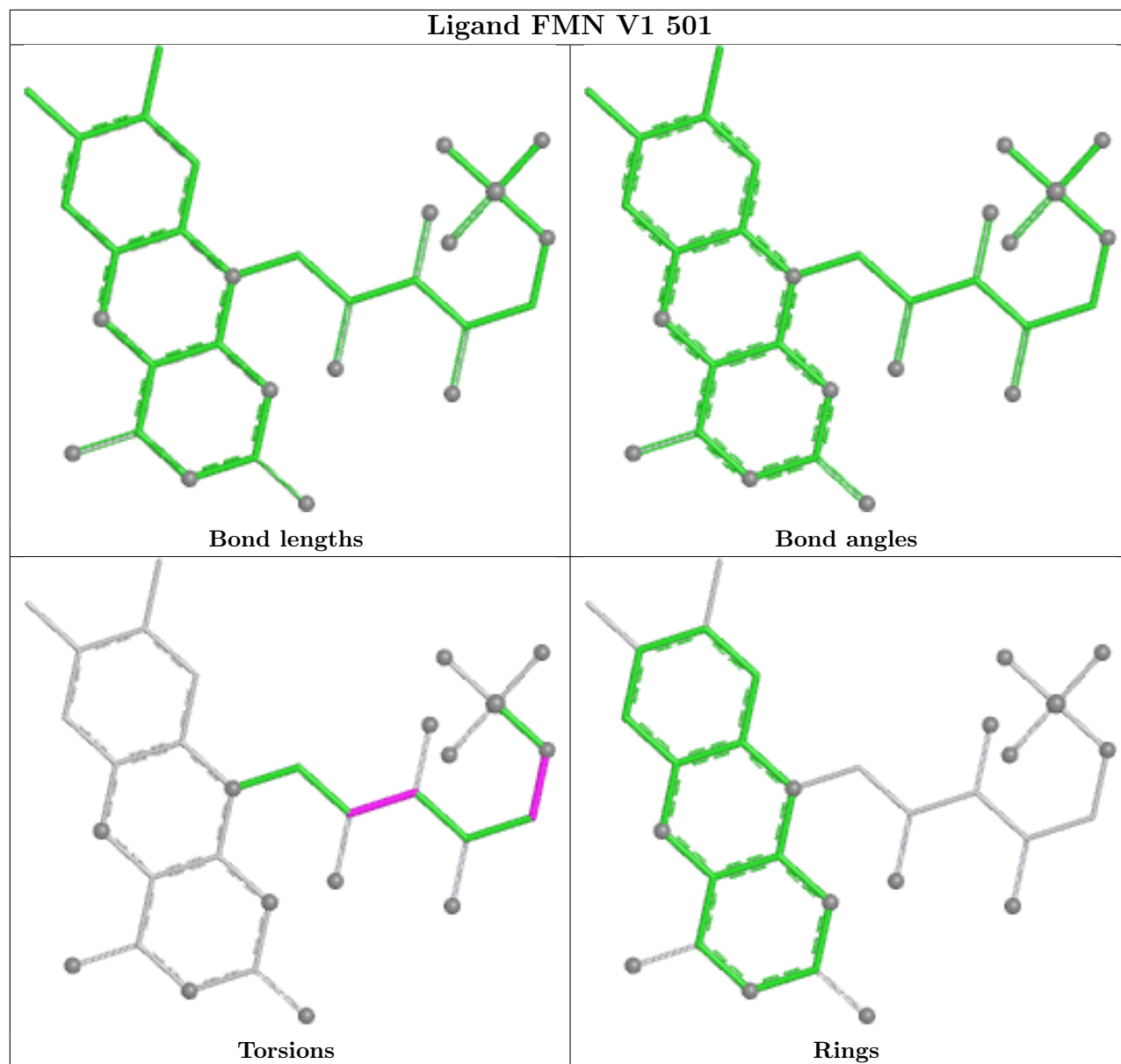
Torsions



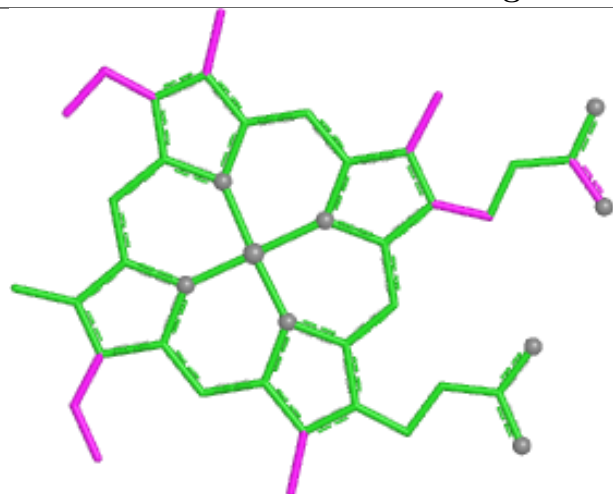
Rings



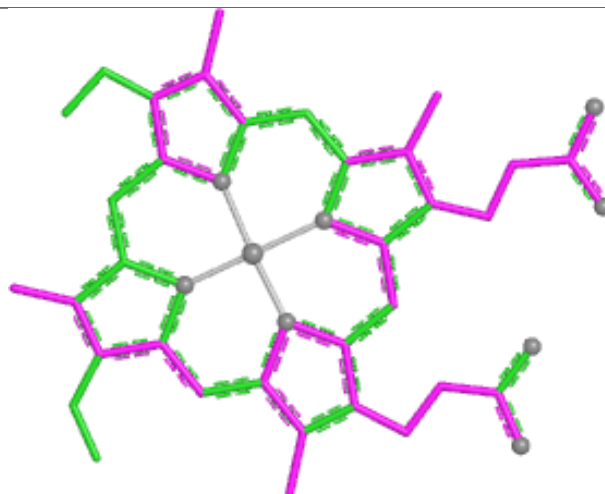
## Ligand FMN V1 501



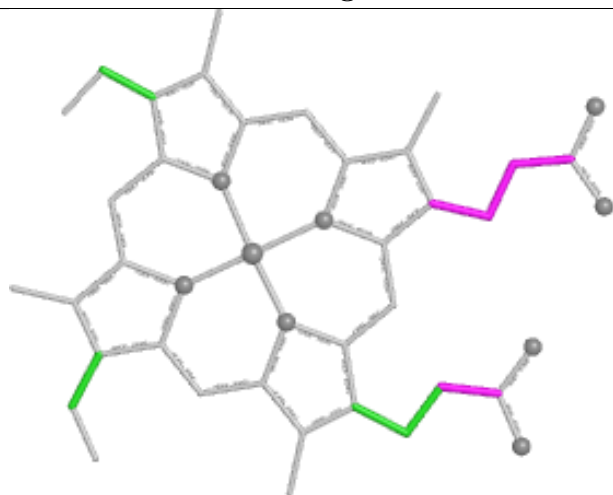
