



# wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 02:17 PM UTC

PDB ID : 6QC3 / pdb\_00006qc3  
EMDB ID : EMD-4495  
Title : Ovine respiratory supercomplex I+III2 open class 1  
Authors : Letts, J.A.; Sazanov, L.A.  
Deposited on : 2018-12-26  
Resolution : 4.20 Å(reported)  
Based on initial model : 1PPJ

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:

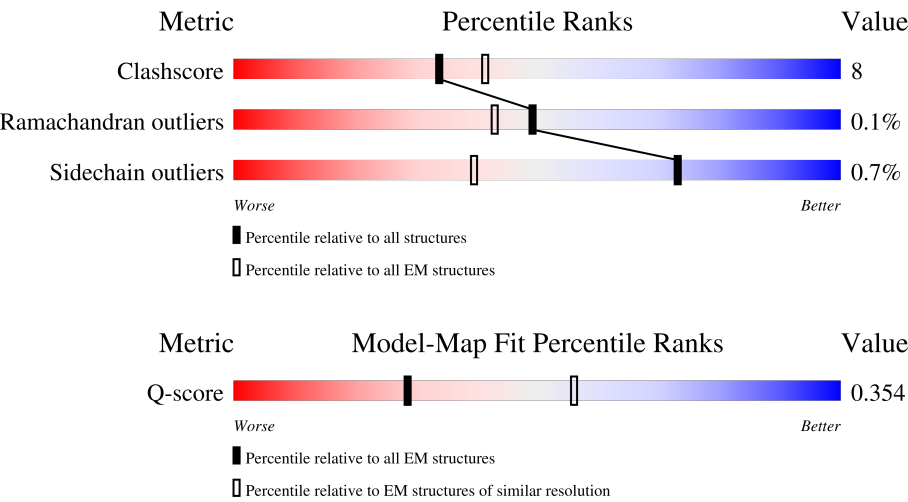
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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) : 2.49

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 4.20 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 5410 ( 3.70 - 4.70 )                                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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   | a1    | 446    | <div><div>52%</div><div>79%</div><div>19%</div><div>..</div></div> |
| 1   | a3    | 446    | <div><div>29%</div><div>83%</div><div>17%</div></div>              |
| 2   | a2    | 439    | <div><div>53%</div><div>78%</div><div>16%</div><div>6%</div></div> |
| 2   | a4    | 439    | <div><div>36%</div><div>71%</div><div>22%</div><div>6%</div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | b1    | 379    |                  |
| 3   | b2    | 379    |                  |
| 4   | c1    | 240    |                  |
| 4   | c2    | 240    |                  |
| 5   | f1    | 196    |                  |
| 5   | f2    | 196    |                  |
| 6   | d1    | 110    |                  |
| 6   | d2    | 110    |                  |
| 7   | q1    | 81     |                  |
| 7   | q2    | 81     |                  |
| 8   | h1    | 78     |                  |
| 8   | h2    | 78     |                  |
| 9   | x1    | 26     |                  |
| 9   | x2    | 26     |                  |
| 10  | i1    | 63     |                  |
| 10  | i2    | 63     |                  |
| 11  | V1    | 445    |                  |
| 12  | V2    | 217    |                  |
| 13  | S1    | 704    |                  |
| 14  | S2    | 430    |                  |
| 15  | S3    | 228    |                  |
| 16  | S7    | 179    |                  |
| 17  | S8    | 176    |                  |
| 18  | V3    | 75     |                  |
| 19  | S6    | 96     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 20  | S4    | 133    |                  |
| 21  | A9    | 338    |                  |
| 22  | A2    | 98     |                  |
| 23  | A5    | 115    |                  |
| 24  | A6    | 127    |                  |
| 25  | A7    | 112    |                  |
| 26  | AL    | 145    |                  |
| 27  | AA    | 88     |                  |
| 27  | AB    | 88     |                  |
| 28  | D3    | 115    |                  |
| 29  | D1    | 318    |                  |
| 30  | D6    | 175    |                  |
| 31  | 4L    | 98     |                  |
| 32  | D5    | 606    |                  |
| 33  | D4    | 459    |                  |
| 34  | D2    | 347    |                  |
| 35  | AK    | 140    |                  |
| 36  | B5    | 143    |                  |
| 37  | A8    | 171    |                  |
| 38  | BJ    | 175    |                  |
| 39  | AJ    | 320    |                  |
| 40  | S5    | 105    |                  |
| 41  | A3    | 83     |                  |
| 42  | B3    | 97     |                  |
| 43  | C2    | 120    |                  |

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| Mol | Chain | Length | Quality of chain                                                                      |
|-----|-------|--------|---------------------------------------------------------------------------------------|
| 44  | B4    | 128    | <div> <div>34%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>                |
| 45  | AM    | 143    | <div> <div>36%</div> <div>74%</div> <div>23%</div> <div>.</div> </div>                |
| 46  | B6    | 127    | <div> <div>30%</div> <div>56%</div> <div>18%</div> <div>.</div> <div>24%</div> </div> |
| 47  | B7    | 119    | <div> <div>40%</div> <div>77%</div> <div>22%</div> <div>.</div> </div>                |
| 48  | B9    | 178    | <div> <div>21%</div> <div>79%</div> <div>20%</div> <div>..</div> </div>               |
| 49  | B2    | 72     | <div> <div>44%</div> <div>75%</div> <div>15%</div> <div>10%</div> </div>              |
| 50  | B8    | 158    | <div> <div>33%</div> <div>75%</div> <div>23%</div> <div>..</div> </div>               |
| 51  | BK    | 125    | <div> <div>33%</div> <div>66%</div> <div>16%</div> <div>18%</div> </div>              |
| 52  | C1    | 49     | <div> <div>33%</div> <div>82%</div> <div>12%</div> <div>6%</div> </div>               |
| 53  | B1    | 57     | <div> <div>40%</div> <div>72%</div> <div>19%</div> <div>9%</div> </div>               |
| 54  | A1    | 70     | <div> <div>36%</div> <div>79%</div> <div>21%</div> </div>                             |

## 2 Entry composition

There are 65 unique types of molecules in this entry. The entry contains 96897 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 UQCRC1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | a1    | 439      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3409  | 2132 | 603 | 654 | 20 |         |       |
| 1   | a3    | 444      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3447  | 2153 | 608 | 666 | 20 |         |       |

- Molecule 2 is a protein called Ubiquinol-cytochrome c reductase core protein 2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | a2    | 414      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3126  | 1963 | 554 | 601 | 8 |         |       |
| 2   | a4    | 413      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3122  | 1961 | 553 | 600 | 8 |         |       |

- Molecule 3 is a protein called Cytochrome b.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | b1    | 378      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3019  | 2029 | 471 | 498 | 21 |         |       |
| 3   | b2    | 378      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3019  | 2029 | 471 | 498 | 21 |         |       |

- Molecule 4 is a protein called Cytochrome c1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | c1    | 239      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1909  | 1219 | 330 | 345 | 15 |         |       |
| 4   | c2    | 238      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1903  | 1216 | 329 | 343 | 15 |         |       |

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | f1    | 196      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1520  | 958 | 263 | 291 | 8 |         |       |
| 5   | f2    | 195      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1514  | 955 | 262 | 289 | 8 |         |       |

- Molecule 6 is a protein called UQCRB.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | d1    | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 886   | 566 | 159 | 159 | 2 |         |       |
| 6   | d2    | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 888   | 566 | 159 | 161 | 2 |         |       |

- Molecule 7 is a protein called Ubiquinol-cytochrome c reductase complex III subunit VII.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 7   | q1    | 73       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 618   | 404 | 116 | 97 | 1 |         |       |
| 7   | q2    | 75       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 631   | 413 | 118 | 99 | 1 |         |       |

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6.

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 8   | h1    | 65       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 532   | 324 | 96 | 107 | 5 |         |       |
| 8   | h2    | 65       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 532   | 324 | 96 | 107 | 5 |         |       |

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 9   | x1    | 23       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 114   | 68 | 23 | 23 |         |       |
| 9   | x2    | 26       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 130   | 78 | 26 | 26 |         |       |

- Molecule 10 is a protein called Ubiquinol-cytochrome c reductase, complex III subunit X.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 10  | i1    | 55       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 459   | 303 | 80 | 76 |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 10  | i2    | 57       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 473   | 312 | 82 | 79 |         |       |

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 11  | V1    | 430      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3312  | 2086 | 593 | 613 | 20 |         |       |

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 12  | V2    | 212      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1647  | 1052 | 277 | 308 | 10 |         |       |

- Molecule 13 is a protein called NADH:ubiquinone oxidoreductase core subunit S1.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 13  | S1    | 688      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5275  | 3301 | 922 | 1011 | 41 |         |       |

- Molecule 14 is a protein called NDUFB11.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 14  | S2    | 424      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3414  | 2180 | 584 | 625 | 25 |         |       |

- Molecule 15 is a protein called NADH:ubiquinone oxidoreductase core subunit S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 15  | S3    | 208      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1726  | 1112 | 296 | 315 | 3 |         |       |

- Molecule 16 is a protein called NDUFB1.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 16  | S7    | 156      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1247  | 795 | 225 | 213 | 14 |         |       |

- Molecule 17 is a protein called NDUFA1.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 17  | S8    | 176      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1414  | 889 | 243 | 270 | 12 |         |       |

- Molecule 18 is a protein called NDUFV3.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 18  | V3    | 41       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 345   | 215 | 63 | 66 | 1 |         |       |

- Molecule 19 is a protein called NDUF6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | S6    | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 737   | 451 | 139 | 144 | 3 |         |       |

- Molecule 20 is a protein called NADH:ubiquinone oxidoreductase subunit S4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | S4    | 126      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1024  | 646 | 182 | 193 | 3 |         |       |

- Molecule 21 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 21  | A9    | 287      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2293  | 1464 | 419 | 405 | 5 |         |       |

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | A2    | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 665   | 419 | 124 | 120 | 2 |         |       |

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | A5    | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 901   | 583 | 151 | 165 | 2 |         |       |

- Molecule 24 is a protein called NADH:ubiquinone oxidoreductase subunit A6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | A6    | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 969   | 619 | 180 | 166 | 4 |         |       |

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | A7    | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 757   | 473 | 144 | 137 | 3 |         |       |

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | AL    | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1201  | 773 | 215 | 209 | 4 |         |       |

- Molecule 27 is a protein called Acyl carrier protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | AA    | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 645   | 416 | 96  | 128 | 5 |         |       |
| 27  | AB    | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 702   | 451 | 103 | 143 | 5 |         |       |

- Molecule 28 is a protein called NADH-ubiquinone oxidoreductase chain 3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | D3    | 90       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 728   | 500 | 103 | 120 | 5 |         |       |

- Molecule 29 is a protein called NADH-ubiquinone oxidoreductase chain 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 29  | D1    | 303      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2415  | 1633 | 368 | 395 | 19 |         |       |

- Molecule 30 is a protein called NADH-ubiquinone oxidoreductase chain 6.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 30  | D6    | 171      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1308  | 878 | 187 | 230 | 13 |         |       |

- Molecule 31 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 31  | 4L    | 98       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 748   | 489 | 112 | 132 | 15 |         |       |

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 32  | D5    | 606      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4805  | 3187 | 746 | 828 | 44 |         |       |

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 33  | D4    | 459      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3646  | 2428 | 571 | 607 | 40 |         |       |

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 34  | D2    | 347      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2724  | 1808 | 416 | 460 | 40 |         |       |

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | AK    | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1025  | 654 | 175 | 190 | 6 |         |       |

- Molecule 36 is a protein called NADH:ubiquinone oxidoreductase subunit B5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | B5    | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1156  | 761 | 194 | 199 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 37  | A8    | 171      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1404  | 889 | 253 | 252 | 10 |         |       |

- Molecule 38 is a protein called MT-ND5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | BJ    | 171      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1441  | 905 | 266 | 262 | 8 |         |       |

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 39  | AJ    | 319      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2583  | 1653 | 430 | 490 | 10 |         |       |

- Molecule 40 is a protein called NADH:ubiquinone oxidoreductase subunit S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | S5    | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 822   | 520 | 154 | 142 | 6 |         |       |

- Molecule 41 is a protein called NADH:ubiquinone oxidoreductase subunit A3.

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 41  | A3    | 74       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 582   | 379 | 96 | 105 | 2 |         |       |

- Molecule 42 is a protein called NADH:ubiquinone oxidoreductase subunit B3.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 42  | B3    | 73       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 578   | 378 | 100 | 98 | 2 |         |       |

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | C2    | 119      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 997   | 647 | 174 | 172 | 4 |         |       |

- Molecule 44 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | B4    | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1059  | 675 | 189 | 194 | 1 |         |       |

- Molecule 45 is a protein called MT-ND1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | AM    | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1143  | 733 | 200 | 201 | 9 |         |       |

- Molecule 46 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | B6    | 96       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 815   | 536 | 139 | 139 | 1 |         |       |

- Molecule 47 is a protein called NADH:ubiquinone oxidoreductase subunit B7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | B7    | 119      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1026  | 641 | 196 | 181 | 8 |         |       |

- Molecule 48 is a protein called NADH:ubiquinone oxidoreductase subunit B9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | B9    | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1515  | 970 | 278 | 261 | 6 |         |       |

- Molecule 49 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 49  | B2    | 65       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 563   | 372 | 93 | 97 | 1 |         |       |

- Molecule 50 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50  | B8    | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1324  | 855 | 217 | 243 | 9 |         |       |

- Molecule 51 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51  | BK    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 853   | 547 | 141 | 161 | 4 |         |       |

- Molecule 52 is a protein called NDUFB4.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 52  | C1    | 46       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 391   | 258 | 67 | 66 |         |       |

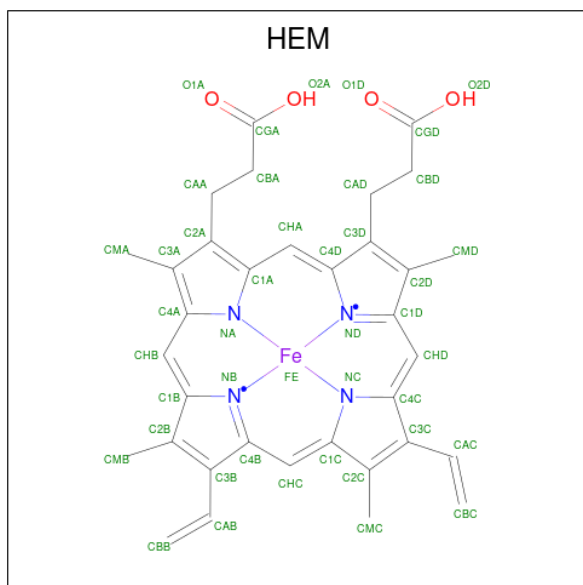
- Molecule 53 is a protein called NDUFA13.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 53  | B1    | 52       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 449   | 296 | 79 | 74 |         |       |

- Molecule 54 is a protein called NDUFA1.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 54  | A1    | 70       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 577   | 369 | 106 | 97 | 5 |         |       |

- Molecule 55 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



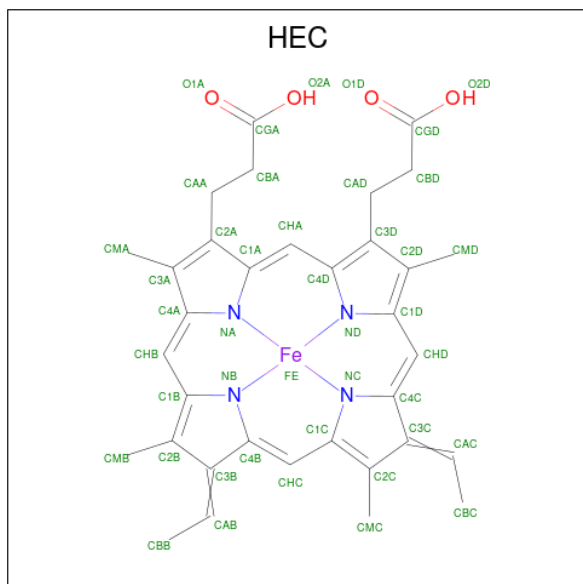
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 55  | b1    | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 55  | b1    | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 55  | b2    | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |

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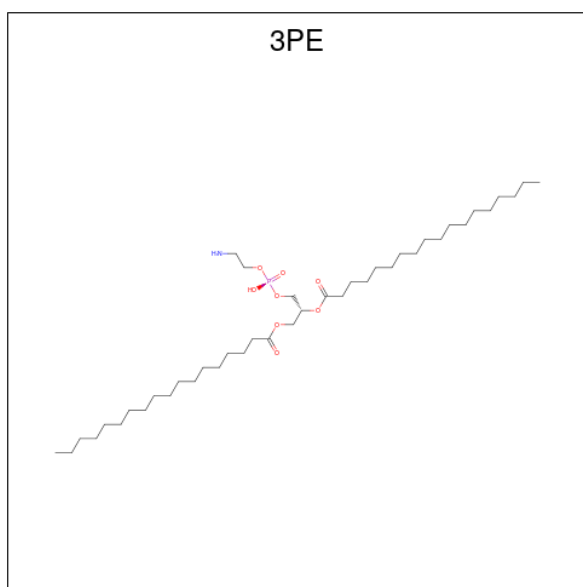
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 55  | b2    | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |

- Molecule 56 is HEME C (CCD ID: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



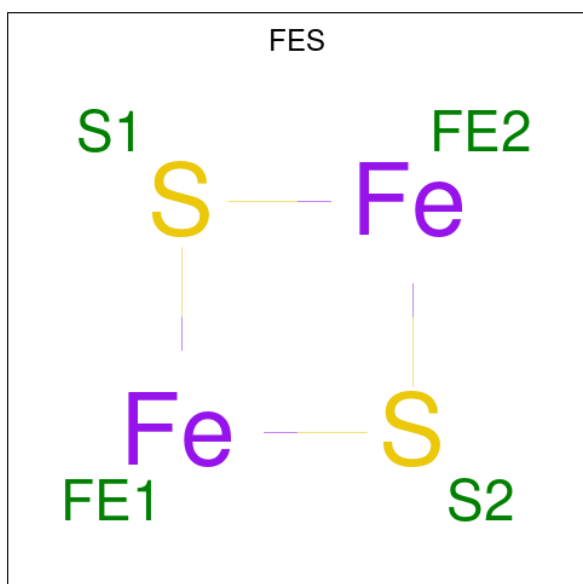
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 56  | c1    | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 56  | c2    | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |

- Molecule 57 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ).



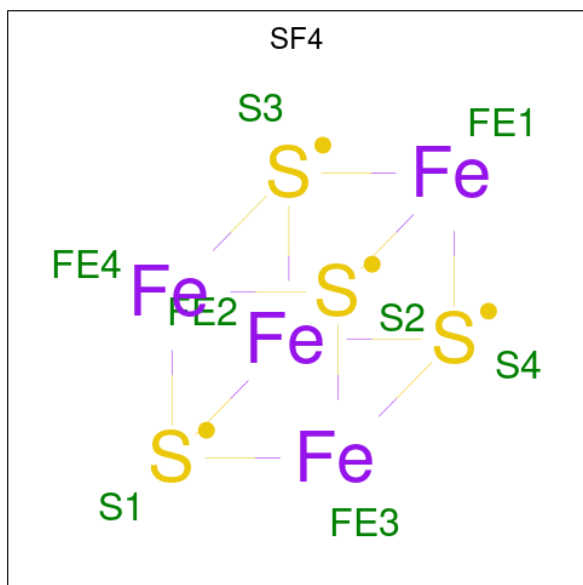
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 57  | c1    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 13    | 5  | 1 | 6 | 1 |         |
| 57  | f2    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 23    | 13 | 1 | 8 | 1 |         |
| 57  | D1    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 26    | 16 | 1 | 8 | 1 |         |
| 57  | D5    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 38    | 28 | 1 | 8 | 1 |         |
| 57  | D4    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 40    | 30 | 1 | 8 | 1 |         |

- Molecule 58 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



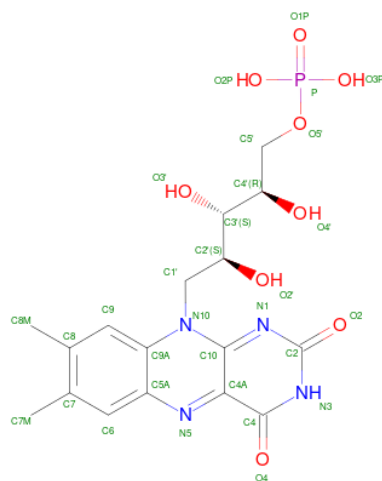
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 58  | f1    | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |
| 58  | f2    | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |
| 58  | V2    | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |
| 58  | S1    | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 59  | V1    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 59  | S1    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 59  | S1    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 59  | S7    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 59  | S8    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 59  | S8    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

- Molecule 60 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula:  $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$ ).

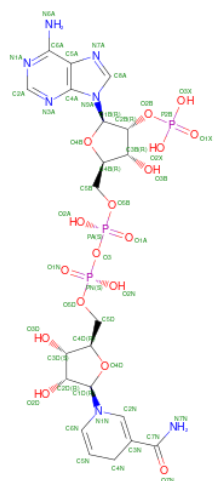


| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 60  | V1    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 31    | 17 | 4 | 9 | 1 |         |

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

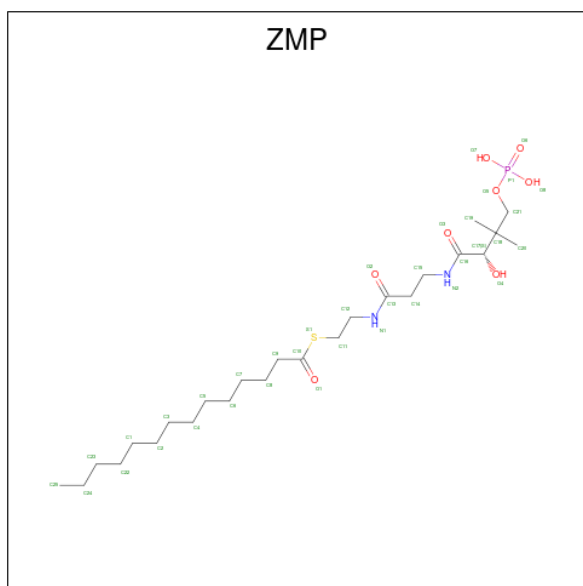
| Mol | Chain | Residues | Atoms           | AltConf |
|-----|-------|----------|-----------------|---------|
| 61  | S6    | 1        | Total Zn<br>1 1 | 0       |

- Molecule 62 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula:  $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$ ).



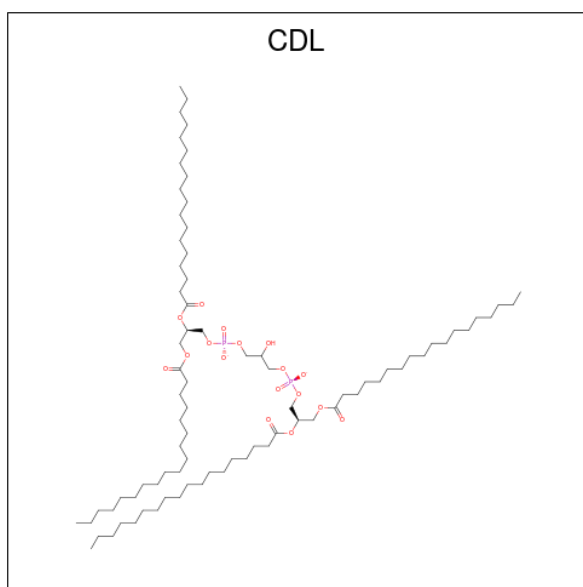
| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 62  | A9    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 48    | 21 | 7 | 17 | 3 |         |

- Molecule 63 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C<sub>25</sub>H<sub>49</sub>N<sub>2</sub>O<sub>8</sub>PS).



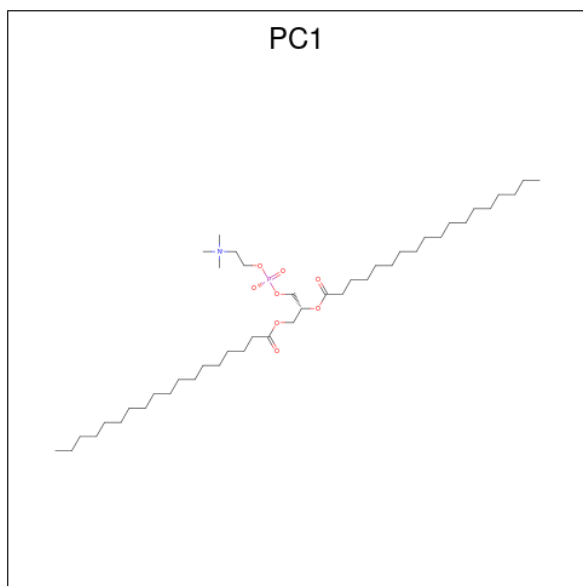
| Mol | Chain | Residues | Atoms       |         |        |        |        |        | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|--------|--------|---------|
| 63  | AA    | 1        | Total<br>34 | C<br>23 | N<br>2 | O<br>7 | P<br>1 | S<br>1 | 0       |
| 63  | AB    | 1        | Total<br>31 | C<br>20 | N<br>2 | O<br>7 | P<br>1 | S<br>1 | 0       |

- Molecule 64 is CARDIOLIPIN (CCD ID: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 64  | D5    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 60    | 41 | 17 | 2 |         |

- Molecule 65 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula:  $C_{44}H_{88}NO_8P$ ).

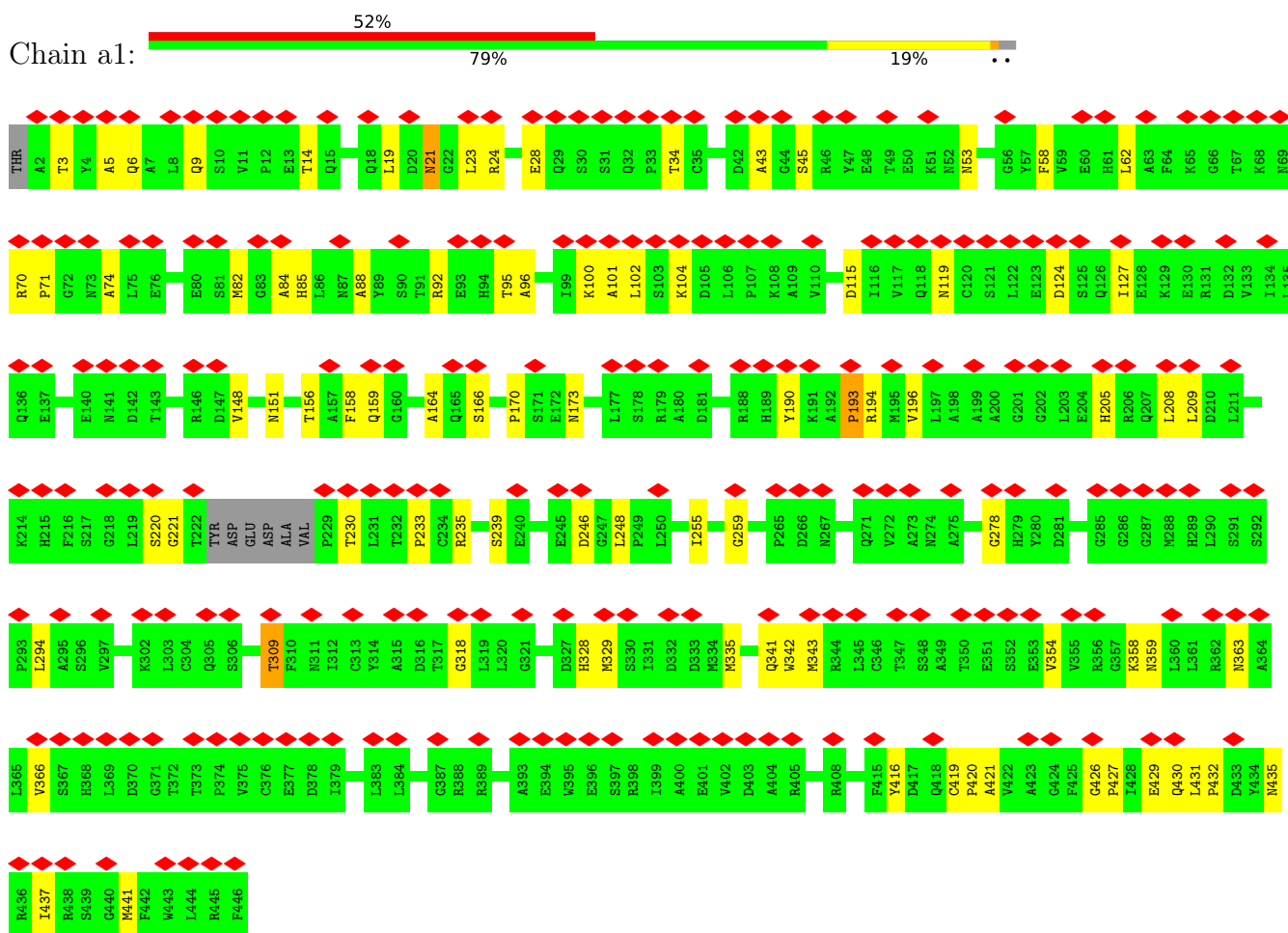


| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 65  | AK    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 28    | 18 | 1 | 8 | 1 |         |

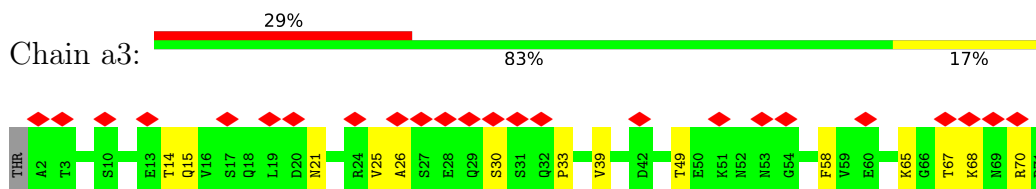
### 3 Residue-property plots

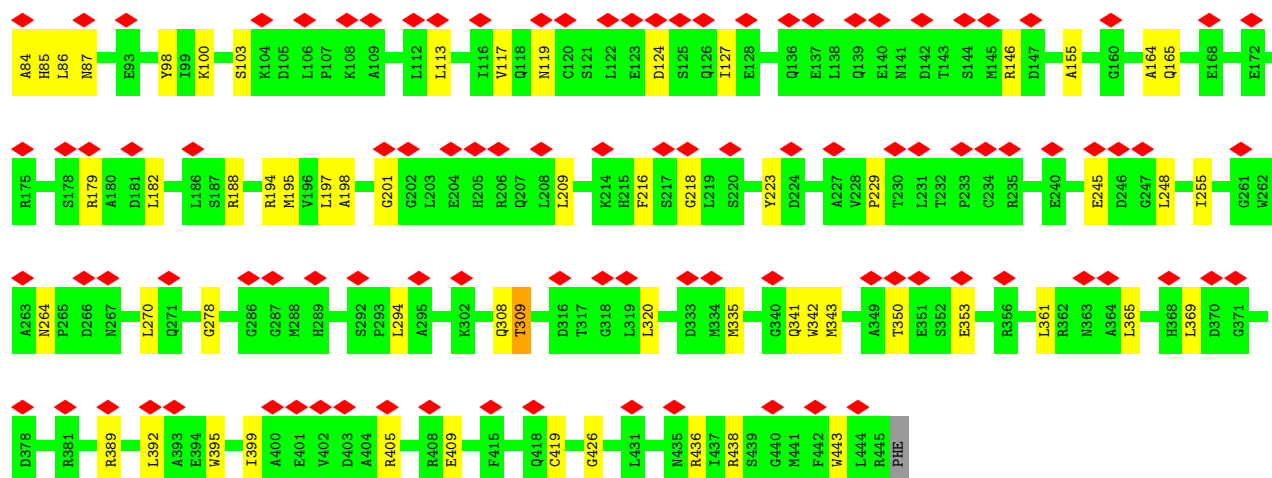
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: UQCRC1

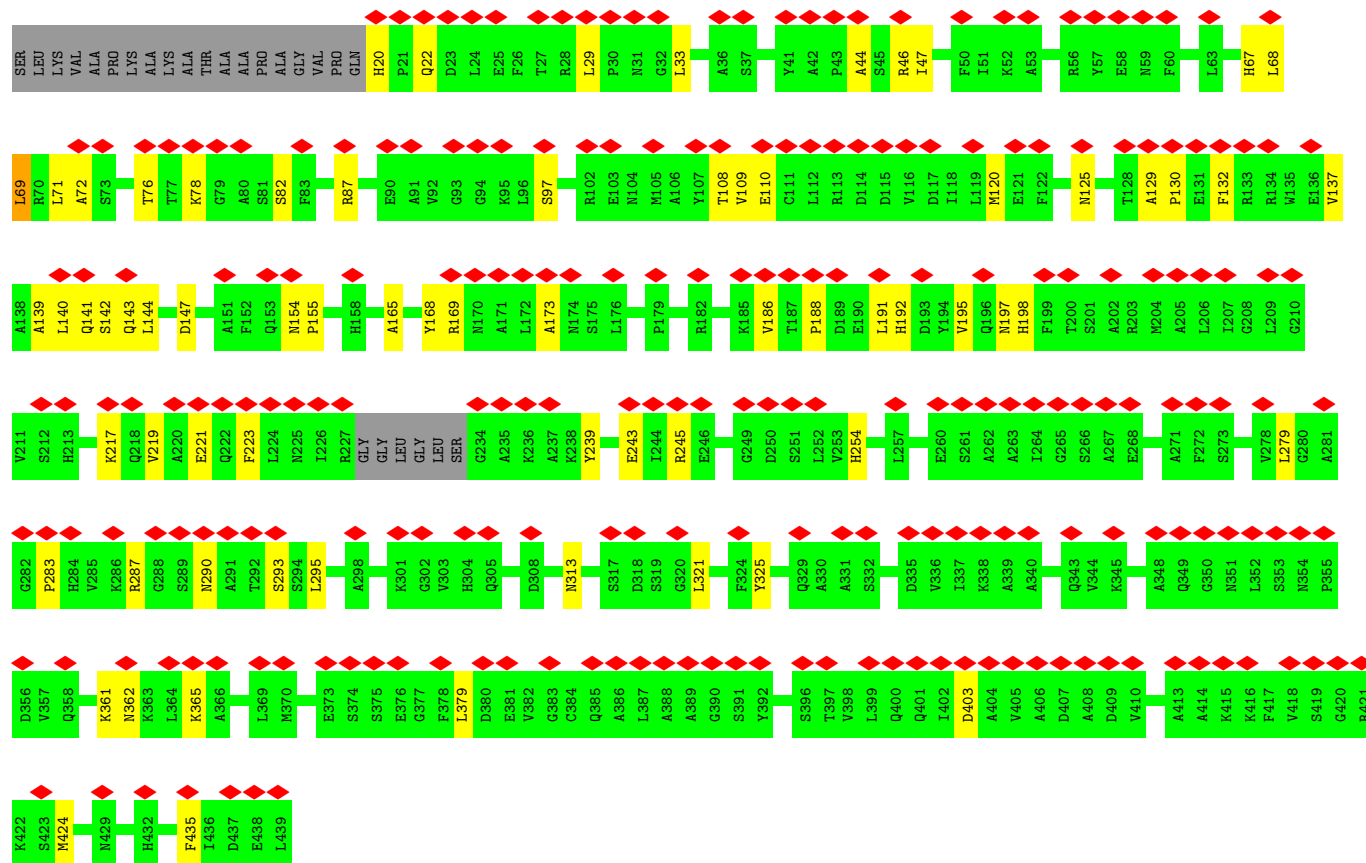
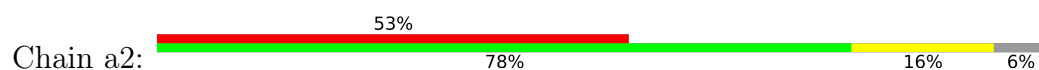


#### • Molecule 1: UQCRC1

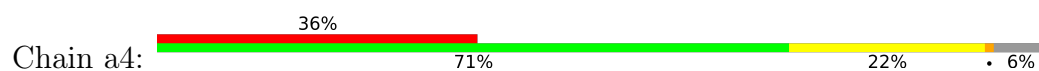


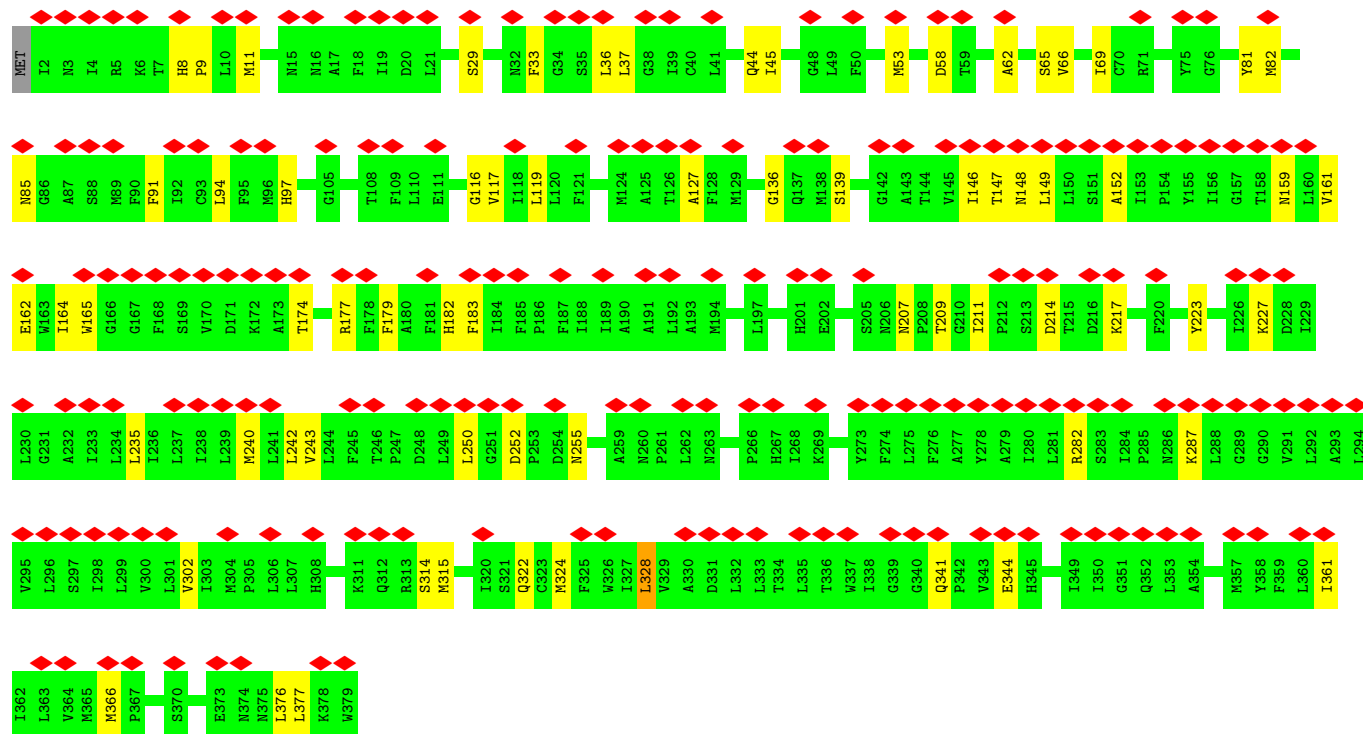


• Molecule 2: Ubiquinol-cytochrome c reductase core protein 2

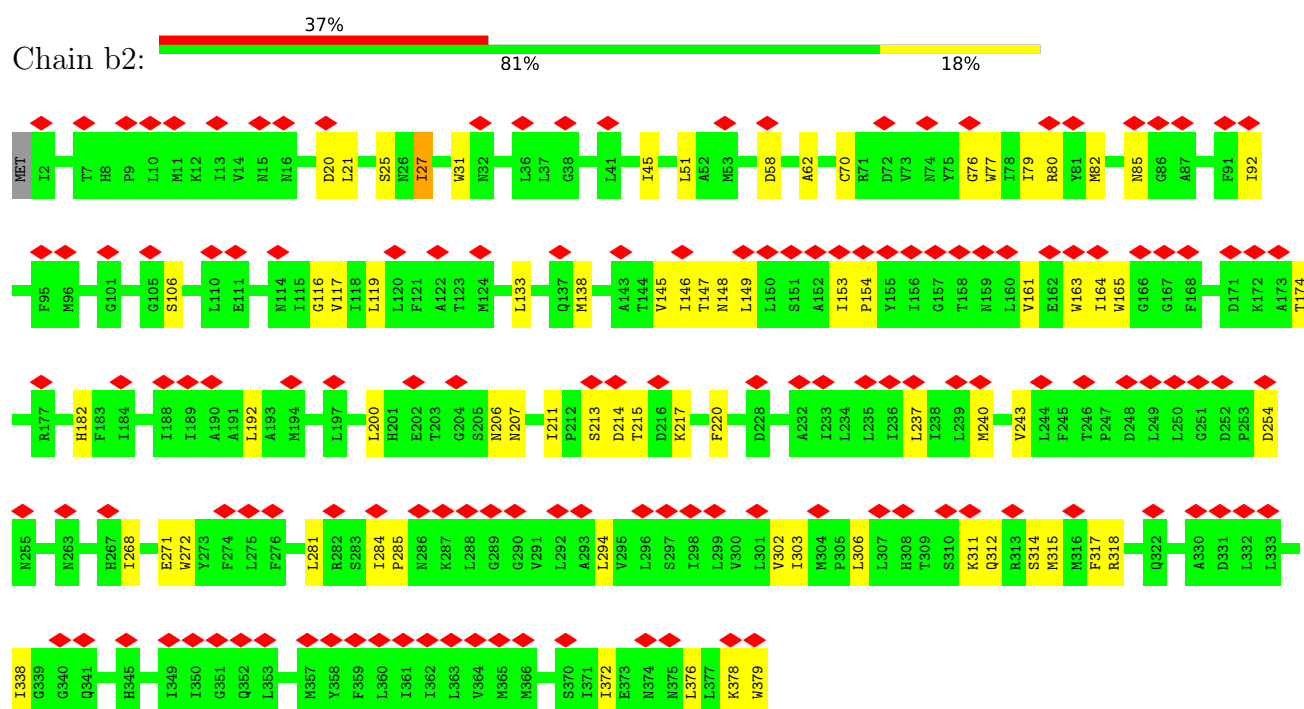


• Molecule 2: Ubiquinol-cytochrome c reductase core protein 2

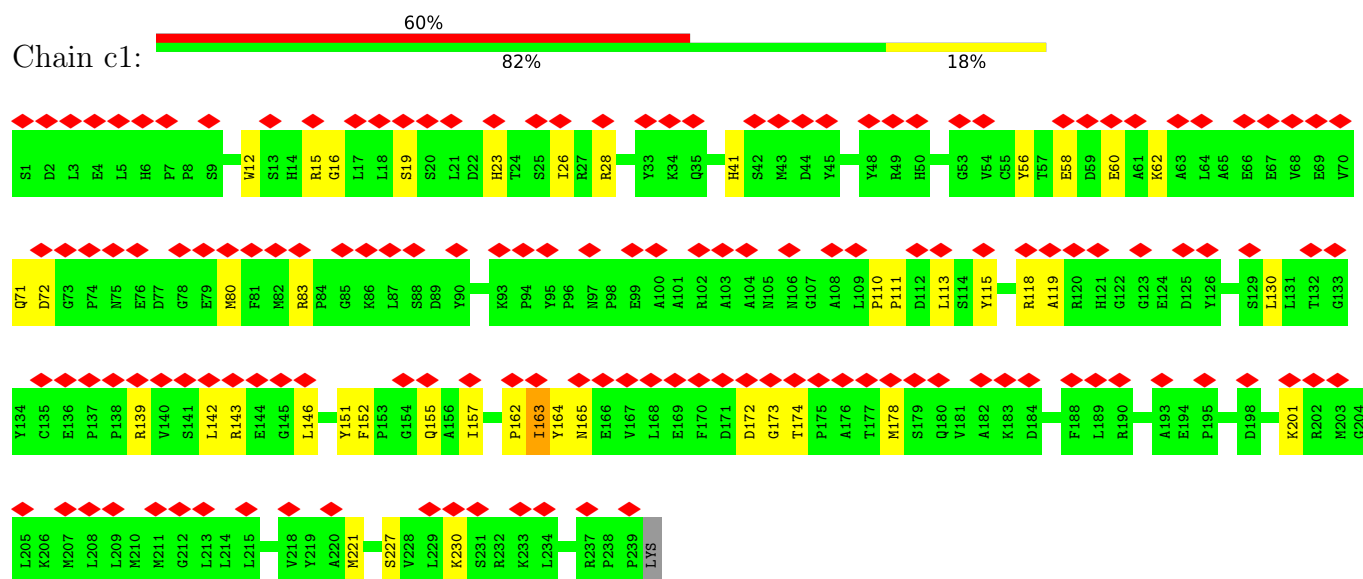




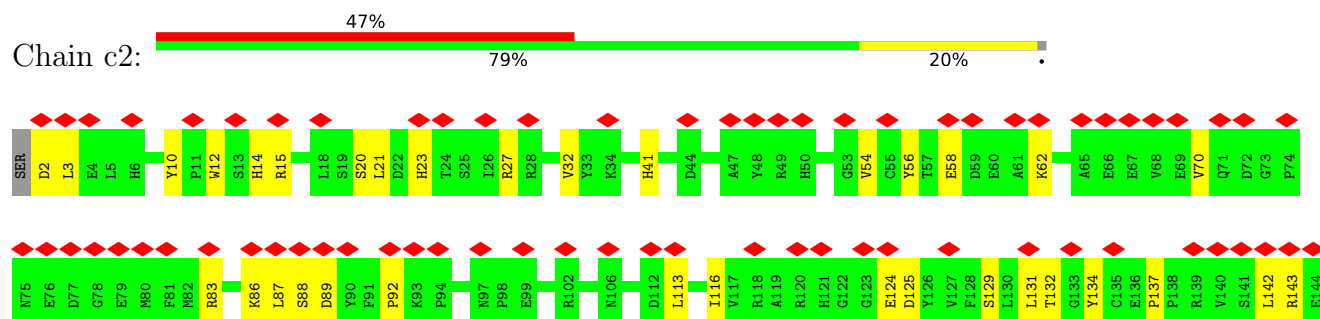
- Molecule 3: Cytochrome b

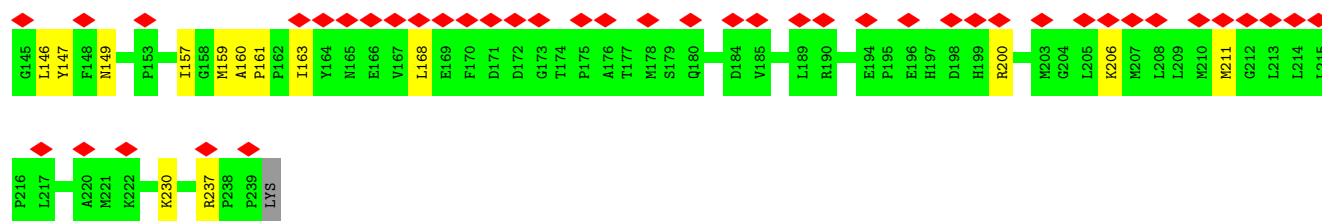


• Molecule 4: Cytochrome c1

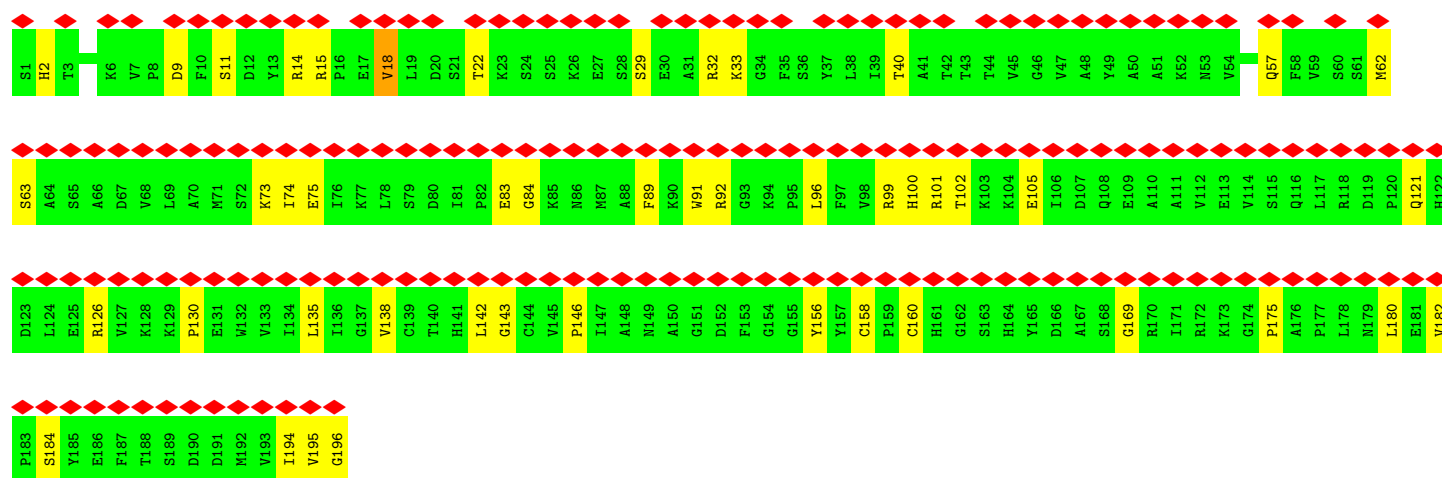
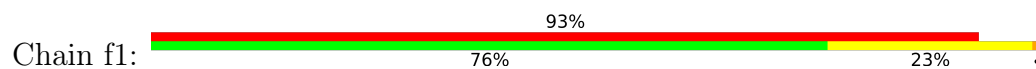