## Ligand HEC 3D 401



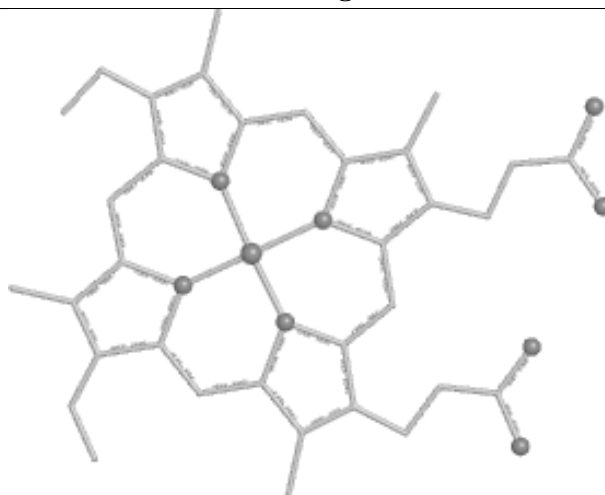
Bond lengths



Bond angles

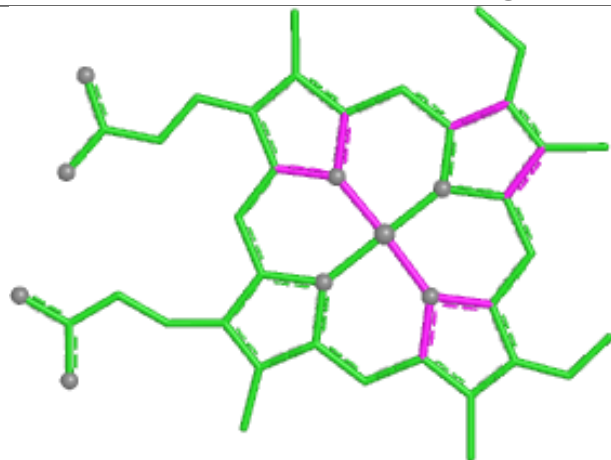


Torsions

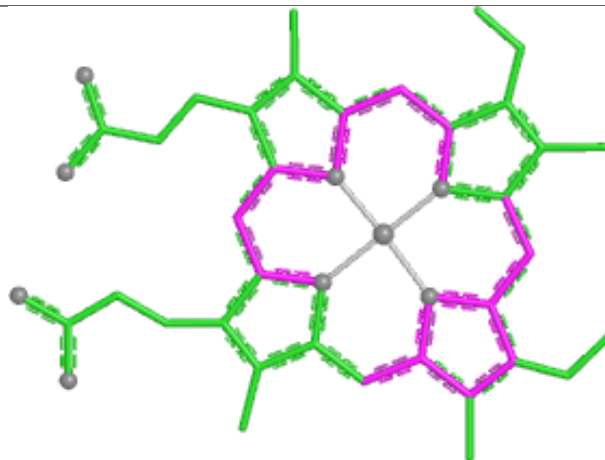


Rings

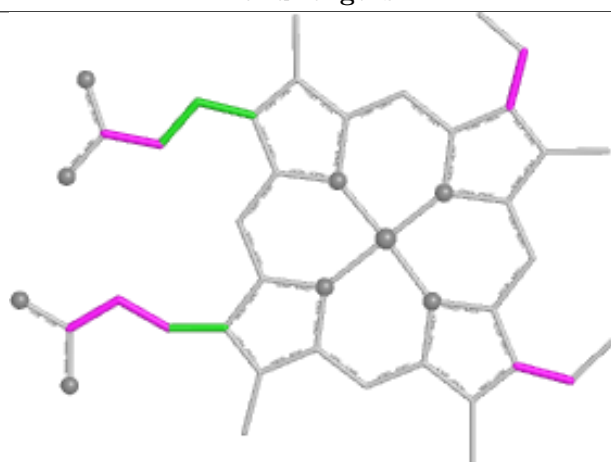
## Ligand HEM 3C 401



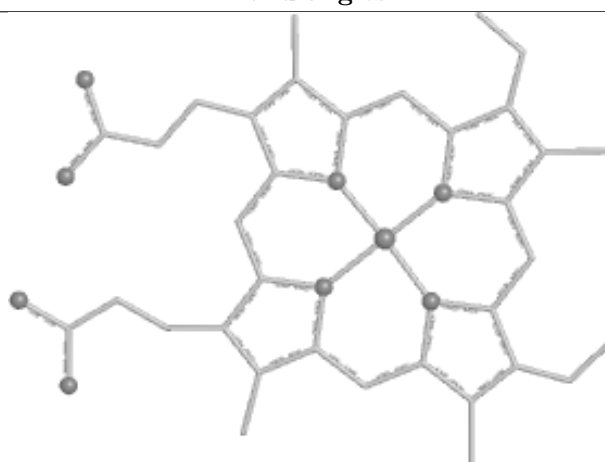
Bond lengths



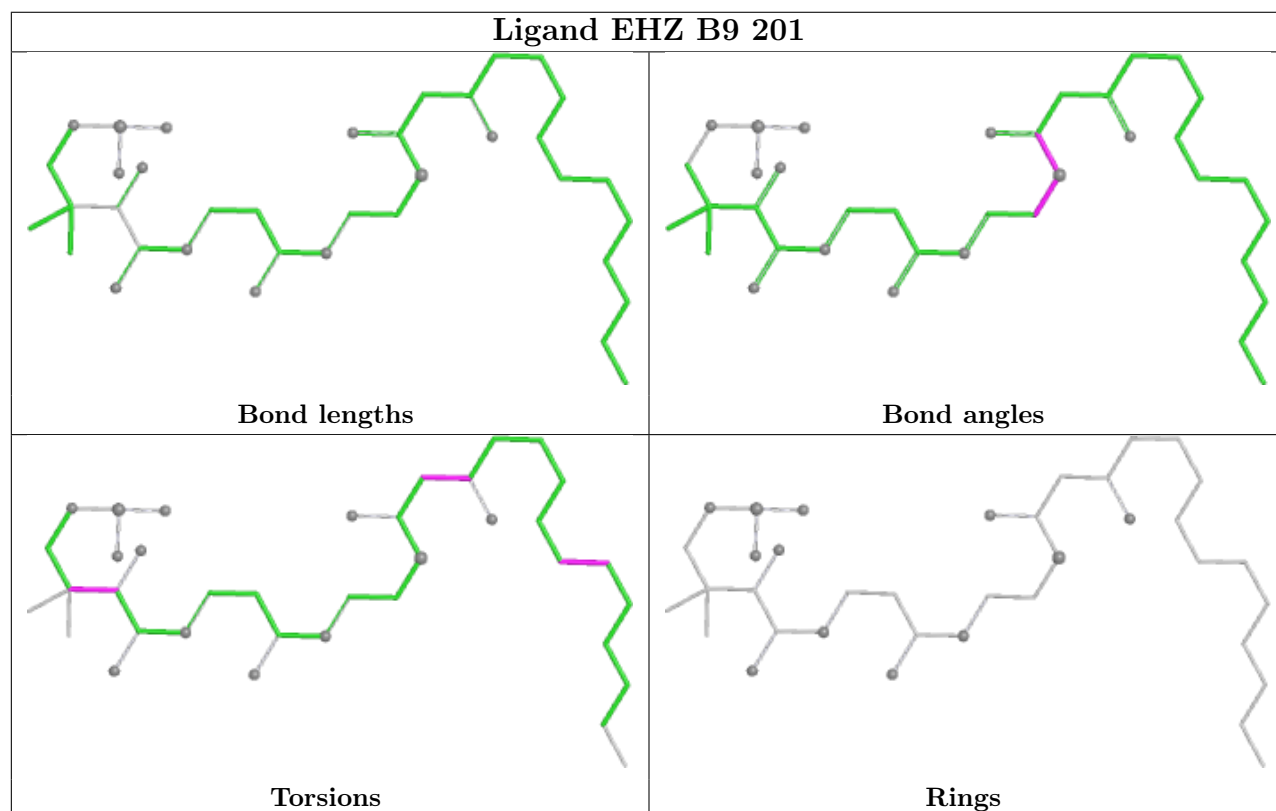
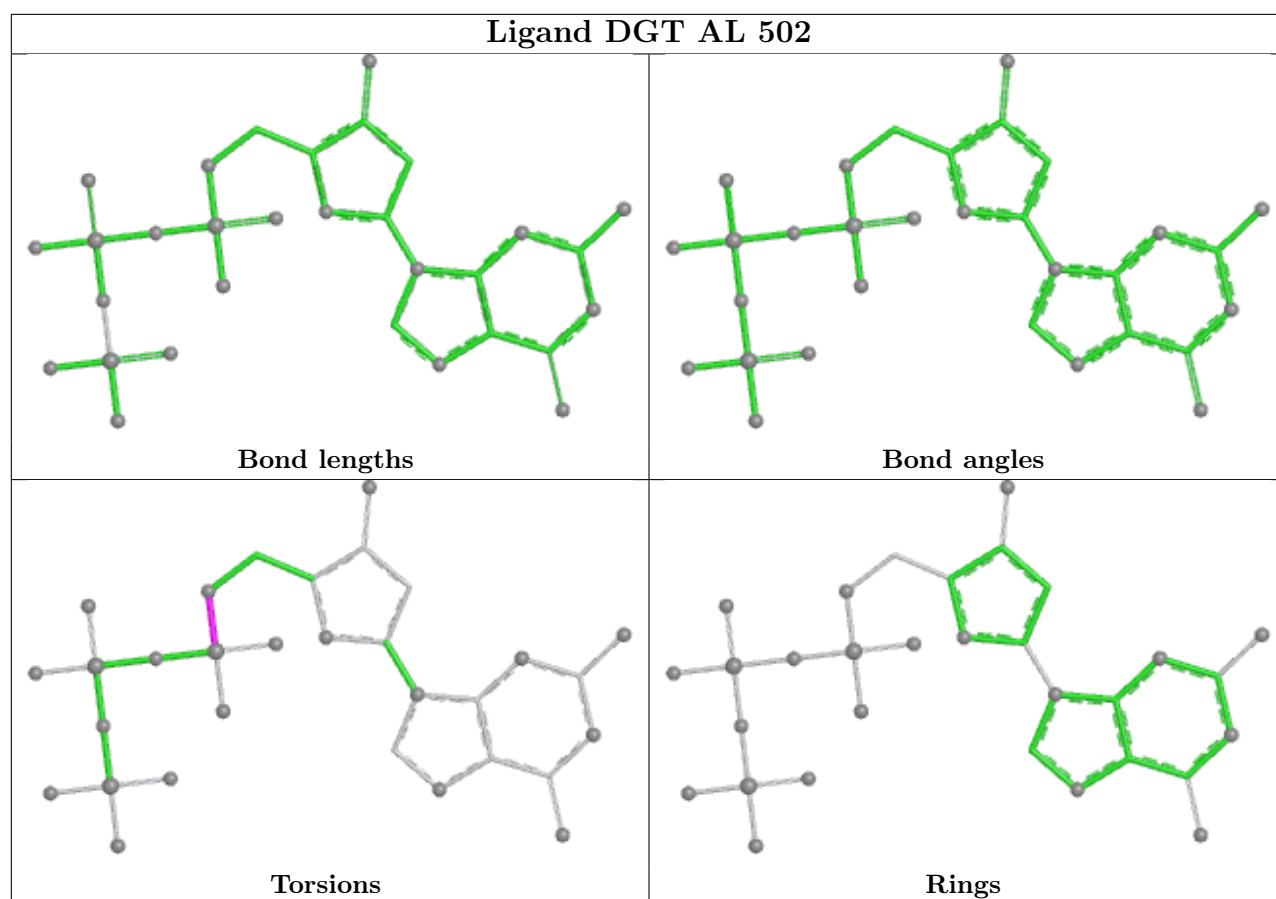
Bond angles