• Molecule 4: Cytochrome c1

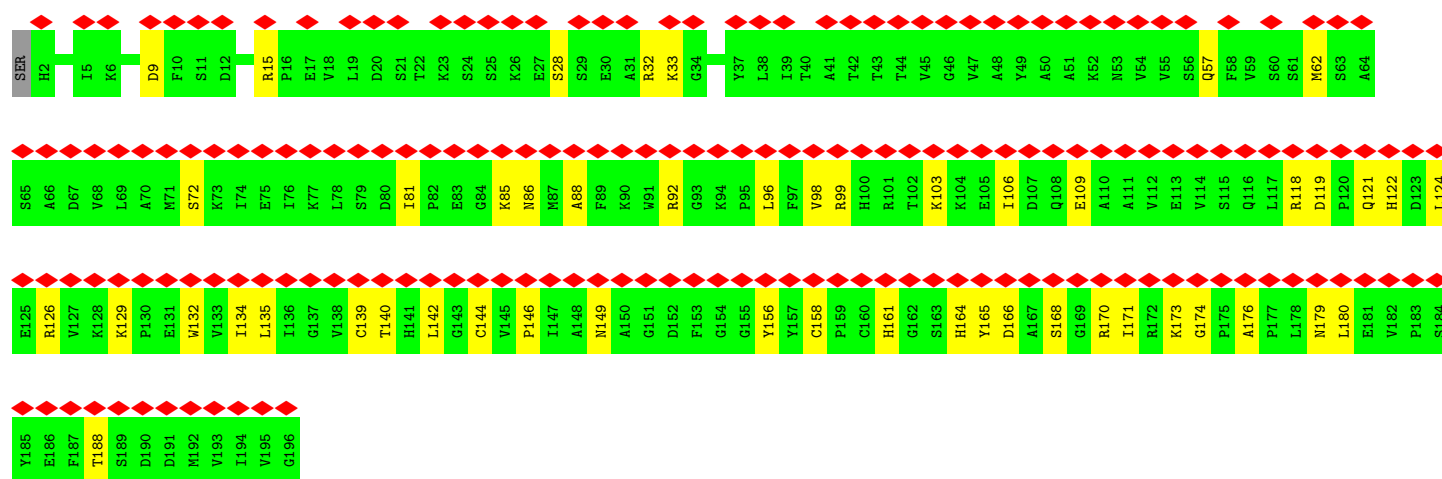
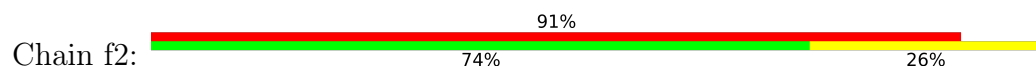




• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

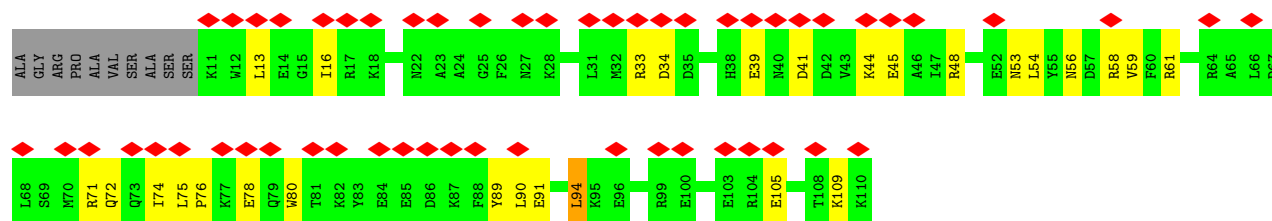


• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

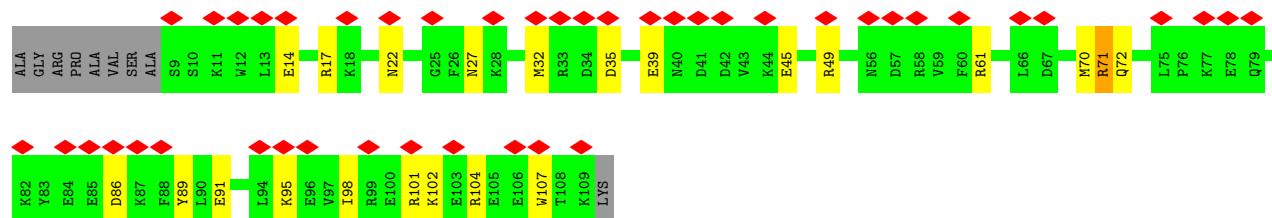
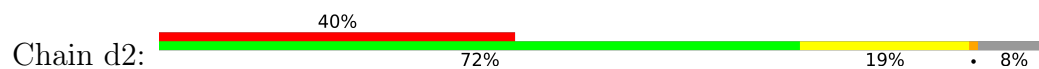


• Molecule 6: UQCRB

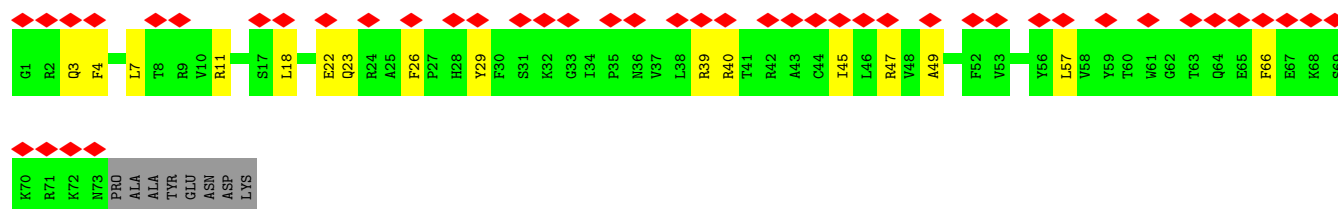
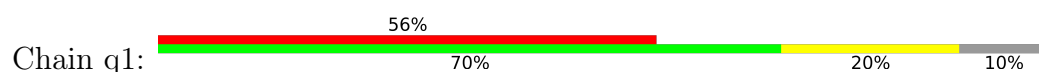




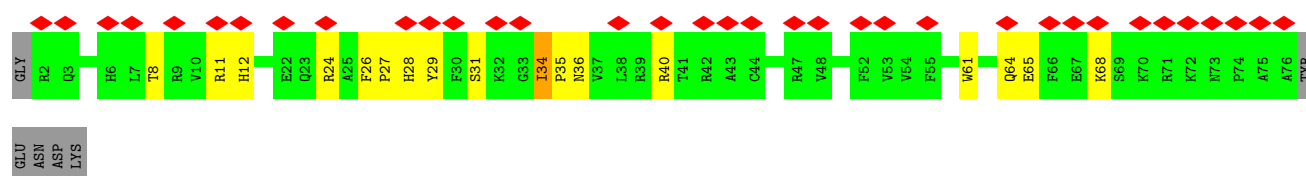
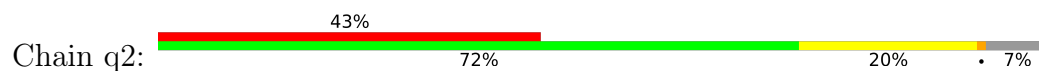
• Molecule 6: UQCRB



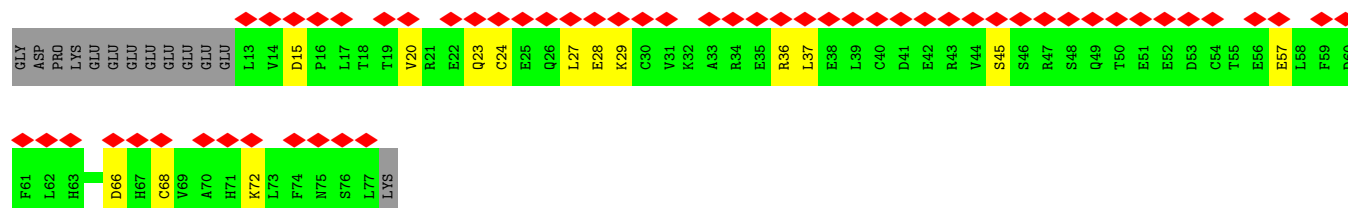
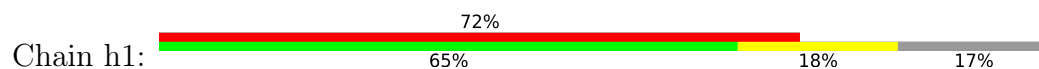
• Molecule 7: Ubiquinol-cytochrome c reductase complex III subunit VII



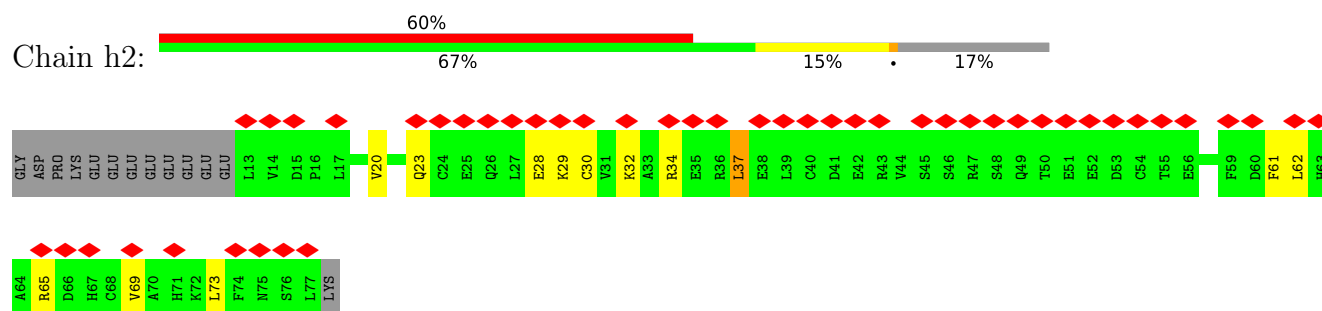
• Molecule 7: Ubiquinol-cytochrome c reductase complex III subunit VII



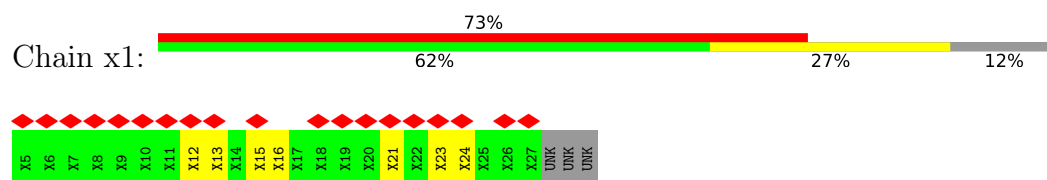
• Molecule 8: Cytochrome b-c1 complex subunit 6



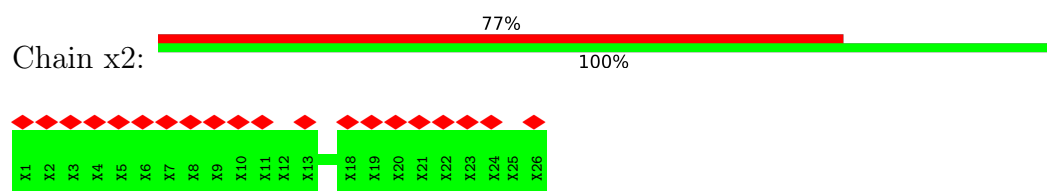
- Molecule 8: Cytochrome b-c1 complex subunit 6



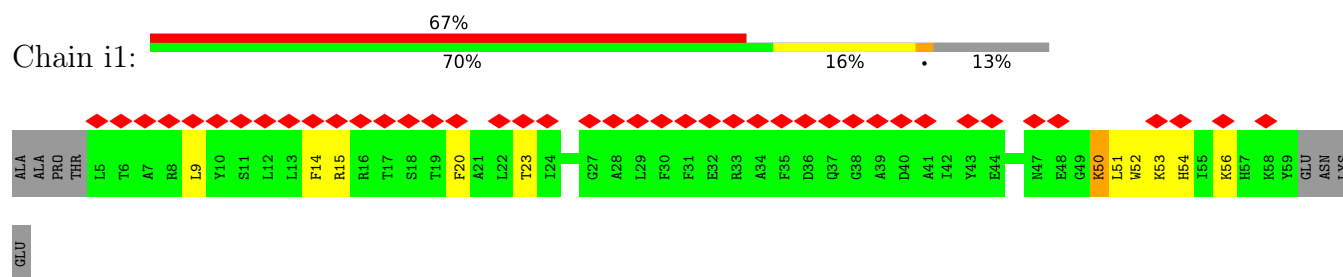
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



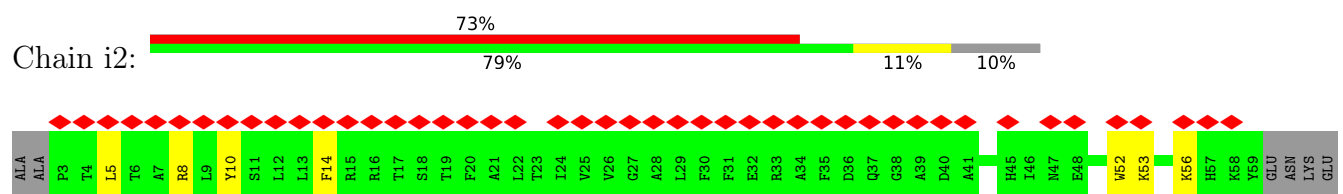
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



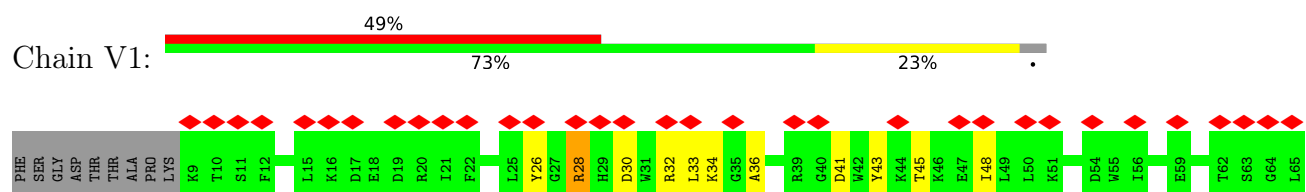
- Molecule 10: Ubiquinol-cytochrome c reductase, complex III subunit X

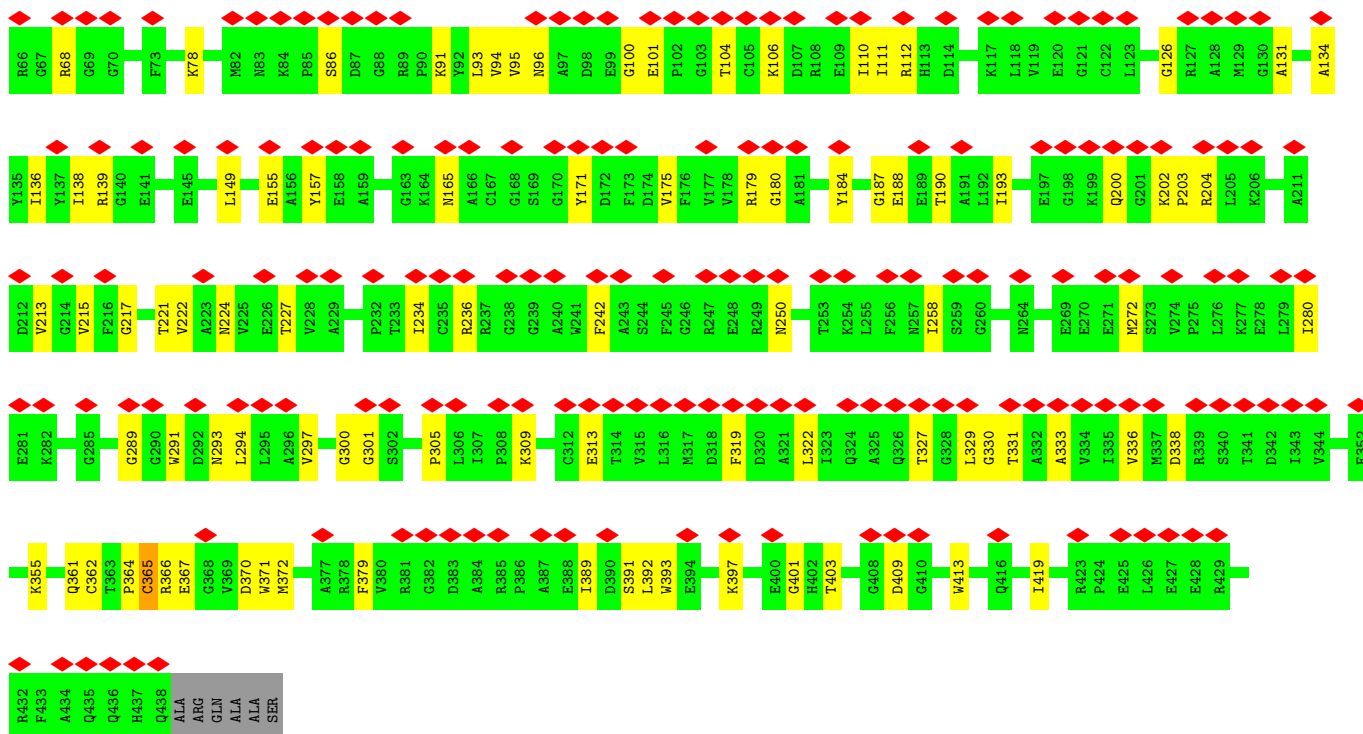


- Molecule 10: Ubiquinol-cytochrome c reductase, complex III subunit X

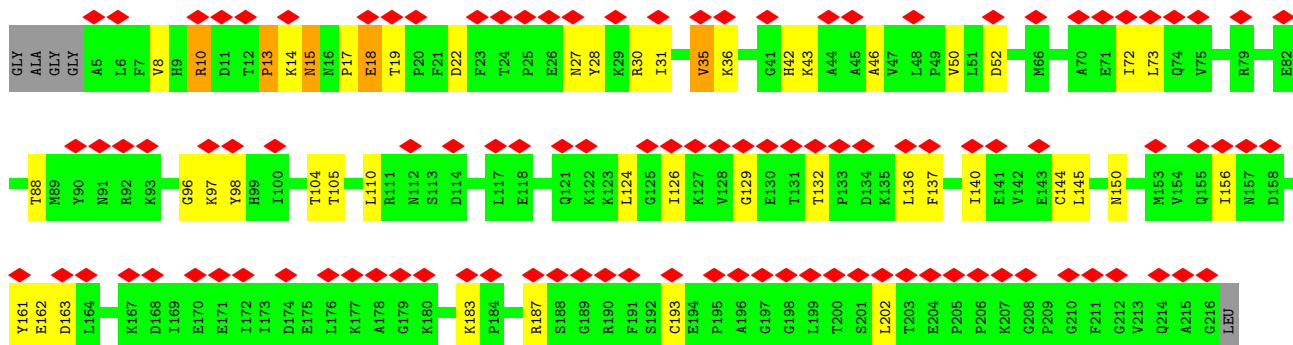
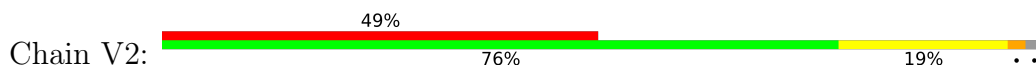