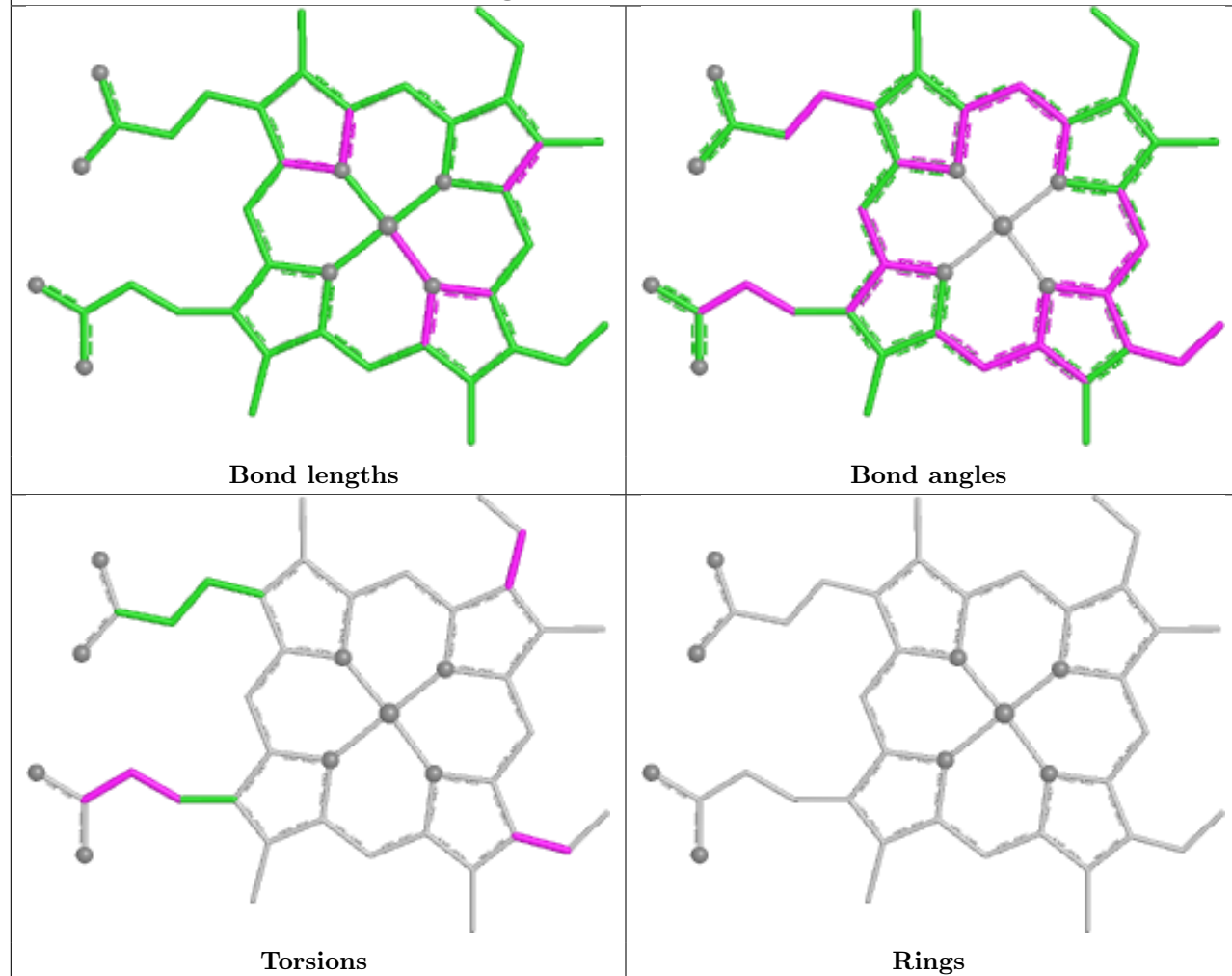
Torsions

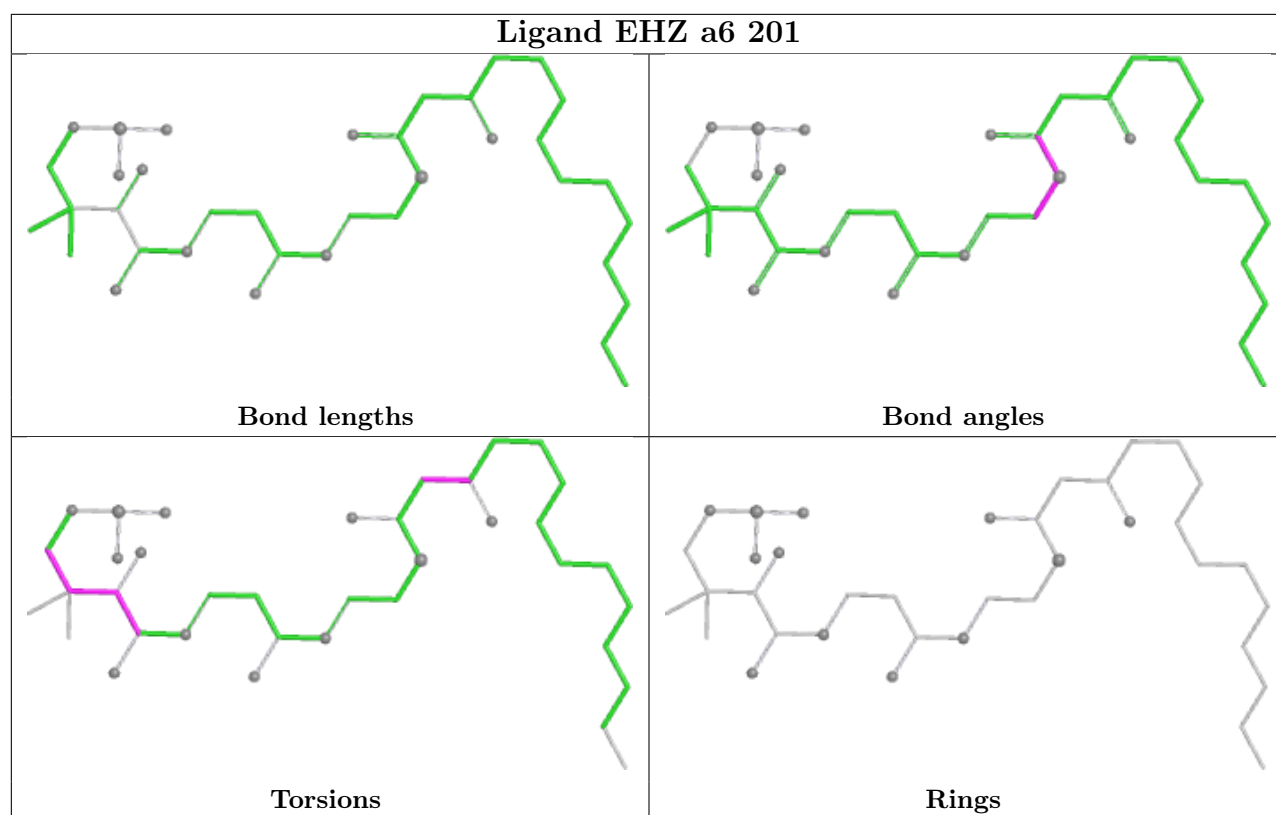


Rings



## Ligand HEM 3C 402





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

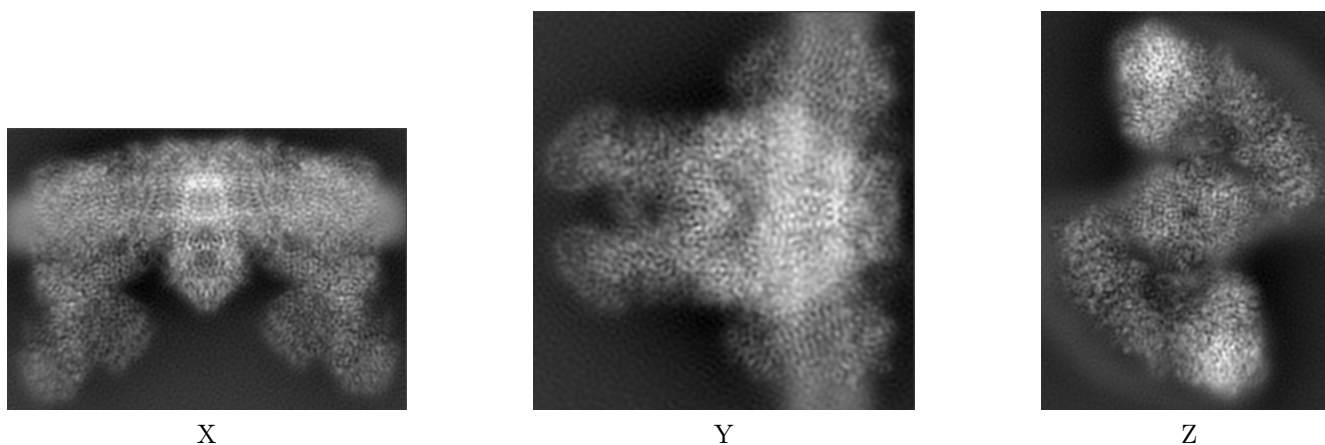
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42122. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

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

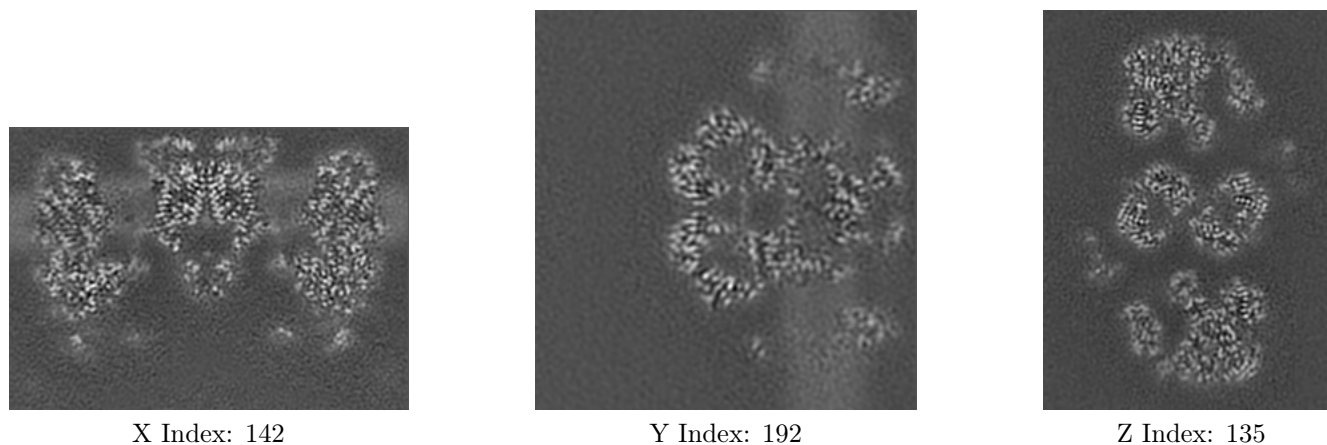
#### 6.1.1 Primary map



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

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

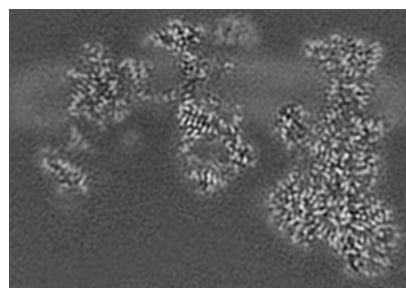
#### 6.2.1 Primary map



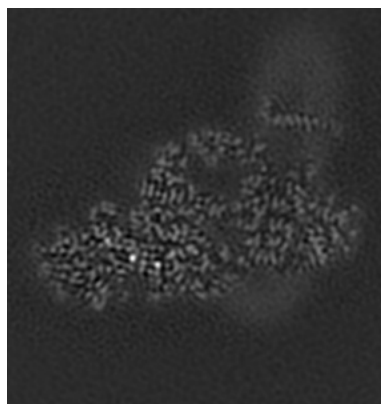
The images above show central slices of the map in three orthogonal directions.

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

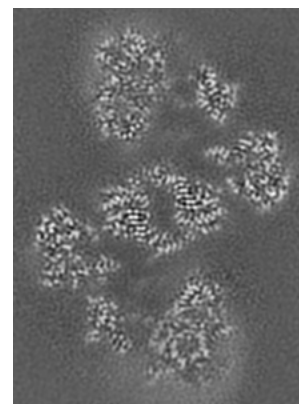
### 6.3.1 Primary map



X Index: 114



Y Index: 323

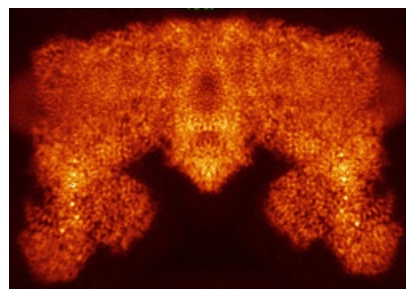


Z Index: 159

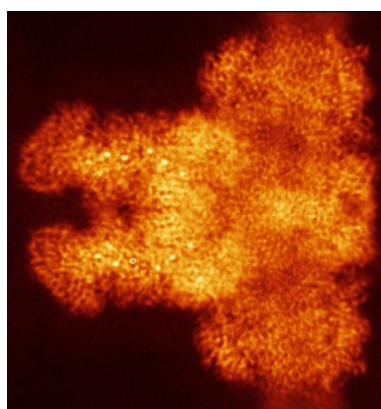
The images above show the largest variance slices of the map in three orthogonal directions.

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

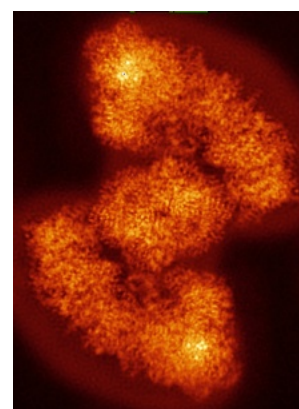
### 6.4.1 Primary map



X



Y

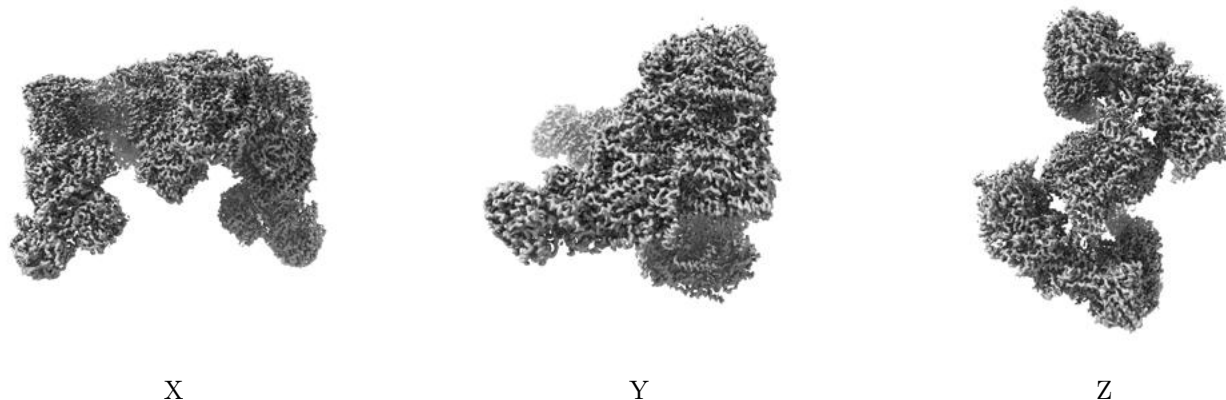


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

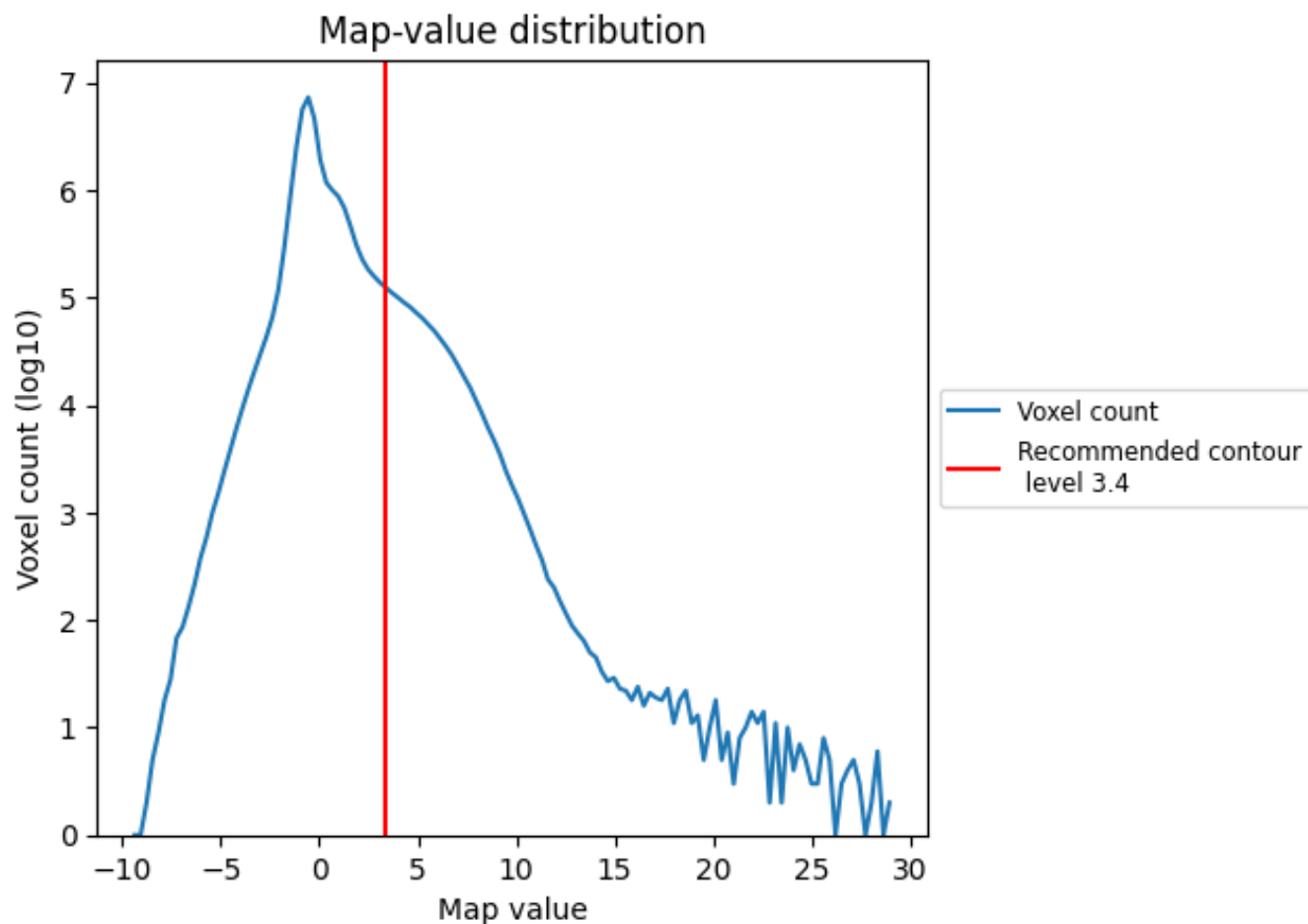
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