- Molecule 11: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

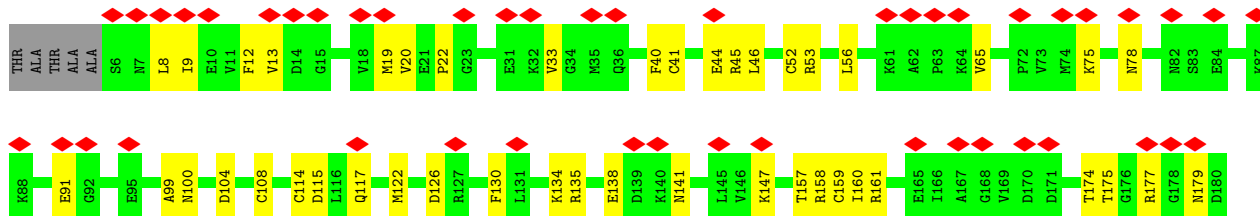


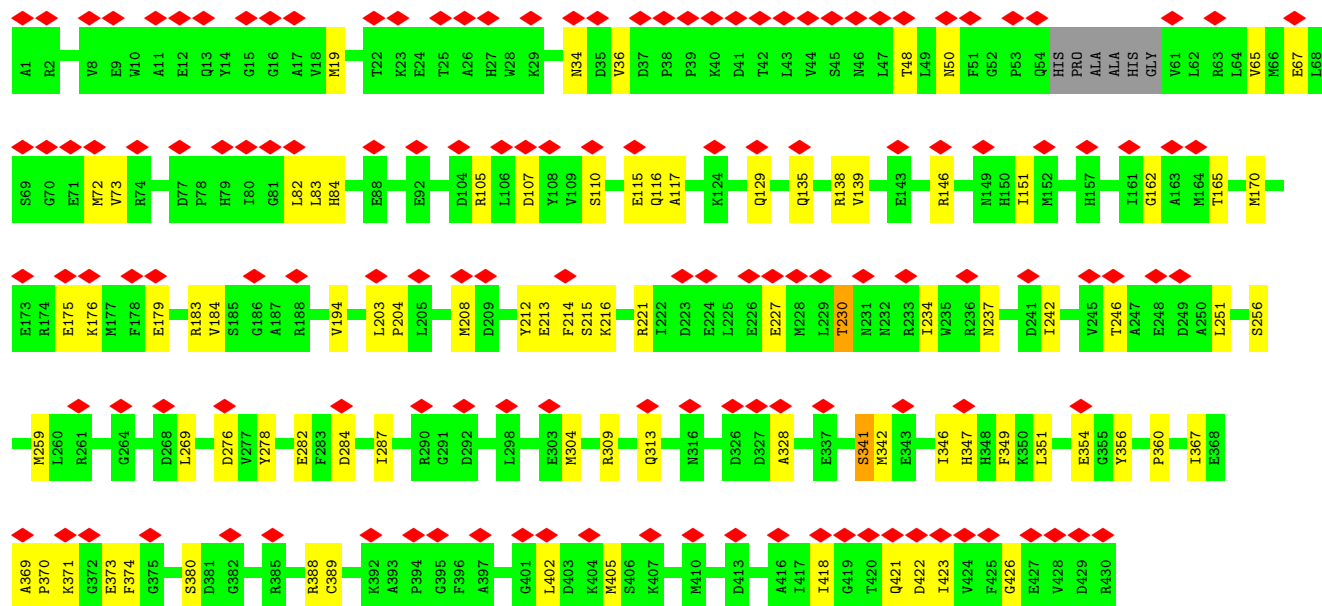


- Molecule 12: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

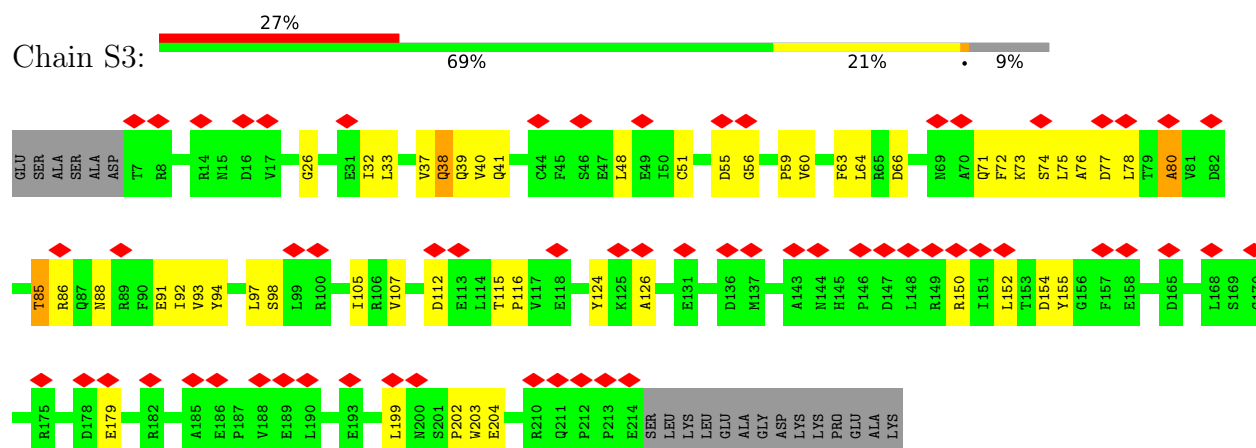


- Molecule 13: NADH:ubiquinone oxidoreductase core subunit S1

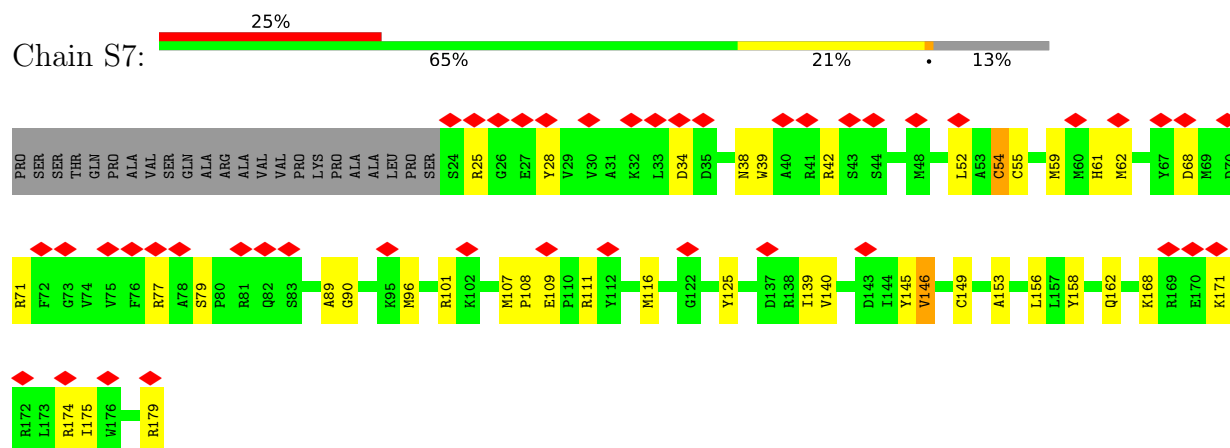




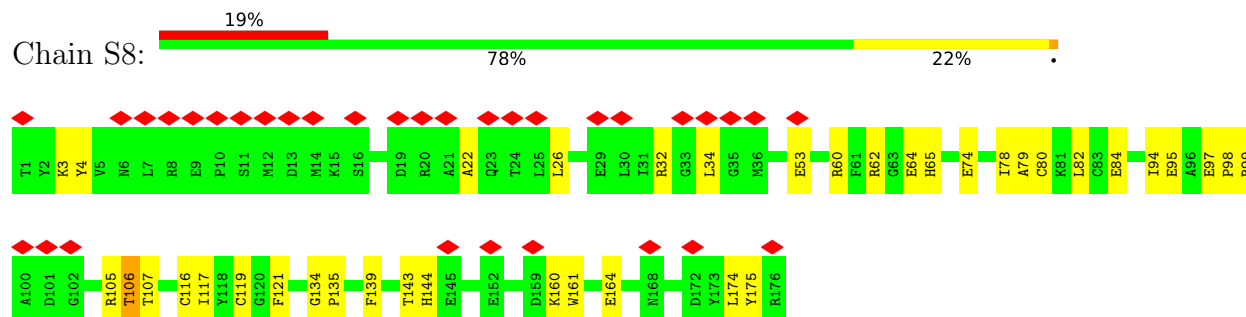
- Molecule 15: NADH:ubiquinone oxidoreductase core subunit S3



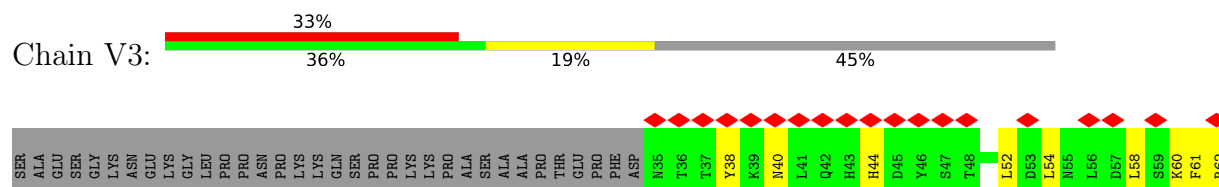
- Molecule 16: NDUFB1

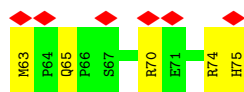


- Molecule 17: NDUFA1

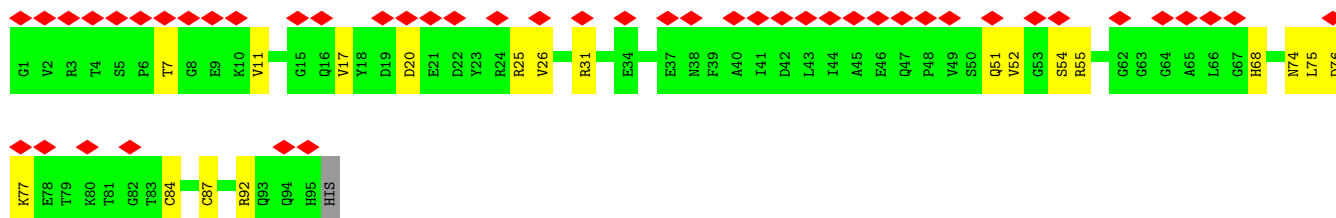
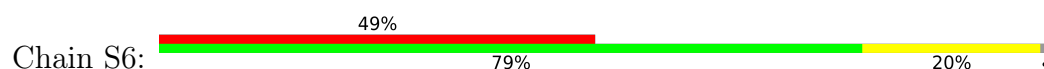


- Molecule 18: NDUFV3

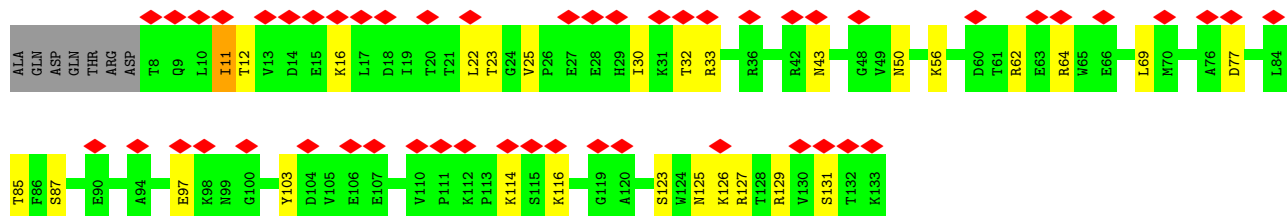
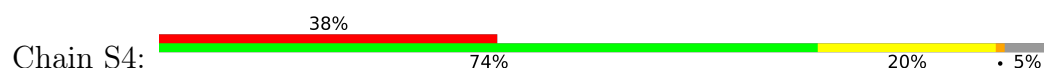




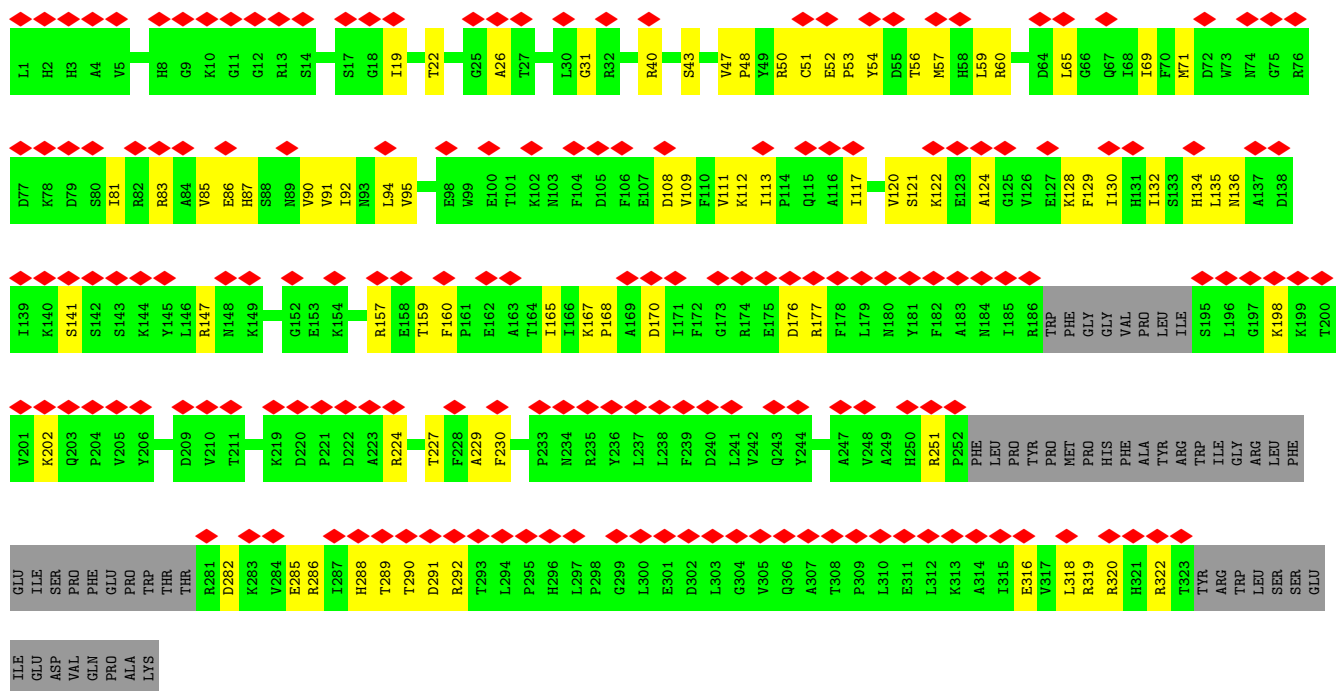
• Molecule 19: NDUFB6



• Molecule 20: NADH:ubiquinone oxidoreductase subunit S4

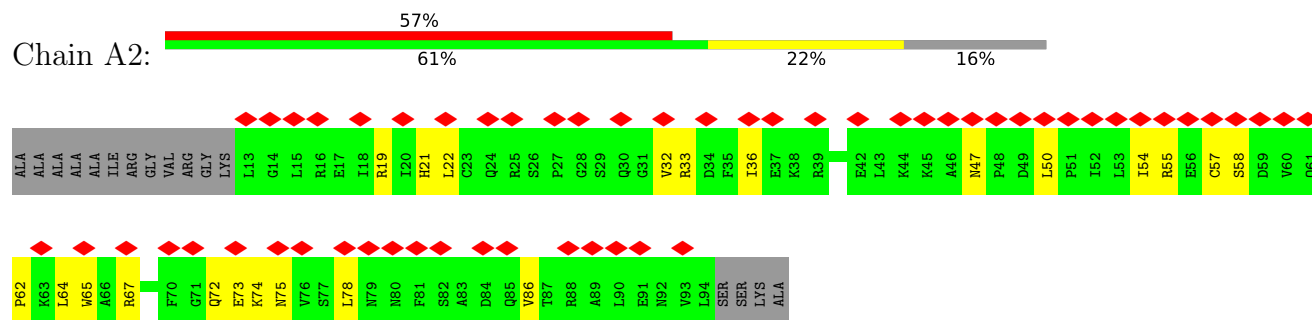


• Molecule 21: NADH:ubiquinone oxidoreductase subunit A9



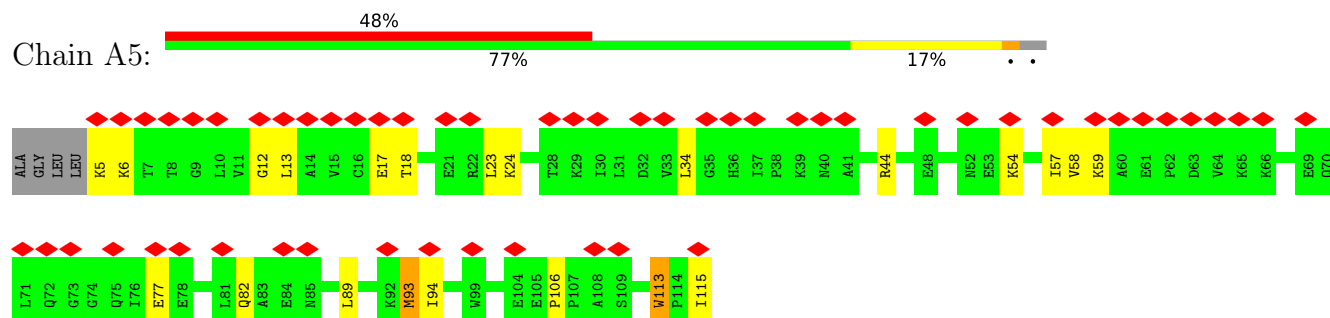
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain A2:



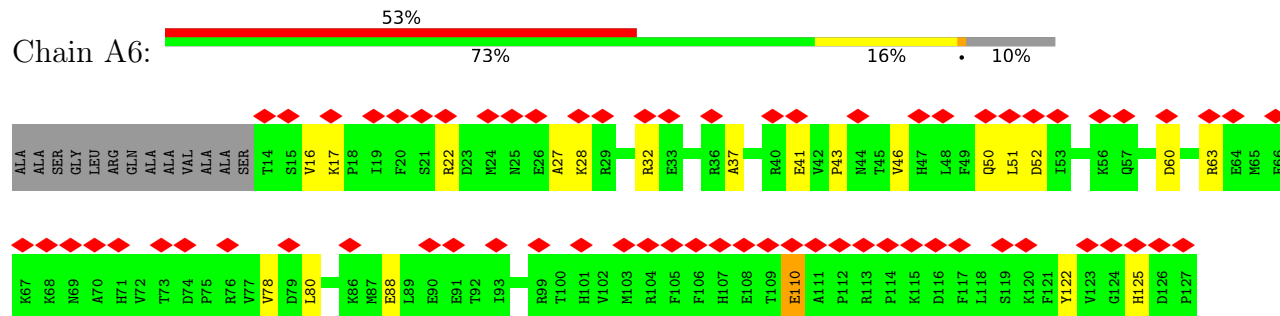
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain A5:



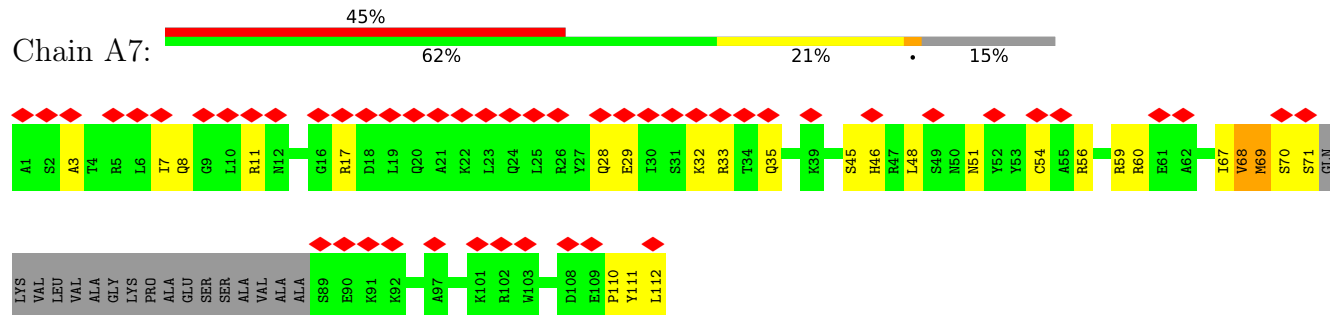
- Molecule 24: NADH:ubiquinone oxidoreductase subunit A6

Chain A6:



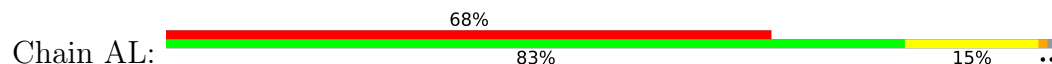
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

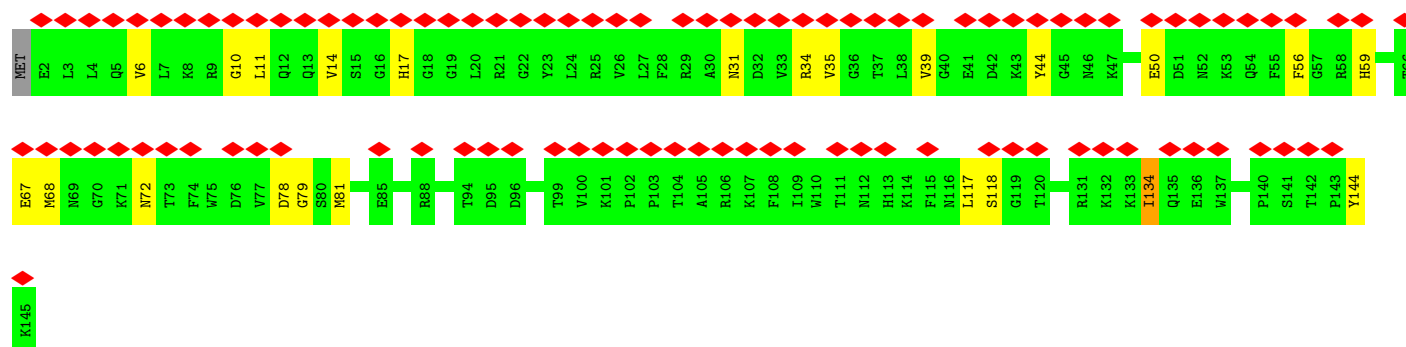
Chain A7:



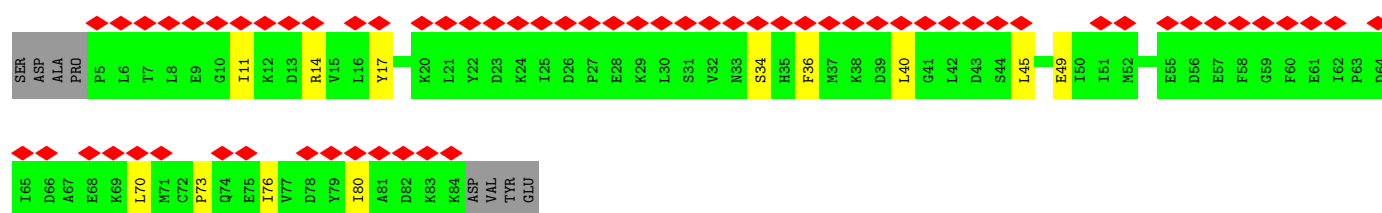
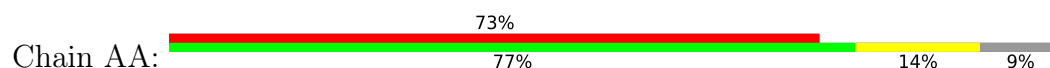
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain AL:

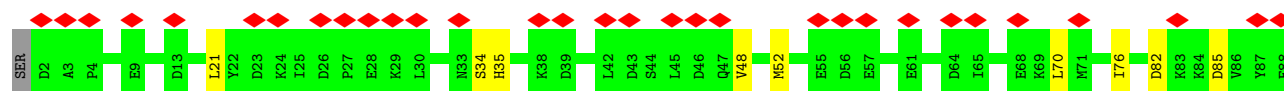
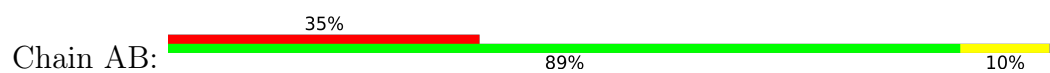