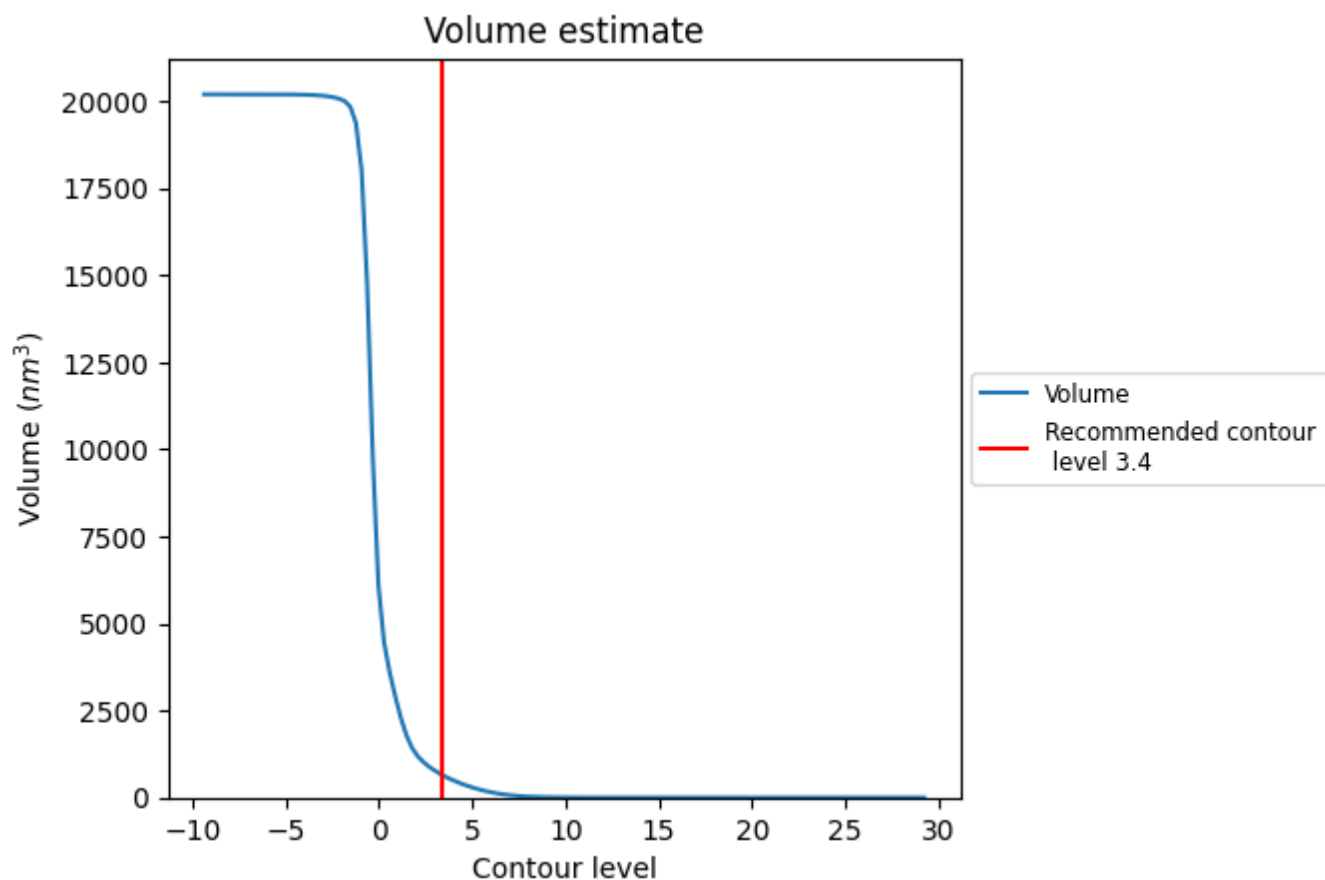
This section contains the results of statistical analysis of the map.

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



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

## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 650 nm<sup>3</sup>; this corresponds to an approximate mass of 587 kDa.

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

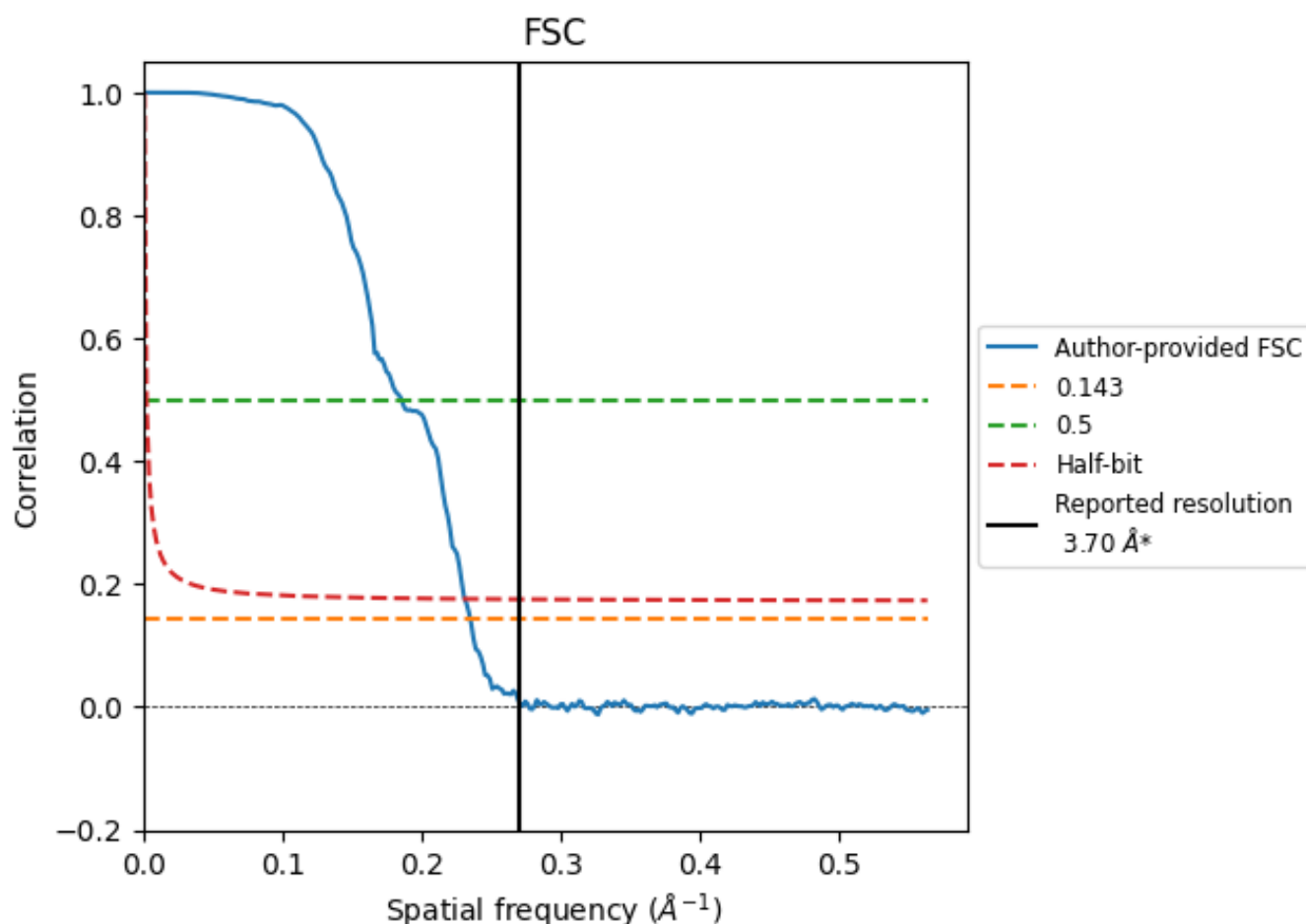
## 7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.270 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