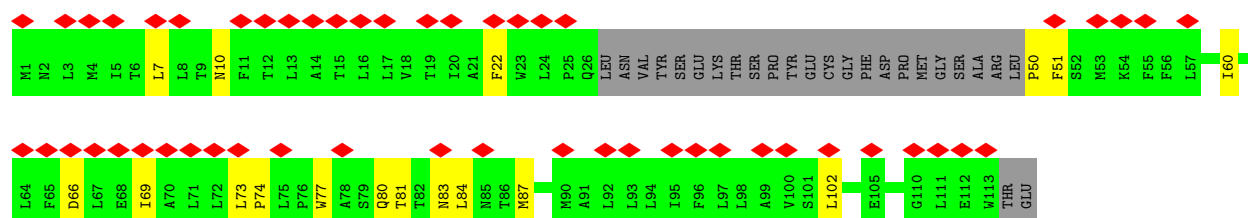
- Molecule 27: Acyl carrier protein



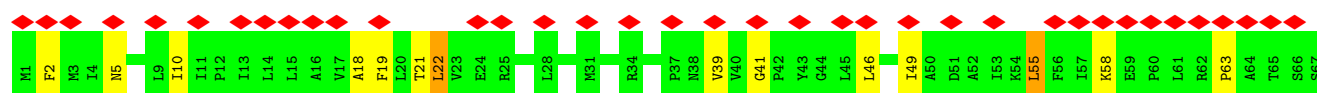
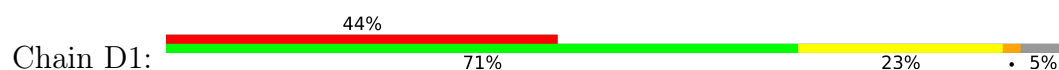
- Molecule 27: Acyl carrier protein

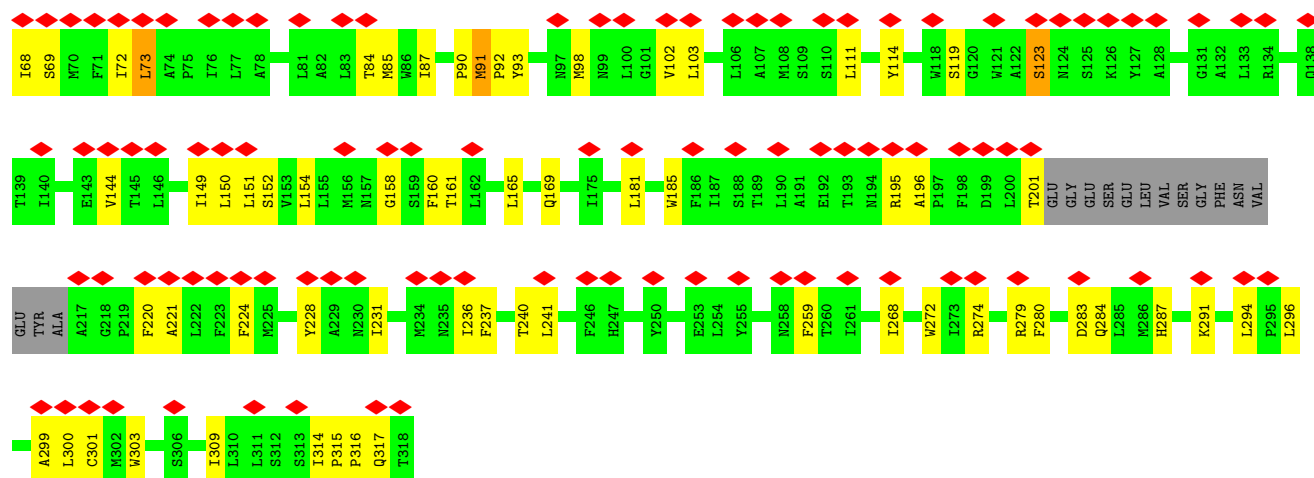


- Molecule 28: NADH-ubiquinone oxidoreductase chain 3

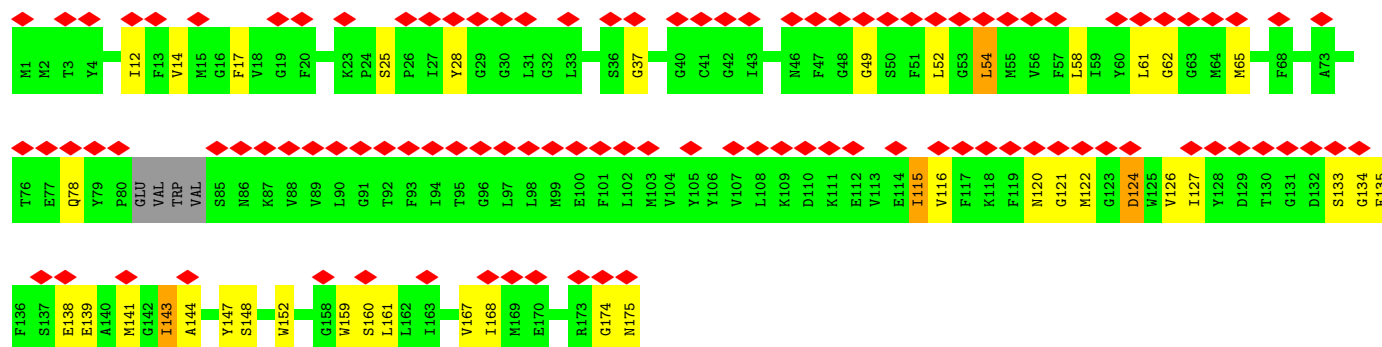
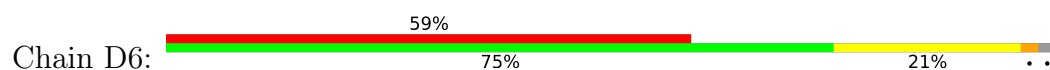


- Molecule 29: NADH-ubiquinone oxidoreductase chain 1

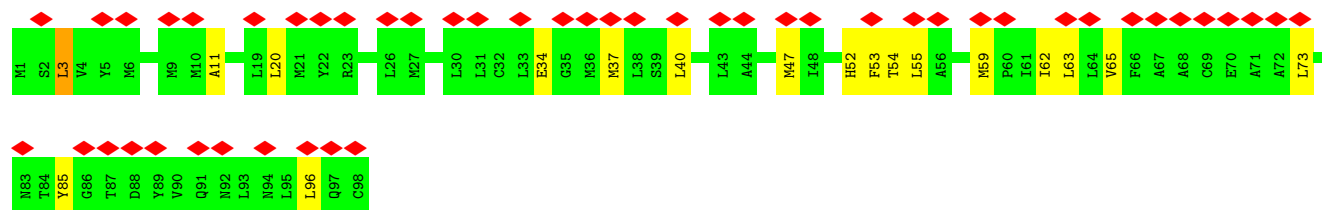
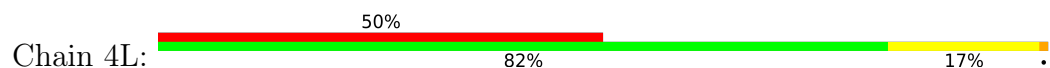




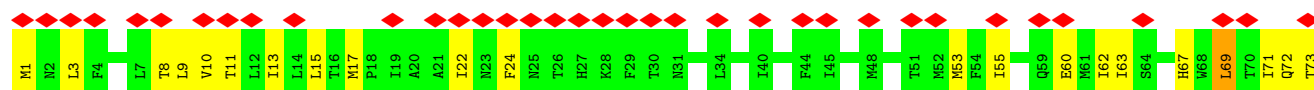
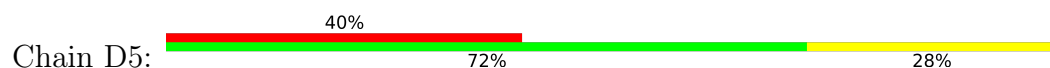
• Molecule 30: NADH-ubiquinone oxidoreductase chain 6

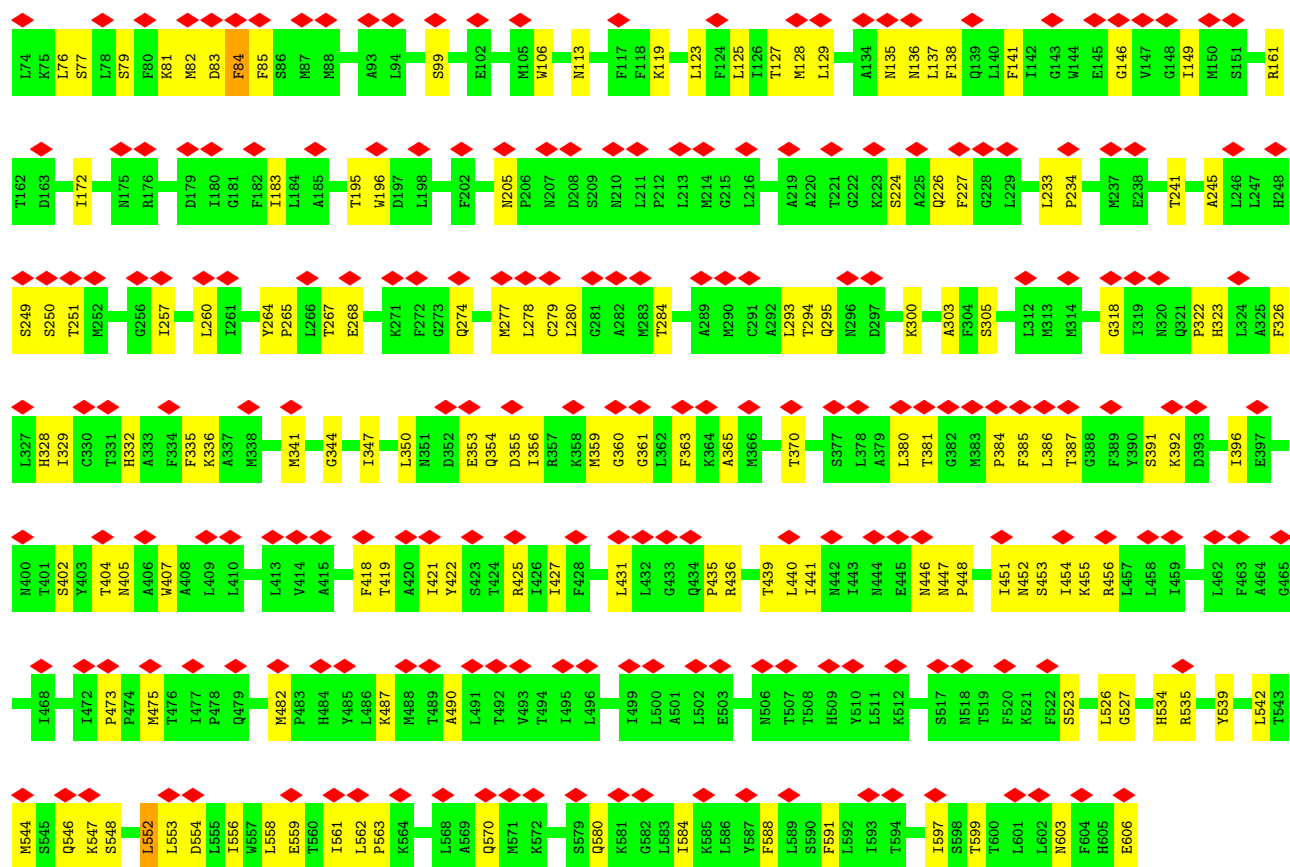


• Molecule 31: NADH-ubiquinone oxidoreductase chain 4L

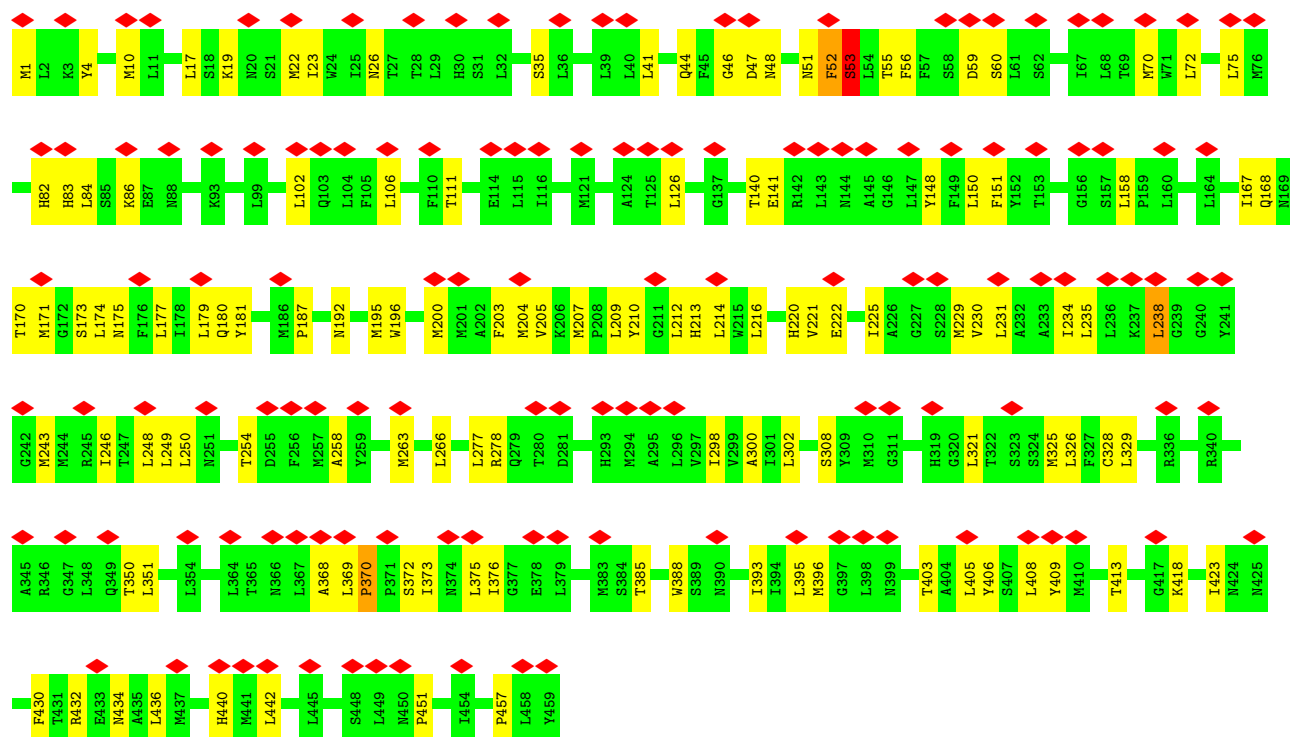
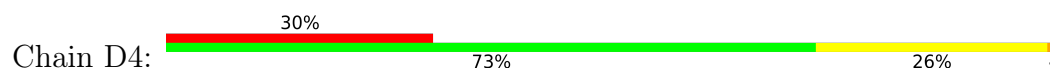


• Molecule 32: NADH-ubiquinone oxidoreductase chain 5

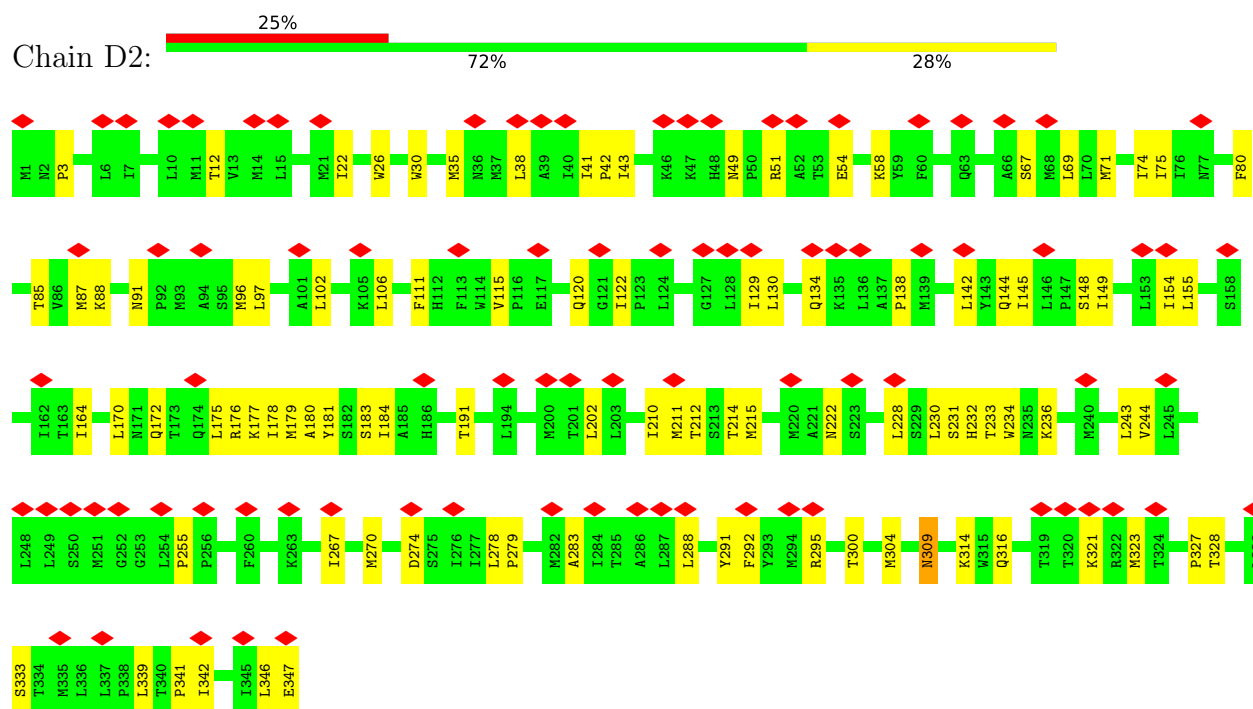




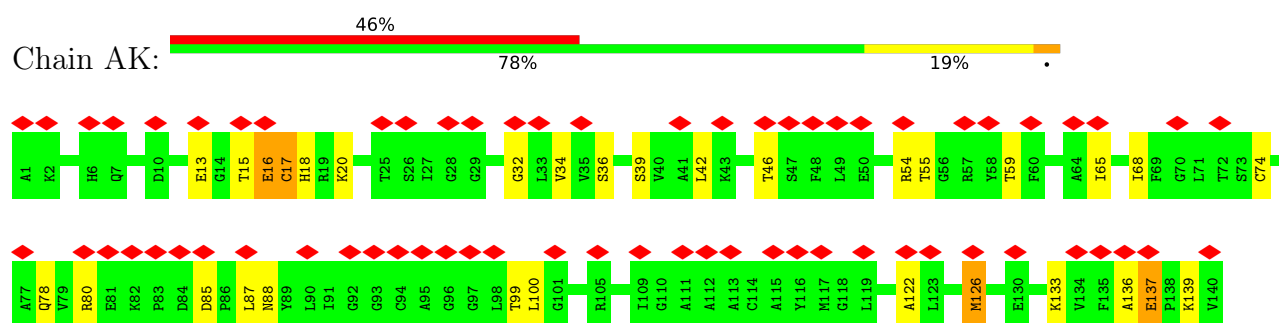
• Molecule 33: NADH-ubiquinone oxidoreductase chain 4



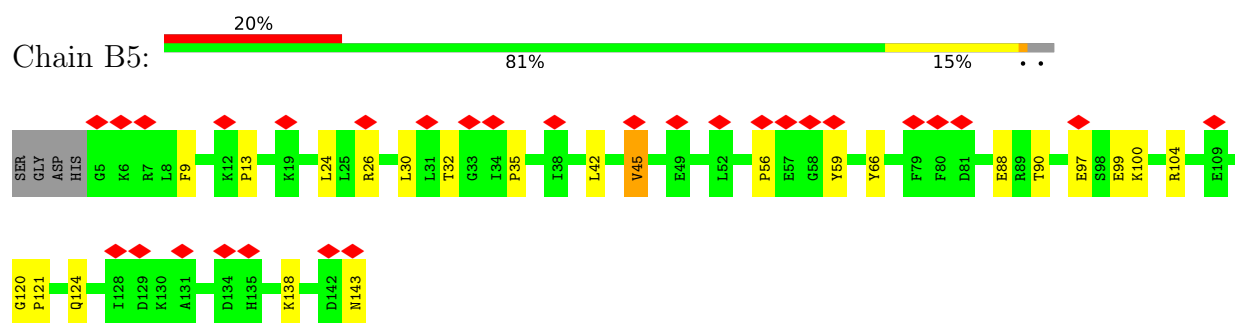
- Molecule 34: NADH-ubiquinone oxidoreductase chain 2



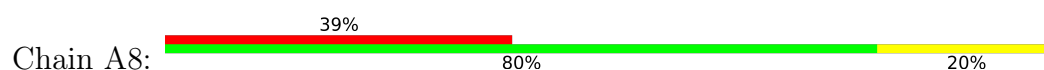
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

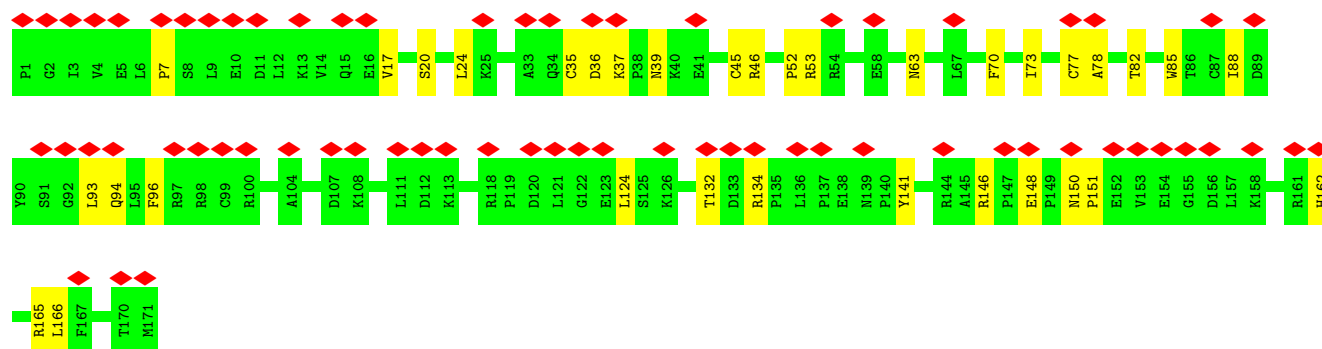


- Molecule 36: NADH:ubiquinone oxidoreductase subunit B5

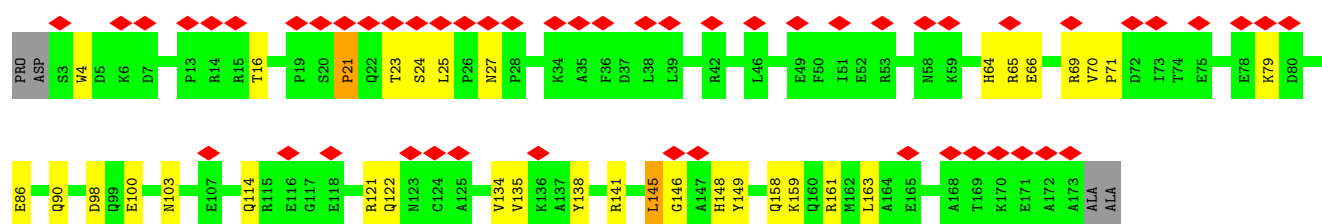
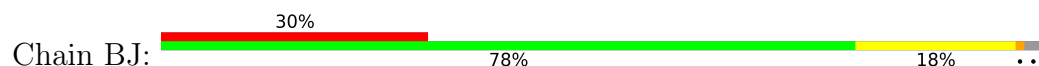


- Molecule 37: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

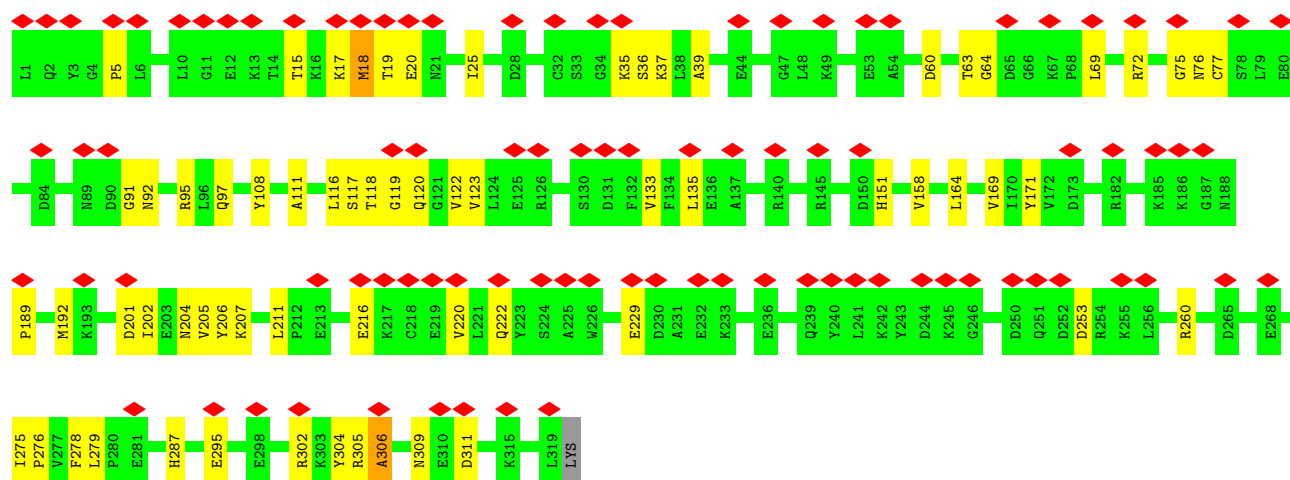
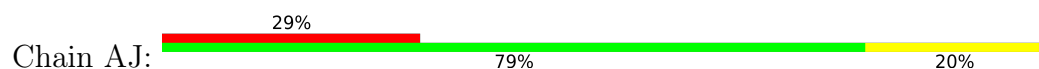




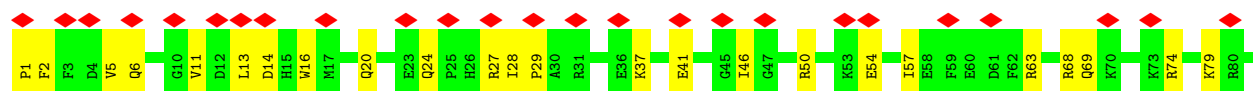
• Molecule 38: MT-ND5

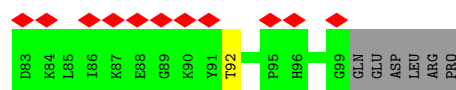


• Molecule 39: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

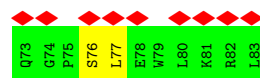
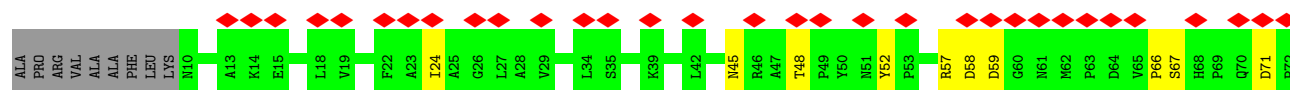
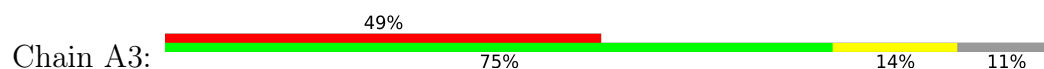


• Molecule 40: NADH:ubiquinone oxidoreductase subunit S5

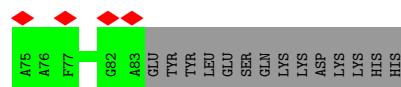
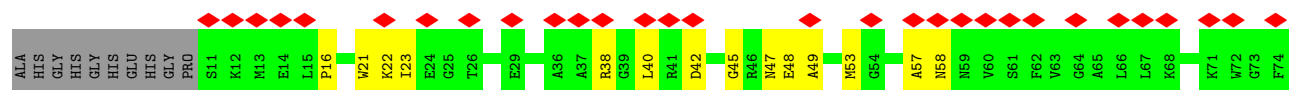




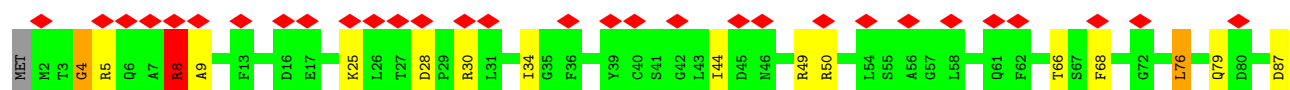
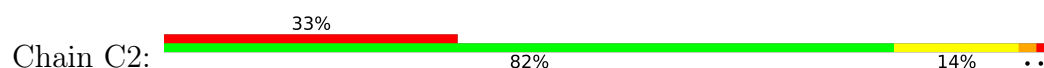
- Molecule 41: NADH:ubiquinone oxidoreductase subunit A3



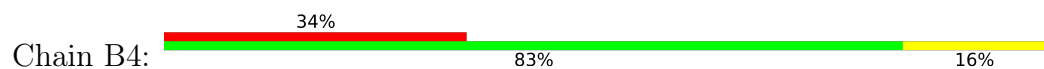
- Molecule 42: NADH:ubiquinone oxidoreductase subunit B3



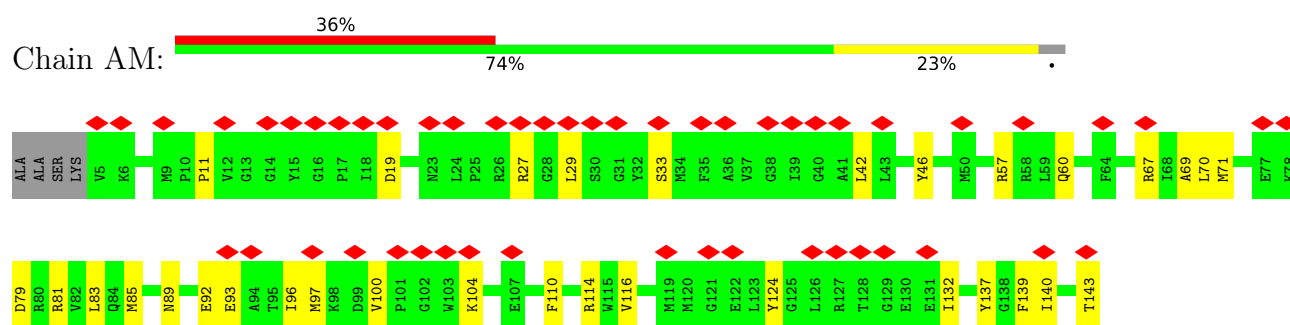
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 subunit C2



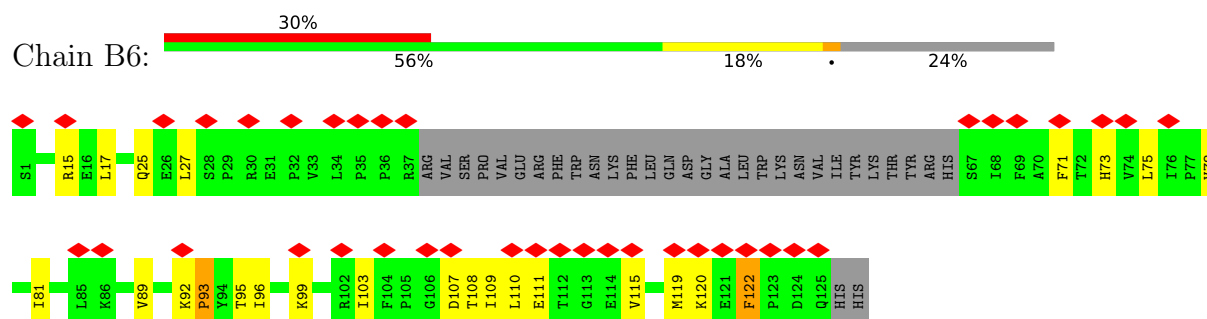
- Molecule 44: NADH:ubiquinone oxidoreductase subunit B4



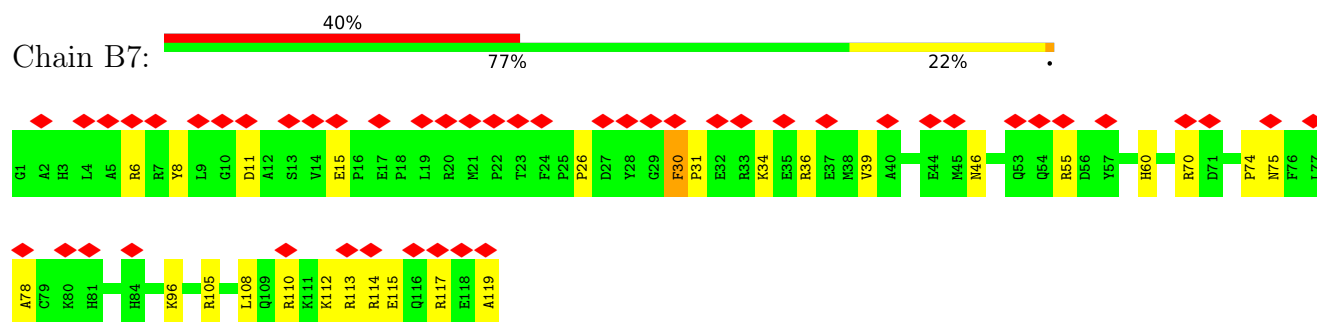
- Molecule 45: MT-ND1



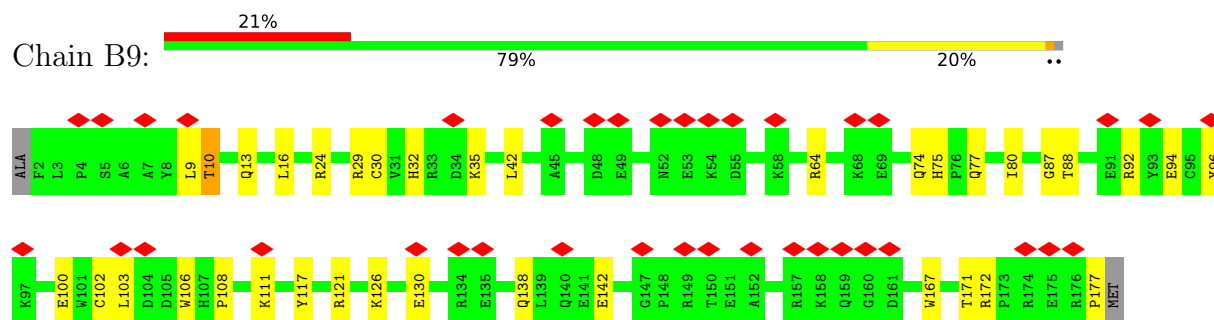
- Molecule 46: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



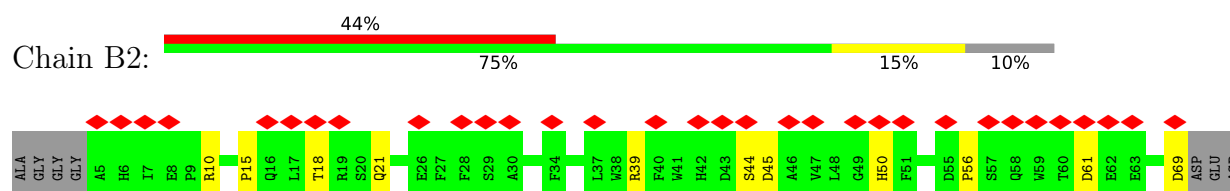
- Molecule 47: NADH:ubiquinone oxidoreductase subunit B7



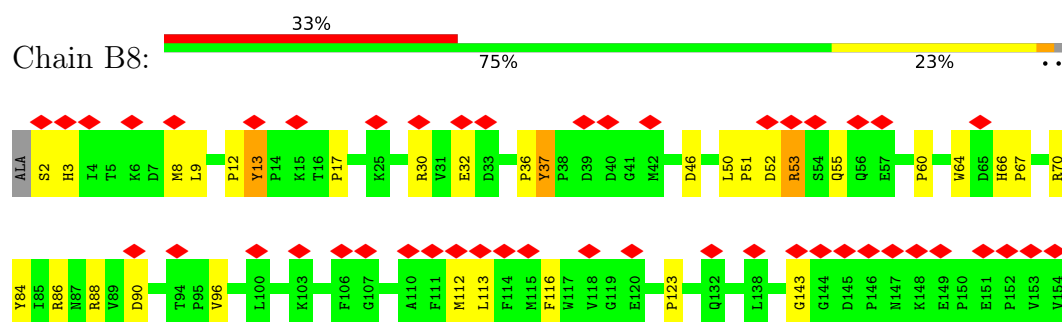
- Molecule 48: NADH:ubiquinone oxidoreductase subunit B9



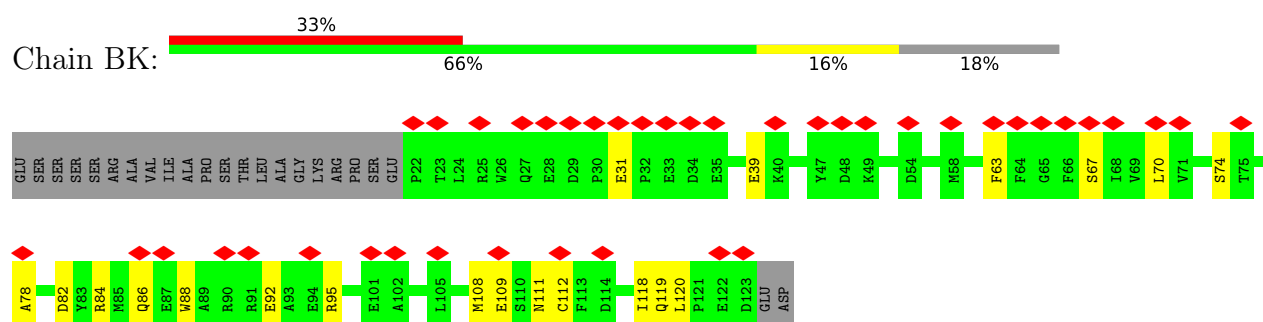
- Molecule 49: NADH:ubiquinone oxidoreductase subunit B2



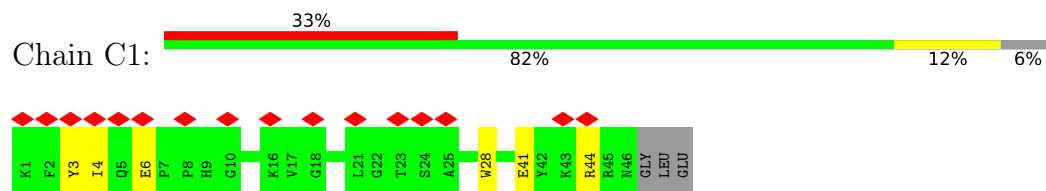
- Molecule 50: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



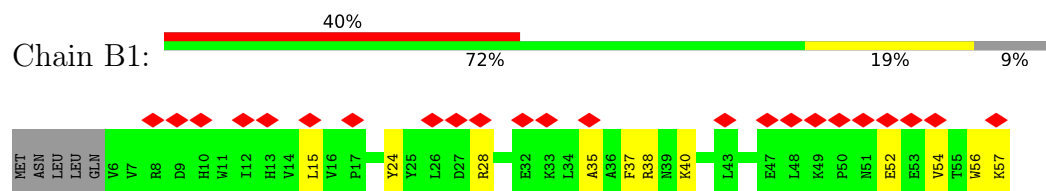
- Molecule 51: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



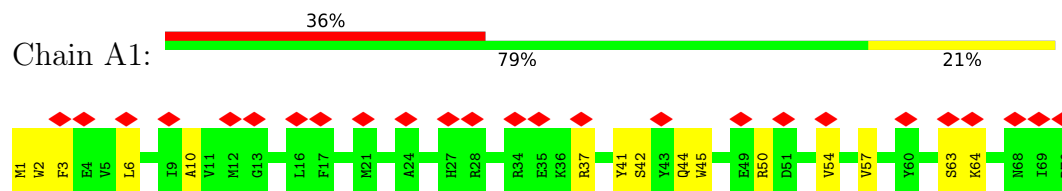
- Molecule 52: NDUFB4



- Molecule 53: NDUFA13



- Molecule 54: NDUFA1



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 35640                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 51                                      | Depositor |
| Minimum defocus (nm)                 | 1500                                    | Depositor |
| Maximum defocus (nm)                 | 3000                                    | Depositor |
| Magnification                        | 100000                                  | Depositor |
| Image detector                       | FEI FALCON II (4k x 4k)                 | Depositor |
| Maximum map value                    | 1.179                                   | Depositor |
| Minimum map value                    | -0.266                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.022                                   | Depositor |
| Recommended contour level            | 0.15                                    | Depositor |
| Map size (Å)                         | 716.8, 716.8, 716.8                     | wwPDB     |
| Map dimensions                       | 512, 512, 512                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.4, 1.4, 1.4                           | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, FMN, SF4, NDP, HEC, 3PE, PC1, ZMP, FES, CDL, HEM

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   | a1    | 0.36         | 0/3479  | 0.66        | 1/4719 (0.0%) |
| 1   | a3    | 0.43         | 0/3518  | 0.69        | 2/4776 (0.0%) |
| 2   | a2    | 0.34         | 0/3183  | 0.60        | 0/4313        |
| 2   | a4    | 0.38         | 0/3179  | 0.63        | 0/4308        |
| 3   | b1    | 0.41         | 0/3119  | 0.64        | 0/4268        |
| 3   | b2    | 0.46         | 0/3119  | 0.68        | 1/4268 (0.0%) |
| 4   | c1    | 0.34         | 0/1968  | 0.65        | 0/2672        |
| 4   | c2    | 0.38         | 0/1962  | 0.68        | 0/2664        |
| 5   | f1    | 0.27         | 0/1554  | 0.55        | 1/2101 (0.0%) |
| 5   | f2    | 0.29         | 0/1548  | 0.56        | 0/2093        |
| 6   | d1    | 0.36         | 0/906   | 0.62        | 0/1213        |
| 6   | d2    | 0.40         | 0/908   | 0.64        | 0/1218        |
| 7   | q1    | 0.35         | 0/638   | 0.65        | 0/862         |
| 7   | q2    | 0.45         | 0/652   | 0.73        | 0/883         |
| 8   | h1    | 0.29         | 0/538   | 0.67        | 0/723         |
| 8   | h2    | 0.35         | 0/538   | 0.78        | 0/723         |
| 10  | i1    | 0.29         | 0/471   | 0.62        | 0/634         |
| 10  | i2    | 0.32         | 0/486   | 0.64        | 0/655         |
| 11  | V1    | 0.39         | 0/3386  | 0.71        | 0/4575        |
| 12  | V2    | 0.39         | 0/1687  | 0.85        | 3/2295 (0.1%) |
| 13  | S1    | 0.43         | 0/5362  | 0.73        | 0/7266        |
| 14  | S2    | 0.52         | 0/3502  | 0.78        | 4/4744 (0.1%) |
| 15  | S3    | 0.49         | 0/1776  | 0.78        | 3/2417 (0.1%) |
| 16  | S7    | 0.52         | 0/1278  | 0.81        | 0/1728        |
| 17  | S8    | 0.59         | 0/1445  | 0.78        | 0/1956        |
| 18  | V3    | 0.33         | 0/355   | 0.76        | 0/480         |
| 19  | S6    | 0.37         | 0/749   | 0.63        | 0/1009        |
| 20  | S4    | 0.41         | 0/1047  | 0.72        | 0/1415        |
| 21  | A9    | 0.37         | 0/2343  | 0.74        | 1/3164 (0.0%) |
| 22  | A2    | 0.32         | 0/676   | 0.72        | 0/911         |
| 23  | A5    | 0.36         | 0/921   | 0.75        | 0/1249        |
| 24  | A6    | 0.38         | 0/993   | 0.71        | 2/1336 (0.1%) |

| Mol | Chain | Bond lengths |         | Bond angles |                  |
|-----|-------|--------------|---------|-------------|------------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5          |
| 25  | A7    | 0.38         | 0/775   | 0.75        | 0/1048           |
| 26  | AL    | 0.37         | 0/1242  | 0.73        | 0/1688           |
| 27  | AA    | 0.31         | 0/655   | 0.75        | 0/881            |
| 27  | AB    | 0.43         | 0/714   | 0.69        | 0/963            |
| 28  | D3    | 0.45         | 0/747   | 0.73        | 1/1022 (0.1%)    |
| 29  | D1    | 0.52         | 0/2487  | 0.86        | 6/3401 (0.2%)    |
| 30  | D6    | 0.41         | 0/1339  | 0.78        | 0/1810           |
| 31  | 4L    | 0.50         | 0/758   | 0.80        | 0/1024           |
| 32  | D5    | 0.49         | 0/4933  | 0.85        | 2/6710 (0.0%)    |
| 33  | D4    | 0.55         | 0/3740  | 0.86        | 1/5095 (0.0%)    |
| 34  | D2    | 0.54         | 0/2788  | 0.79        | 1/3795 (0.0%)    |
| 35  | AK    | 0.40         | 0/1046  | 0.81        | 6/1419 (0.4%)    |
| 36  | B5    | 0.44         | 0/1189  | 0.66        | 0/1607           |
| 37  | A8    | 0.40         | 0/1441  | 0.75        | 0/1942           |
| 38  | BJ    | 0.44         | 0/1475  | 0.75        | 3/1989 (0.2%)    |
| 39  | AJ    | 0.44         | 0/2644  | 0.77        | 8/3579 (0.2%)    |
| 40  | S5    | 0.45         | 0/843   | 0.77        | 0/1128           |
| 41  | A3    | 0.37         | 0/602   | 0.76        | 0/828            |
| 42  | B3    | 0.44         | 0/595   | 0.88        | 1/803 (0.1%)     |
| 43  | C2    | 0.44         | 0/1028  | 0.79        | 4/1388 (0.3%)    |
| 44  | B4    | 0.44         | 0/1085  | 0.73        | 0/1467           |
| 45  | AM    | 0.40         | 0/1172  | 0.75        | 0/1579           |
| 46  | B6    | 0.44         | 0/841   | 0.88        | 1/1144 (0.1%)    |
| 47  | B7    | 0.39         | 0/1051  | 0.73        | 2/1408 (0.1%)    |
| 48  | B9    | 0.49         | 0/1568  | 0.75        | 2/2123 (0.1%)    |
| 49  | B2    | 0.41         | 0/590   | 0.83        | 4/810 (0.5%)     |
| 50  | B8    | 0.48         | 0/1379  | 0.92        | 6/1884 (0.3%)    |
| 51  | BK    | 0.44         | 0/880   | 0.76        | 0/1196           |
| 52  | C1    | 0.35         | 0/404   | 0.71        | 2/548 (0.4%)     |
| 53  | B1    | 0.37         | 0/462   | 0.69        | 0/624            |
| 54  | A1    | 0.38         | 0/592   | 0.70        | 1/795 (0.1%)     |
| All | All   | 0.43         | 0/98351 | 0.74        | 69/133336 (0.1%) |

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 |
|-----|-------|---------------------|---------------------|
| 1   | a1    | 0                   | 3                   |
| 1   | a3    | 0                   | 1                   |
| 2   | a4    | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 3   | b2    | 0                   | 1                   |
| 4   | c1    | 0                   | 1                   |
| 4   | c2    | 0                   | 2                   |
| 5   | f2    | 0                   | 1                   |
| 6   | d1    | 0                   | 1                   |
| 6   | d2    | 0                   | 1                   |
| 11  | V1    | 0                   | 2                   |
| 12  | V2    | 0                   | 4                   |
| 13  | S1    | 0                   | 6                   |
| 14  | S2    | 0                   | 4                   |
| 15  | S3    | 0                   | 3                   |
| 17  | S8    | 0                   | 1                   |
| 18  | V3    | 0                   | 2                   |
| 20  | S4    | 0                   | 2                   |
| 22  | A2    | 0                   | 1                   |
| 23  | A5    | 0                   | 2                   |
| 25  | A7    | 0                   | 2                   |
| 29  | D1    | 0                   | 3                   |
| 30  | D6    | 0                   | 2                   |
| 32  | D5    | 0                   | 4                   |
| 33  | D4    | 0                   | 4                   |
| 34  | D2    | 0                   | 1                   |
| 35  | AK    | 0                   | 3                   |
| 37  | A8    | 0                   | 2                   |
| 38  | BJ    | 0                   | 2                   |
| 39  | AJ    | 0                   | 3                   |
| 40  | S5    | 0                   | 1                   |
| 41  | A3    | 0                   | 1                   |
| 42  | B3    | 0                   | 3                   |
| 43  | C2    | 0                   | 1                   |
| 44  | B4    | 0                   | 1                   |
| 46  | B6    | 0                   | 1                   |
| 47  | B7    | 0                   | 1                   |
| 49  | B2    | 0                   | 1                   |
| 50  | B8    | 0                   | 3                   |
| 51  | BK    | 0                   | 1                   |
| 52  | C1    | 0                   | 1                   |
| 53  | B1    | 0                   | 1                   |
| 54  | A1    | 0                   | 1                   |
| All | All   | 0                   | 82                  |

There are no bond length outliers.