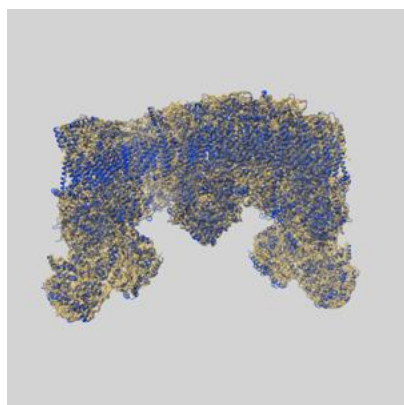
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.70                               | -    | -        |
| Author-provided FSC curve | 4.25                               | 5.39 | 4.32     |
| Unmasked-calculated*      | -                                  | -    | -        |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.25 differs from the reported value 3.7 by more than 10 %

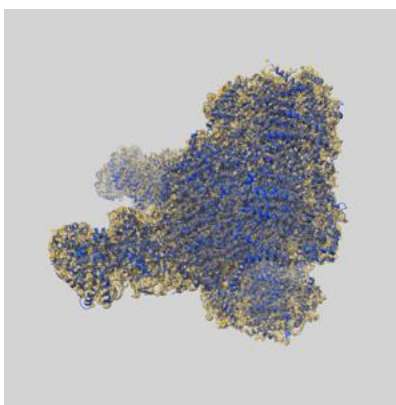
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42122 and PDB model 8UCA. Per-residue inclusion information can be found in section [3](#) on page [26](#).

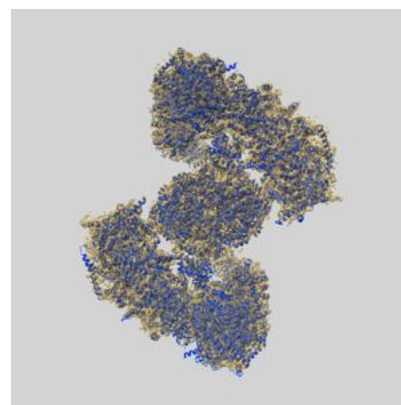
### 9.1 Map-model overlay [i](#)



X



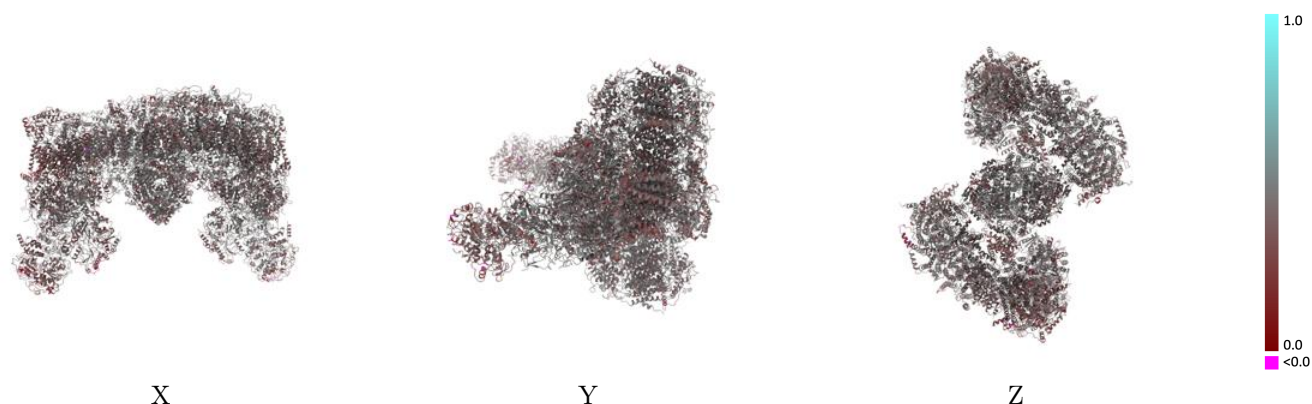
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