The worst 5 of 69 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 38  | BJ    | 21  | PRO  | CA-C-N | 7.70 | 135.56      | 121.70   |
| 38  | BJ    | 21  | PRO  | C-N-CA | 7.70 | 135.56      | 121.70   |
| 39  | AJ    | 229 | GLU  | CA-C-N | 7.50 | 135.21      | 121.70   |
| 39  | AJ    | 229 | GLU  | C-N-CA | 7.50 | 135.21      | 121.70   |
| 49  | B2    | 44  | SER  | CA-C-N | 7.38 | 134.99      | 121.70   |

There are no chirality outliers.

5 of 82 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | a1    | 190 | TYR  | Peptide |
| 1   | a1    | 193 | PRO  | Peptide |
| 1   | a1    | 309 | THR  | Peptide |
| 4   | c1    | 173 | GLY  | Peptide |
| 6   | d1    | 39  | GLU  | Peptide |

## 5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | a1    | 3409  | 0        | 3322     | 53      | 0            |
| 1   | a3    | 3447  | 0        | 3350     | 49      | 0            |
| 2   | a2    | 3126  | 0        | 3093     | 41      | 0            |
| 2   | a4    | 3122  | 0        | 3090     | 61      | 0            |
| 3   | b1    | 3019  | 0        | 3082     | 48      | 0            |
| 3   | b2    | 3019  | 0        | 3082     | 49      | 0            |
| 4   | c1    | 1909  | 0        | 1858     | 29      | 0            |
| 4   | c2    | 1903  | 0        | 1850     | 33      | 0            |
| 5   | f1    | 1520  | 0        | 1505     | 34      | 0            |
| 5   | f2    | 1514  | 0        | 1497     | 36      | 0            |
| 6   | d1    | 886   | 0        | 883      | 16      | 0            |
| 6   | d2    | 888   | 0        | 880      | 15      | 0            |
| 7   | q1    | 618   | 0        | 628      | 15      | 0            |
| 7   | q2    | 631   | 0        | 639      | 14      | 0            |
| 8   | h1    | 532   | 0        | 509      | 9       | 0            |
| 8   | h2    | 532   | 0        | 509      | 7       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9   | x1    | 114   | 0        | 28       | 4       | 0            |
| 9   | x2    | 130   | 0        | 33       | 0       | 0            |
| 10  | i1    | 459   | 0        | 462      | 8       | 0            |
| 10  | i2    | 473   | 0        | 477      | 4       | 0            |
| 11  | V1    | 3312  | 0        | 3266     | 67      | 0            |
| 12  | V2    | 1647  | 0        | 1657     | 33      | 0            |
| 13  | S1    | 5275  | 0        | 5300     | 141     | 0            |
| 14  | S2    | 3414  | 0        | 3360     | 60      | 0            |
| 15  | S3    | 1726  | 0        | 1676     | 40      | 0            |
| 16  | S7    | 1247  | 0        | 1256     | 29      | 0            |
| 17  | S8    | 1414  | 0        | 1370     | 33      | 0            |
| 18  | V3    | 345   | 0        | 323      | 9       | 0            |
| 19  | S6    | 737   | 0        | 710      | 14      | 0            |
| 20  | S4    | 1024  | 0        | 1023     | 25      | 0            |
| 21  | A9    | 2293  | 0        | 2326     | 55      | 0            |
| 22  | A2    | 665   | 0        | 678      | 16      | 0            |
| 23  | A5    | 901   | 0        | 936      | 13      | 0            |
| 24  | A6    | 969   | 0        | 980      | 20      | 0            |
| 25  | A7    | 757   | 0        | 771      | 22      | 0            |
| 26  | AL    | 1201  | 0        | 1170     | 14      | 0            |
| 27  | AA    | 645   | 0        | 649      | 7       | 0            |
| 27  | AB    | 702   | 0        | 692      | 8       | 0            |
| 28  | D3    | 728   | 0        | 773      | 17      | 0            |
| 29  | D1    | 2415  | 0        | 2542     | 55      | 0            |
| 30  | D6    | 1308  | 0        | 1329     | 35      | 0            |
| 31  | 4L    | 748   | 0        | 794      | 20      | 0            |
| 32  | D5    | 4805  | 0        | 4950     | 116     | 0            |
| 33  | D4    | 3646  | 0        | 3850     | 87      | 0            |
| 34  | D2    | 2724  | 0        | 2930     | 76      | 0            |
| 35  | AK    | 1025  | 0        | 1033     | 20      | 0            |
| 36  | B5    | 1156  | 0        | 1177     | 20      | 0            |
| 37  | A8    | 1404  | 0        | 1384     | 26      | 0            |
| 38  | BJ    | 1441  | 0        | 1417     | 25      | 0            |
| 39  | AJ    | 2583  | 0        | 2547     | 38      | 0            |
| 40  | S5    | 822   | 0        | 820      | 23      | 0            |
| 41  | A3    | 582   | 0        | 583      | 9       | 0            |
| 42  | B3    | 578   | 0        | 570      | 8       | 0            |
| 43  | C2    | 997   | 0        | 983      | 19      | 0            |
| 44  | B4    | 1059  | 0        | 1062     | 19      | 0            |
| 45  | AM    | 1143  | 0        | 1137     | 28      | 0            |
| 46  | B6    | 815   | 0        | 837      | 22      | 0            |
| 47  | B7    | 1026  | 0        | 995      | 23      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 48  | B9    | 1515  | 0        | 1469     | 26      | 0            |
| 49  | B2    | 563   | 0        | 509      | 9       | 0            |
| 50  | B8    | 1324  | 0        | 1219     | 27      | 0            |
| 51  | BK    | 853   | 0        | 800      | 20      | 0            |
| 52  | C1    | 391   | 0        | 391      | 4       | 0            |
| 53  | B1    | 449   | 0        | 453      | 6       | 0            |
| 54  | A1    | 577   | 0        | 570      | 11      | 0            |
| 55  | b1    | 86    | 0        | 60       | 7       | 0            |
| 55  | b2    | 86    | 0        | 60       | 5       | 0            |
| 56  | c1    | 43    | 0        | 30       | 3       | 0            |
| 56  | c2    | 43    | 0        | 30       | 2       | 0            |
| 57  | D1    | 26    | 0        | 26       | 2       | 0            |
| 57  | D4    | 40    | 0        | 54       | 3       | 0            |
| 57  | D5    | 38    | 0        | 50       | 2       | 0            |
| 57  | c1    | 13    | 0        | 12       | 1       | 0            |
| 57  | f2    | 23    | 0        | 20       | 2       | 0            |
| 58  | S1    | 4     | 0        | 0        | 0       | 0            |
| 58  | V2    | 4     | 0        | 0        | 1       | 0            |
| 58  | f1    | 4     | 0        | 0        | 0       | 0            |
| 58  | f2    | 4     | 0        | 0        | 0       | 0            |
| 59  | S1    | 16    | 0        | 0        | 1       | 0            |
| 59  | S7    | 8     | 0        | 0        | 1       | 0            |
| 59  | S8    | 16    | 0        | 0        | 1       | 0            |
| 59  | V1    | 8     | 0        | 0        | 1       | 0            |
| 60  | V1    | 31    | 0        | 19       | 3       | 0            |
| 61  | S6    | 1     | 0        | 0        | 0       | 0            |
| 62  | A9    | 48    | 0        | 26       | 3       | 0            |
| 63  | AA    | 34    | 0        | 40       | 0       | 0            |
| 63  | AB    | 31    | 0        | 34       | 1       | 0            |
| 64  | D5    | 60    | 0        | 64       | 4       | 0            |
| 65  | AK    | 28    | 0        | 30       | 0       | 0            |
| All | All   | 96897 | 0        | 96599    | 1593    | 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 8.

The worst 5 of 1593 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) |
|-----------------|----------------|--------------------------|-------------------|
| 15:S3:80:ALA:HA | 15:S3:91:GLU:O | 1.15                     | 1.24              |
| 4:c2:237:ARG:O  | 7:q2:12:HIS:HA | 1.51                     | 1.10              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 13:S1:449:PRO:O | 13:S1:489:VAL:HA | 1.60                     | 1.02              |
| 15:S3:80:ALA:CA | 15:S3:91:GLU:O   | 2.11                     | 0.98              |
| 15:S3:38:GLN:HA | 25:A7:70:SER:O   | 1.64                     | 0.97              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1   | a1    | 435/446 (98%) | 391 (90%) | 44 (10%) | 0        | 100         | 100 |
| 1   | a3    | 442/446 (99%) | 400 (90%) | 42 (10%) | 0        | 100         | 100 |
| 2   | a2    | 410/439 (93%) | 367 (90%) | 43 (10%) | 0        | 100         | 100 |
| 2   | a4    | 409/439 (93%) | 369 (90%) | 40 (10%) | 0        | 100         | 100 |
| 3   | b1    | 376/379 (99%) | 351 (93%) | 25 (7%)  | 0        | 100         | 100 |
| 3   | b2    | 376/379 (99%) | 349 (93%) | 27 (7%)  | 0        | 100         | 100 |
| 4   | c1    | 237/240 (99%) | 195 (82%) | 42 (18%) | 0        | 100         | 100 |
| 4   | c2    | 236/240 (98%) | 202 (86%) | 34 (14%) | 0        | 100         | 100 |
| 5   | f1    | 194/196 (99%) | 179 (92%) | 15 (8%)  | 0        | 100         | 100 |
| 5   | f2    | 193/196 (98%) | 168 (87%) | 25 (13%) | 0        | 100         | 100 |
| 6   | d1    | 98/110 (89%)  | 93 (95%)  | 5 (5%)   | 0        | 100         | 100 |
| 6   | d2    | 99/110 (90%)  | 96 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 7   | q1    | 71/81 (88%)   | 68 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 7   | q2    | 73/81 (90%)   | 67 (92%)  | 6 (8%)   | 0        | 100         | 100 |
| 8   | h1    | 63/78 (81%)   | 57 (90%)  | 6 (10%)  | 0        | 100         | 100 |
| 8   | h2    | 63/78 (81%)   | 56 (89%)  | 7 (11%)  | 0        | 100         | 100 |
| 10  | i1    | 53/63 (84%)   | 49 (92%)  | 4 (8%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 10  | i2    | 55/63 (87%)    | 53 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 11  | V1    | 428/445 (96%)  | 380 (89%) | 48 (11%) | 0        | 100         | 100 |
| 12  | V2    | 210/217 (97%)  | 165 (79%) | 45 (21%) | 0        | 100         | 100 |
| 13  | S1    | 686/704 (97%)  | 595 (87%) | 90 (13%) | 1 (0%)   | 48          | 82  |
| 14  | S2    | 420/430 (98%)  | 373 (89%) | 47 (11%) | 0        | 100         | 100 |
| 15  | S3    | 206/228 (90%)  | 176 (85%) | 30 (15%) | 0        | 100         | 100 |
| 16  | S7    | 154/179 (86%)  | 136 (88%) | 17 (11%) | 1 (1%)   | 21          | 58  |
| 17  | S8    | 174/176 (99%)  | 155 (89%) | 19 (11%) | 0        | 100         | 100 |
| 18  | V3    | 39/75 (52%)    | 31 (80%)  | 8 (20%)  | 0        | 100         | 100 |
| 19  | S6    | 93/96 (97%)    | 83 (89%)  | 10 (11%) | 0        | 100         | 100 |
| 20  | S4    | 124/133 (93%)  | 108 (87%) | 16 (13%) | 0        | 100         | 100 |
| 21  | A9    | 281/338 (83%)  | 245 (87%) | 36 (13%) | 0        | 100         | 100 |
| 22  | A2    | 80/98 (82%)    | 69 (86%)  | 11 (14%) | 0        | 100         | 100 |
| 23  | A5    | 109/115 (95%)  | 93 (85%)  | 16 (15%) | 0        | 100         | 100 |
| 24  | A6    | 112/127 (88%)  | 104 (93%) | 8 (7%)   | 0        | 100         | 100 |
| 25  | A7    | 91/112 (81%)   | 73 (80%)  | 17 (19%) | 1 (1%)   | 11          | 45  |
| 26  | AL    | 142/145 (98%)  | 111 (78%) | 31 (22%) | 0        | 100         | 100 |
| 27  | AA    | 78/88 (89%)    | 67 (86%)  | 11 (14%) | 0        | 100         | 100 |
| 27  | AB    | 85/88 (97%)    | 77 (91%)  | 8 (9%)   | 0        | 100         | 100 |
| 28  | D3    | 86/115 (75%)   | 83 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 29  | D1    | 299/318 (94%)  | 273 (91%) | 25 (8%)  | 1 (0%)   | 36          | 71  |
| 30  | D6    | 167/175 (95%)  | 144 (86%) | 23 (14%) | 0        | 100         | 100 |
| 31  | 4L    | 96/98 (98%)    | 89 (93%)  | 6 (6%)   | 1 (1%)   | 12          | 47  |
| 32  | D5    | 604/606 (100%) | 524 (87%) | 78 (13%) | 2 (0%)   | 36          | 71  |
| 33  | D4    | 457/459 (100%) | 411 (90%) | 44 (10%) | 2 (0%)   | 30          | 66  |
| 34  | D2    | 345/347 (99%)  | 320 (93%) | 25 (7%)  | 0        | 100         | 100 |
| 35  | AK    | 138/140 (99%)  | 129 (94%) | 9 (6%)   | 0        | 100         | 100 |
| 36  | B5    | 137/143 (96%)  | 120 (88%) | 17 (12%) | 0        | 100         | 100 |
| 37  | A8    | 169/171 (99%)  | 138 (82%) | 31 (18%) | 0        | 100         | 100 |
| 38  | BJ    | 169/175 (97%)  | 150 (89%) | 18 (11%) | 1 (1%)   | 21          | 58  |
| 39  | AJ    | 317/320 (99%)  | 270 (85%) | 46 (14%) | 1 (0%)   | 36          | 71  |

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| Mol | Chain | Analysed          | Favoured    | Allowed    | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|------------|----------|-------------|-----|
| 40  | S5    | 97/105 (92%)      | 82 (84%)    | 15 (16%)   | 0        | 100         | 100 |
| 41  | A3    | 72/83 (87%)       | 58 (81%)    | 14 (19%)   | 0        | 100         | 100 |
| 42  | B3    | 71/97 (73%)       | 59 (83%)    | 12 (17%)   | 0        | 100         | 100 |
| 43  | C2    | 117/120 (98%)     | 100 (86%)   | 17 (14%)   | 0        | 100         | 100 |
| 44  | B4    | 126/128 (98%)     | 112 (89%)   | 14 (11%)   | 0        | 100         | 100 |
| 45  | AM    | 137/143 (96%)     | 126 (92%)   | 11 (8%)    | 0        | 100         | 100 |
| 46  | B6    | 92/127 (72%)      | 79 (86%)    | 12 (13%)   | 1 (1%)   | 11          | 45  |
| 47  | B7    | 117/119 (98%)     | 97 (83%)    | 19 (16%)   | 1 (1%)   | 14          | 49  |
| 48  | B9    | 174/178 (98%)     | 144 (83%)   | 29 (17%)   | 1 (1%)   | 21          | 58  |
| 49  | B2    | 63/72 (88%)       | 51 (81%)    | 12 (19%)   | 0        | 100         | 100 |
| 50  | B8    | 155/158 (98%)     | 115 (74%)   | 38 (24%)   | 2 (1%)   | 9           | 41  |
| 51  | BK    | 100/125 (80%)     | 83 (83%)    | 17 (17%)   | 0        | 100         | 100 |
| 52  | C1    | 44/49 (90%)       | 38 (86%)    | 6 (14%)    | 0        | 100         | 100 |
| 53  | B1    | 50/57 (88%)       | 46 (92%)    | 4 (8%)     | 0        | 100         | 100 |
| 54  | A1    | 68/70 (97%)       | 63 (93%)    | 5 (7%)     | 0        | 100         | 100 |
| All | All   | 11862/12556 (94%) | 10455 (88%) | 1391 (12%) | 16 (0%)  | 49          | 82  |

5 of 16 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | D5    | 84  | PHE  |
| 33  | D4    | 53  | SER  |
| 16  | S7    | 54  | CYS  |
| 25  | A7    | 69  | MET  |
| 32  | D5    | 527 | GLY  |

### 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   | a1    | 366/372 (98%) | 364 (100%) | 2 (0%)   | 81          | 81 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | a3    | 370/372 (100%) | 369 (100%) | 1 (0%)   | 86          | 84  |
| 2   | a2    | 326/341 (96%)  | 324 (99%)  | 2 (1%)   | 78          | 80  |
| 2   | a4    | 326/341 (96%)  | 323 (99%)  | 3 (1%)   | 70          | 75  |
| 3   | b1    | 330/331 (100%) | 328 (99%)  | 2 (1%)   | 78          | 80  |
| 3   | b2    | 330/331 (100%) | 328 (99%)  | 2 (1%)   | 78          | 80  |
| 4   | c1    | 205/206 (100%) | 204 (100%) | 1 (0%)   | 81          | 81  |
| 4   | c2    | 204/206 (99%)  | 203 (100%) | 1 (0%)   | 81          | 81  |
| 5   | f1    | 168/168 (100%) | 168 (100%) | 0        | 100         | 100 |
| 5   | f2    | 167/168 (99%)  | 167 (100%) | 0        | 100         | 100 |
| 6   | d1    | 93/99 (94%)    | 92 (99%)   | 1 (1%)   | 65          | 73  |
| 6   | d2    | 94/99 (95%)    | 93 (99%)   | 1 (1%)   | 65          | 73  |
| 7   | q1    | 66/72 (92%)    | 66 (100%)  | 0        | 100         | 100 |
| 7   | q2    | 67/72 (93%)    | 65 (97%)   | 2 (3%)   | 36          | 57  |
| 8   | h1    | 62/74 (84%)    | 60 (97%)   | 2 (3%)   | 34          | 56  |
| 8   | h2    | 62/74 (84%)    | 61 (98%)   | 1 (2%)   | 55          | 69  |
| 10  | i1    | 46/52 (88%)    | 45 (98%)   | 1 (2%)   | 45          | 64  |
| 10  | i2    | 48/52 (92%)    | 48 (100%)  | 0        | 100         | 100 |
| 11  | V1    | 344/354 (97%)  | 342 (99%)  | 2 (1%)   | 78          | 80  |
| 12  | V2    | 182/183 (100%) | 179 (98%)  | 3 (2%)   | 55          | 69  |
| 13  | S1    | 578/588 (98%)  | 573 (99%)  | 5 (1%)   | 70          | 75  |
| 14  | S2    | 368/371 (99%)  | 364 (99%)  | 4 (1%)   | 65          | 73  |
| 15  | S3    | 189/204 (93%)  | 188 (100%) | 1 (0%)   | 81          | 81  |
| 16  | S7    | 132/150 (88%)  | 130 (98%)  | 2 (2%)   | 57          | 70  |
| 17  | S8    | 151/151 (100%) | 150 (99%)  | 1 (1%)   | 76          | 78  |
| 18  | V3    | 40/68 (59%)    | 39 (98%)   | 1 (2%)   | 42          | 62  |
| 19  | S6    | 79/80 (99%)    | 79 (100%)  | 0        | 100         | 100 |
| 20  | S4    | 113/119 (95%)  | 113 (100%) | 0        | 100         | 100 |
| 21  | A9    | 246/292 (84%)  | 245 (100%) | 1 (0%)   | 84          | 82  |
| 22  | A2    | 73/81 (90%)    | 73 (100%)  | 0        | 100         | 100 |
| 23  | A5    | 99/101 (98%)   | 98 (99%)   | 1 (1%)   | 68          | 75  |
| 24  | A6    | 107/113 (95%)  | 107 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 25  | A7    | 83/94 (88%)    | 83 (100%)  | 0        | 100         | 100 |
| 26  | AL    | 130/131 (99%)  | 128 (98%)  | 2 (2%)   | 57          | 70  |
| 27  | AA    | 74/81 (91%)    | 73 (99%)   | 1 (1%)   | 59          | 70  |
| 27  | AB    | 80/81 (99%)    | 80 (100%)  | 0        | 100         | 100 |
| 28  | D3    | 81/103 (79%)   | 81 (100%)  | 0        | 100         | 100 |
| 29  | D1    | 266/278 (96%)  | 262 (98%)  | 4 (2%)   | 57          | 70  |
| 30  | D6    | 140/144 (97%)  | 137 (98%)  | 3 (2%)   | 47          | 65  |
| 31  | 4L    | 87/87 (100%)   | 87 (100%)  | 0        | 100         | 100 |
| 32  | D5    | 539/539 (100%) | 534 (99%)  | 5 (1%)   | 70          | 75  |
| 33  | D4    | 412/412 (100%) | 407 (99%)  | 5 (1%)   | 63          | 73  |
| 34  | D2    | 315/315 (100%) | 314 (100%) | 1 (0%)   | 86          | 84  |
| 35  | AK    | 101/101 (100%) | 101 (100%) | 0        | 100         | 100 |
| 36  | B5    | 122/125 (98%)  | 120 (98%)  | 2 (2%)   | 55          | 69  |
| 37  | A8    | 154/154 (100%) | 154 (100%) | 0        | 100         | 100 |
| 38  | BJ    | 155/157 (99%)  | 153 (99%)  | 2 (1%)   | 61          | 71  |
| 39  | AJ    | 283/284 (100%) | 283 (100%) | 0        | 100         | 100 |
| 40  | S5    | 88/94 (94%)    | 87 (99%)   | 1 (1%)   | 65          | 73  |
| 41  | A3    | 65/71 (92%)    | 65 (100%)  | 0        | 100         | 100 |
| 42  | B3    | 55/75 (73%)    | 55 (100%)  | 0        | 100         | 100 |
| 43  | C2    | 106/107 (99%)  | 105 (99%)  | 1 (1%)   | 70          | 75  |
| 44  | B4    | 114/114 (100%) | 113 (99%)  | 1 (1%)   | 70          | 75  |
| 45  | AM    | 119/121 (98%)  | 119 (100%) | 0        | 100         | 100 |
| 46  | B6    | 92/121 (76%)   | 90 (98%)   | 2 (2%)   | 45          | 64  |
| 47  | B7    | 108/108 (100%) | 107 (99%)  | 1 (1%)   | 70          | 75  |
| 48  | B9    | 159/160 (99%)  | 159 (100%) | 0        | 100         | 100 |
| 49  | B2    | 59/62 (95%)    | 59 (100%)  | 0        | 100         | 100 |
| 50  | B8    | 142/142 (100%) | 140 (99%)  | 2 (1%)   | 59          | 70  |
| 51  | BK    | 93/112 (83%)   | 92 (99%)   | 1 (1%)   | 65          | 73  |
| 52  | C1    | 42/44 (96%)    | 42 (100%)  | 0        | 100         | 100 |
| 53  | B1    | 48/53 (91%)    | 48 (100%)  | 0        | 100         | 100 |
| 54  | A1    | 59/59 (100%)   | 58 (98%)   | 1 (2%)   | 53          | 67  |