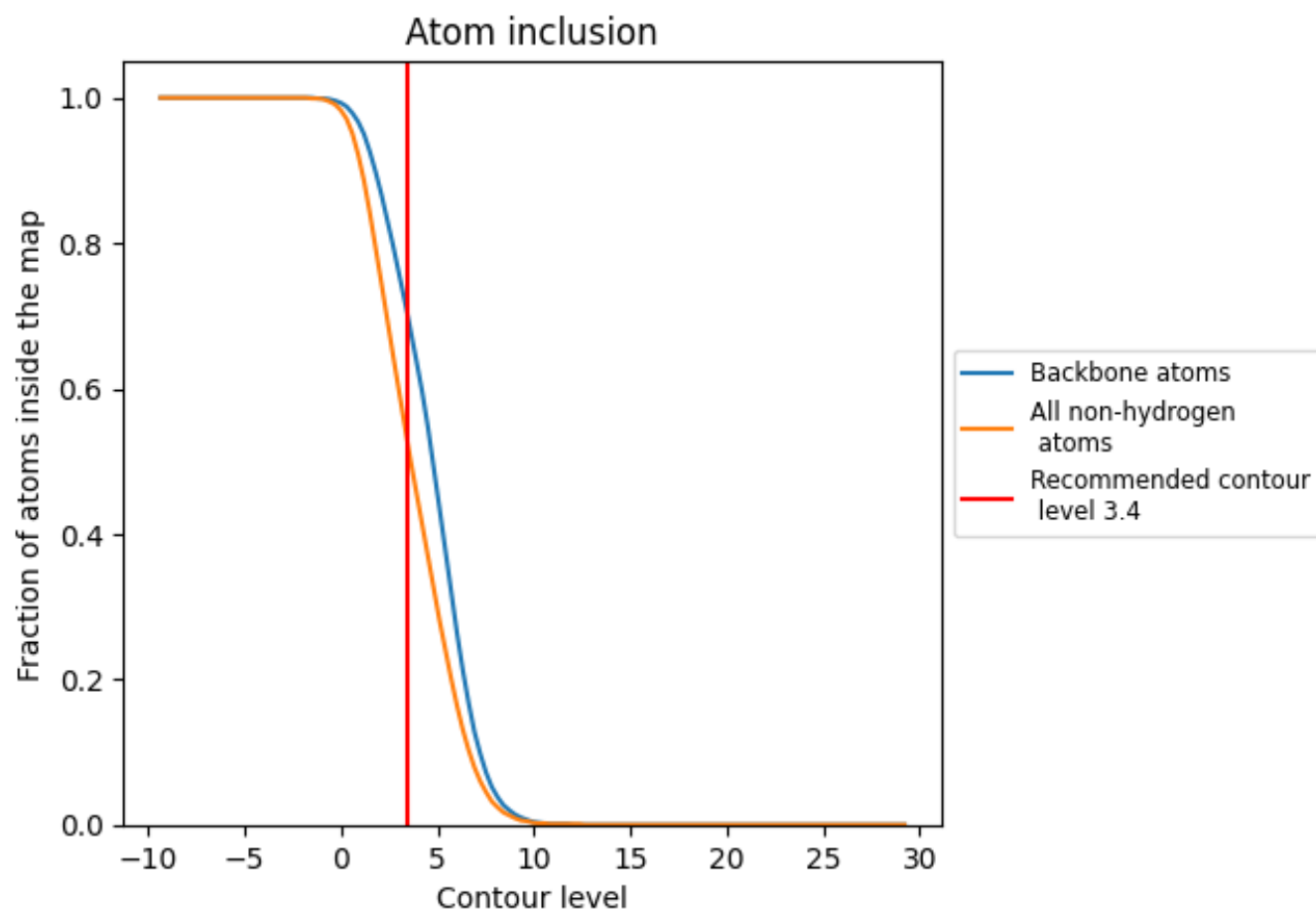
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.4).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 53% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (3.4) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.5330   |  0.4110   |
| 1     |  0.5210   |  0.4050   |
| 1a    |  0.3980   |  0.3640   |
| 2     |  0.5480   |  0.4290   |
| 2a    |  0.5150   |  0.4220   |
| 3     |  0.4490   |  0.3920   |
| 3A    |  0.6140   |  0.4350   |
| 3B    |  0.5740   |  0.4260   |
| 3C    |  0.5920   |  0.4440   |
| 3D    |  0.6190   |  0.4400   |
| 3E    |  0.5060   |  0.4320   |
| 3F    |  0.5480   |  0.4460   |
| 3G    |  0.5250   |  0.4390   |
| 3H    |  0.4370   |  0.3540   |
| 3J    |  0.5230  |  0.4200  |
| 3K    |  0.3370 |  0.4010 |
| 3L    |  0.6100 |  0.4420 |
| 3M    |  0.6080 |  0.4430 |
| 3N    |  0.5740 |  0.4400 |
| 3O    |  0.6000 |  0.4380 |
| 3P    |  0.4920 |  0.4320 |
| 3Q    |  0.4910 |  0.4430 |
| 3R    |  0.4900 |  0.4270 |
| 3S    |  0.2980 |  0.3010 |
| 3T    |  0.3250 |  0.3810 |
| 3U    |  0.4510 |  0.3890 |
| 3V    |  0.3610 |  0.3500 |
| 3a    |  0.3660 |  0.3720 |
| 4     |  0.5710 |  0.4400 |
| 4L    |  0.4940 |  0.3990 |
| 4a    |  0.5440 |  0.4360 |
| 4l    |  0.4650 |  0.4130 |
| 5     |  0.5710 |  0.4280 |
| 5a    |  0.5540 |  0.4230 |
| 6     |  0.4030 |  0.3940 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| 6a    |  0.3330   |  0.3610   |
| A1    |  0.5710   |  0.3930   |
| A2    |  0.5350   |  0.3830   |
| A3    |  0.4360   |  0.3900   |
| A5    |  0.4740   |  0.4070   |
| A6    |  0.5330   |  0.4290   |
| A7    |  0.5730   |  0.4530   |
| A8    |  0.5680   |  0.4150   |
| A9    |  0.5830   |  0.4350   |
| AB    |  0.2790   |  0.3290   |
| AC    |  0.5610   |  0.4100   |
| AL    |  0.5300   |  0.4090   |
| AM    |  0.4050   |  0.3950   |
| AN    |  0.6070   |  0.4500   |
| AO    |  0.5450   |  0.4120   |
| B1    |  0.4540   |  0.4070   |
| B2    |  0.4670   |  0.3660   |
| B3    |  0.5120  |  0.4090  |
| B4    |  0.5100 |  0.4150 |
| B5    |  0.5930 |  0.4440 |
| B6    |  0.5750 |  0.4330 |
| B7    |  0.4950 |  0.3860 |
| B8    |  0.5450 |  0.4300 |
| B9    |  0.5830 |  0.4230 |
| BL    |  0.5800 |  0.4180 |
| BM    |  0.5440 |  0.4290 |
| C1    |  0.4070 |  0.4080 |
| C2    |  0.5450 |  0.4330 |
| S1    |  0.6080 |  0.4110 |
| S2    |  0.5980 |  0.4350 |
| S3    |  0.6310 |  0.4510 |
| S4    |  0.5670 |  0.4530 |
| S5    |  0.5270 |  0.4110 |
| S6    |  0.5800 |  0.4490 |
| S7    |  0.6000 |  0.4040 |
| S8    |  0.6340 |  0.4100 |
| V1    |  0.5730 |  0.3660 |
| V2    |  0.5350 |  0.3580 |
| V3    |  0.5210 |  0.3920 |
| a1    |  0.4350 |  0.3780 |
| a2    |  0.4740 |  0.3900 |
| a3    |  0.2510 |  0.3150 |

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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| a5    |  0.4020   |  0.3610   |
| a6    |  0.4820   |  0.4280   |
| a7    |  0.4450   |  0.3780   |
| a8    |  0.4440   |  0.3740   |
| a9    |  0.5320   |  0.4220   |
| ab    |  0.1850   |  0.2990   |
| ac    |  0.5540   |  0.4370   |
| al    |  0.4470   |  0.3890   |
| am    |  0.3710   |  0.3860   |
| an    |  0.5170   |  0.4170   |
| ao    |  0.4310   |  0.3790   |
| b1    |  0.3650   |  0.3860   |
| b2    |  0.5240   |  0.4110   |
| b3    |  0.5820   |  0.4150   |
| b4    |  0.5010   |  0.4210   |
| b5    |  0.5430   |  0.4240   |
| b6    |  0.5630   |  0.4360   |
| b7    |  0.5070   |  0.3960   |
| b8    |  0.5220  |  0.4340  |
| b9    |  0.5740 |  0.4340 |
| bl    |  0.5090 |  0.3970 |
| bm    |  0.5130 |  0.4180 |
| c1    |  0.3390 |  0.3770 |
| c2    |  0.4940 |  0.4180 |
| s1    |  0.5610 |  0.3800 |
| s2    |  0.5210 |  0.4040 |
| s3    |  0.5670 |  0.4270 |
| s4    |  0.5520 |  0.4300 |
| s5    |  0.4720 |  0.4000 |
| s6    |  0.5510 |  0.4290 |
| s7    |  0.5790 |  0.3810 |
| s8    |  0.5730 |  0.3740 |
| v1    |  0.4820 |  0.3250 |
| v2    |  0.5020 |  0.3540 |
| v3    |  0.5320 |  0.3610 |