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| Mol | Chain | Analysed          | Rotameric   | Outliers | Percentiles |    |
|-----|-------|-------------------|-------------|----------|-------------|----|
| All | All   | 10402/10814 (96%) | 10324 (99%) | 78 (1%)  | 73          | 78 |

5 of 78 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | D5    | 553 | LEU  |
| 46  | B6    | 89  | VAL  |
| 33  | D4    | 126 | LEU  |
| 36  | B5    | 66  | TYR  |
| 50  | B8    | 96  | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 226 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | S7    | 127 | HIS  |
| 53  | B1    | 51  | ASN  |
| 29  | D1    | 5   | ASN  |
| 51  | BK    | 45  | HIS  |
| 43  | C2    | 59  | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 28 ligands modelled in this entry, 1 is monoatomic - leaving 27 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 |
| 58  | FES  | f1    | 501 | 5    | 0,4,4        | -    | -        | -           |      |          |
| 56  | HEC  | c1    | 501 | 4    | 46,50,50     | 2.00 | 9 (19%)  | 58,82,82    | 1.88 | 9 (15%)  |
| 58  | FES  | f2    | 202 | 5    | 0,4,4        | -    | -        | -           |      |          |
| 59  | SF4  | V1    | 500 | 11   | 0,12,12      | -    | -        | -           |      |          |
| 55  | HEM  | b2    | 402 | 3    | 50,50,50     | 1.66 | 9 (18%)  | 67,82,82    | 1.77 | 15 (22%) |
| 58  | FES  | S1    | 803 | 13   | 0,4,4        | -    | -        | -           |      |          |
| 59  | SF4  | S8    | 201 | 17   | 0,12,12      | -    | -        | -           |      |          |
| 59  | SF4  | S8    | 202 | 17   | 0,12,12      | -    | -        | -           |      |          |
| 57  | 3PE  | D1    | 501 | -    | 25,25,50     | 0.40 | 0        | 28,30,55    | 0.46 | 0        |
| 56  | HEC  | c2    | 501 | 4    | 46,50,50     | 2.00 | 9 (19%)  | 58,82,82    | 2.06 | 7 (12%)  |
| 57  | 3PE  | c1    | 502 | -    | 12,12,50     | 0.63 | 0        | 13,15,55    | 0.66 | 0        |
| 63  | ZMP  | AB    | 101 | 27   | 25,30,36     | 0.67 | 0        | 29,37,45    | 1.47 | 4 (13%)  |
| 59  | SF4  | S1    | 801 | 13   | 0,12,12      | -    | -        | -           |      |          |
| 57  | 3PE  | f2    | 201 | -    | 22,22,50     | 0.44 | 0        | 25,27,55    | 0.47 | 0        |
| 63  | ZMP  | AA    | 101 | 27   | 28,33,36     | 0.57 | 0        | 32,40,45    | 1.08 | 2 (6%)   |
| 60  | FMN  | V1    | 501 | -    | 33,33,33     | 0.45 | 0        | 48,50,50    | 0.39 | 0        |
| 62  | NDP  | A9    | 401 | -    | 51,52,52     | 0.50 | 1 (1%)   | 71,80,80    | 0.64 | 1 (1%)   |
| 55  | HEM  | b1    | 402 | 3    | 50,50,50     | 1.55 | 7 (14%)  | 67,82,82    | 1.87 | 15 (22%) |
| 57  | 3PE  | D5    | 902 | -    | 37,37,50     | 0.36 | 0        | 40,42,55    | 0.41 | 0        |
| 59  | SF4  | S7    | 300 | 16   | 0,12,12      | -    | -        | -           |      |          |
| 55  | HEM  | b1    | 401 | 3    | 50,50,50     | 1.51 | 7 (14%)  | 67,82,82    | 1.76 | 14 (20%) |
| 65  | PC1  | AK    | 201 | -    | 27,27,53     | 0.41 | 0        | 33,35,61    | 0.41 | 0        |
| 64  | CDL  | D5    | 901 | -    | 59,59,99     | 0.40 | 0        | 65,71,111   | 0.57 | 1 (1%)   |
| 59  | SF4  | S1    | 802 | 13   | 0,12,12      | -    | -        | -           |      |          |
| 57  | 3PE  | D4    | 501 | -    | 39,39,50     | 0.34 | 0        | 42,44,55    | 0.39 | 0        |
| 55  | HEM  | b2    | 401 | 3    | 50,50,50     | 1.54 | 9 (18%)  | 67,82,82    | 1.79 | 18 (26%) |
| 58  | FES  | V2    | 300 | 12   | 0,4,4        | -    | -        | -           |      |          |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 58  | FES  | f1    | 501 | 5    | -       | -        | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions     | Rings   |
|-----|------|-------|-----|------|---------|--------------|---------|
| 56  | HEC  | c1    | 501 | 4    | -       | 8/14/54/54   | -       |
| 58  | FES  | f2    | 202 | 5    | -       | -            | 0/1/1/1 |
| 59  | SF4  | V1    | 500 | 11   | -       | -            | 0/6/5/5 |
| 55  | HEM  | b2    | 402 | 3    | -       | 6/14/54/54   | -       |
| 58  | FES  | S1    | 803 | 13   | -       | -            | 0/1/1/1 |
| 59  | SF4  | S8    | 201 | 17   | -       | -            | 0/6/5/5 |
| 59  | SF4  | S8    | 202 | 17   | -       | -            | 0/6/5/5 |
| 57  | 3PE  | D1    | 501 | -    | -       | 12/28/28/54  | -       |
| 56  | HEC  | c2    | 501 | 4    | -       | 7/14/54/54   | -       |
| 57  | 3PE  | c1    | 502 | -    | -       | 7/13/13/54   | -       |
| 63  | ZMP  | AB    | 101 | 27   | -       | 17/35/37/43  | -       |
| 59  | SF4  | S1    | 801 | 13   | -       | -            | 0/6/5/5 |
| 57  | 3PE  | f2    | 201 | -    | -       | 7/26/26/54   | -       |
| 63  | ZMP  | AA    | 101 | 27   | -       | 16/38/40/43  | -       |
| 60  | FMN  | V1    | 501 | -    | -       | 7/18/18/18   | 0/3/3/3 |
| 62  | NDP  | A9    | 401 | -    | -       | 9/34/77/77   | 0/5/5/5 |
| 55  | HEM  | b1    | 402 | 3    | -       | 9/14/54/54   | -       |
| 57  | 3PE  | D5    | 902 | -    | -       | 12/41/41/54  | -       |
| 59  | SF4  | S7    | 300 | 16   | -       | -            | 0/6/5/5 |
| 55  | HEM  | b1    | 401 | 3    | -       | 9/14/54/54   | -       |
| 65  | PC1  | AK    | 201 | -    | -       | 8/31/31/57   | -       |
| 64  | CDL  | D5    | 901 | -    | -       | 12/70/70/110 | -       |
| 59  | SF4  | S1    | 802 | 13   | -       | -            | 0/6/5/5 |
| 57  | 3PE  | D4    | 501 | -    | -       | 7/43/43/54   | -       |
| 55  | HEM  | b2    | 401 | 3    | -       | 5/14/54/54   | -       |
| 58  | FES  | V2    | 300 | 12   | -       | -            | 0/1/1/1 |

The worst 5 of 51 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 56  | c1    | 501 | HEC  | CAC-C3C | 7.10  | 1.58        | 1.35     |
| 56  | c2    | 501 | HEC  | CAC-C3C | 6.64  | 1.56        | 1.35     |
| 56  | c1    | 501 | HEC  | CAB-C3B | 6.48  | 1.56        | 1.35     |
| 56  | c2    | 501 | HEC  | CAB-C3B | 6.33  | 1.55        | 1.35     |
| 55  | b1    | 401 | HEM  | C4D-ND  | -4.51 | 1.32        | 1.40     |

The worst 5 of 86 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 56  | c2    | 501 | HEC  | CBC-CAC-C3C | -9.20 | 109.04      | 127.43   |
| 56  | c2    | 501 | HEC  | CBB-CAB-C3B | -8.64 | 110.17      | 127.43   |
| 56  | c1    | 501 | HEC  | CBB-CAB-C3B | -7.77 | 111.90      | 127.43   |
| 55  | b1    | 402 | HEM  | CHC-C4B-NB  | 6.38  | 131.28      | 124.42   |
| 55  | b1    | 401 | HEM  | CHC-C4B-NB  | 6.26  | 131.16      | 124.42   |

There are no chirality outliers.

5 of 158 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 55  | b1    | 401 | HEM  | C2B-C3B-CAB-CBB |
| 55  | b1    | 401 | HEM  | C4B-C3B-CAB-CBB |
| 55  | b1    | 401 | HEM  | C2C-C3C-CAC-CBC |
| 55  | b1    | 402 | HEM  | C2B-C3B-CAB-CBB |
| 55  | b1    | 402 | HEM  | C4B-C3B-CAB-CBB |

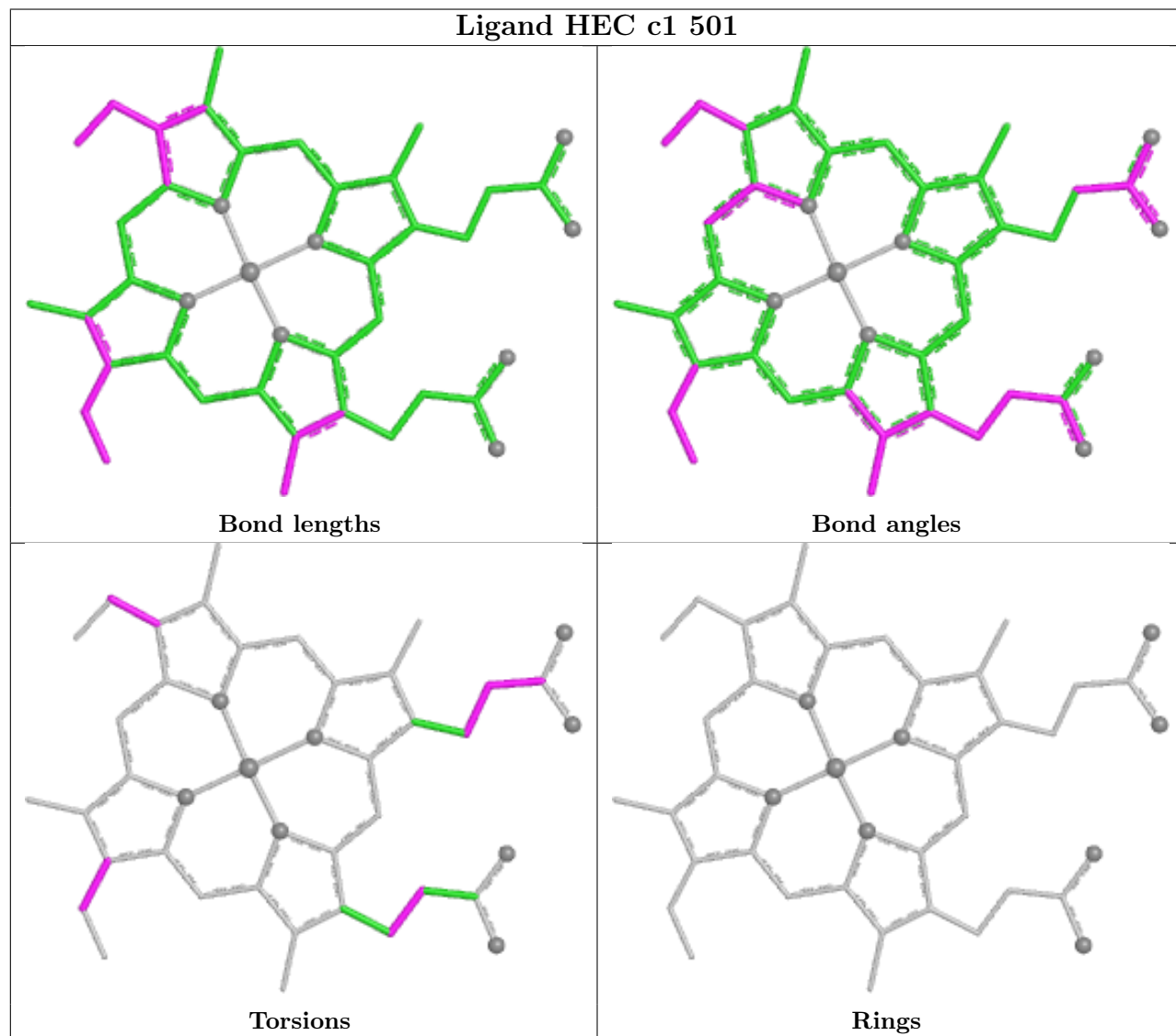
There are no ring outliers.

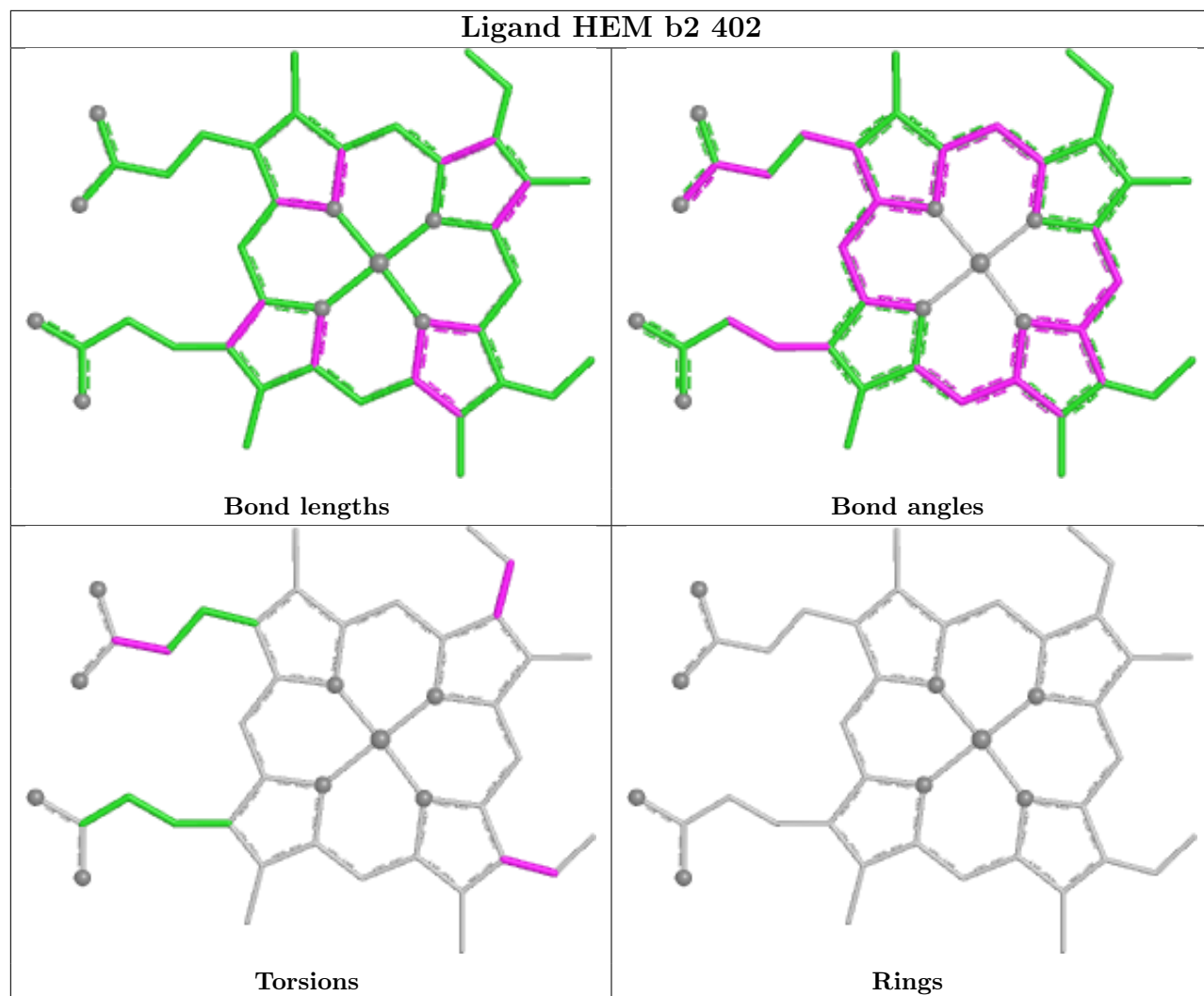
20 monomers are involved in 43 short contacts:

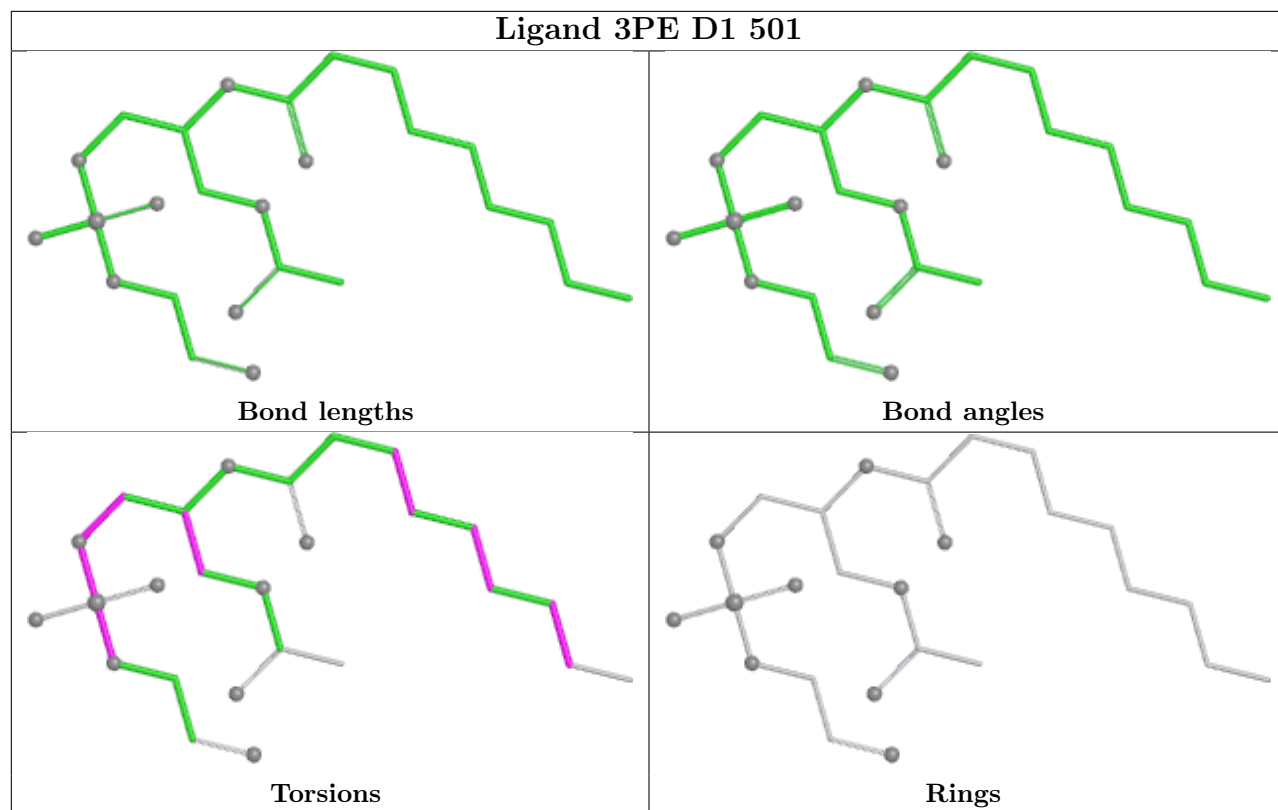
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 56  | c1    | 501 | HEC  | 3       | 0            |
| 59  | V1    | 500 | SF4  | 1       | 0            |
| 55  | b2    | 402 | HEM  | 2       | 0            |
| 59  | S8    | 202 | SF4  | 1       | 0            |
| 57  | D1    | 501 | 3PE  | 2       | 0            |
| 56  | c2    | 501 | HEC  | 2       | 0            |
| 57  | c1    | 502 | 3PE  | 1       | 0            |
| 63  | AB    | 101 | ZMP  | 1       | 0            |
| 59  | S1    | 801 | SF4  | 1       | 0            |
| 57  | f2    | 201 | 3PE  | 2       | 0            |
| 60  | V1    | 501 | FMN  | 3       | 0            |
| 62  | A9    | 401 | NDP  | 3       | 0            |
| 55  | b1    | 402 | HEM  | 3       | 0            |
| 57  | D5    | 902 | 3PE  | 2       | 0            |
| 59  | S7    | 300 | SF4  | 1       | 0            |
| 55  | b1    | 401 | HEM  | 4       | 0            |
| 64  | D5    | 901 | CDL  | 4       | 0            |
| 57  | D4    | 501 | 3PE  | 3       | 0            |
| 55  | b2    | 401 | HEM  | 3       | 0            |
| 58  | V2    | 300 | FES  | 1       | 0            |

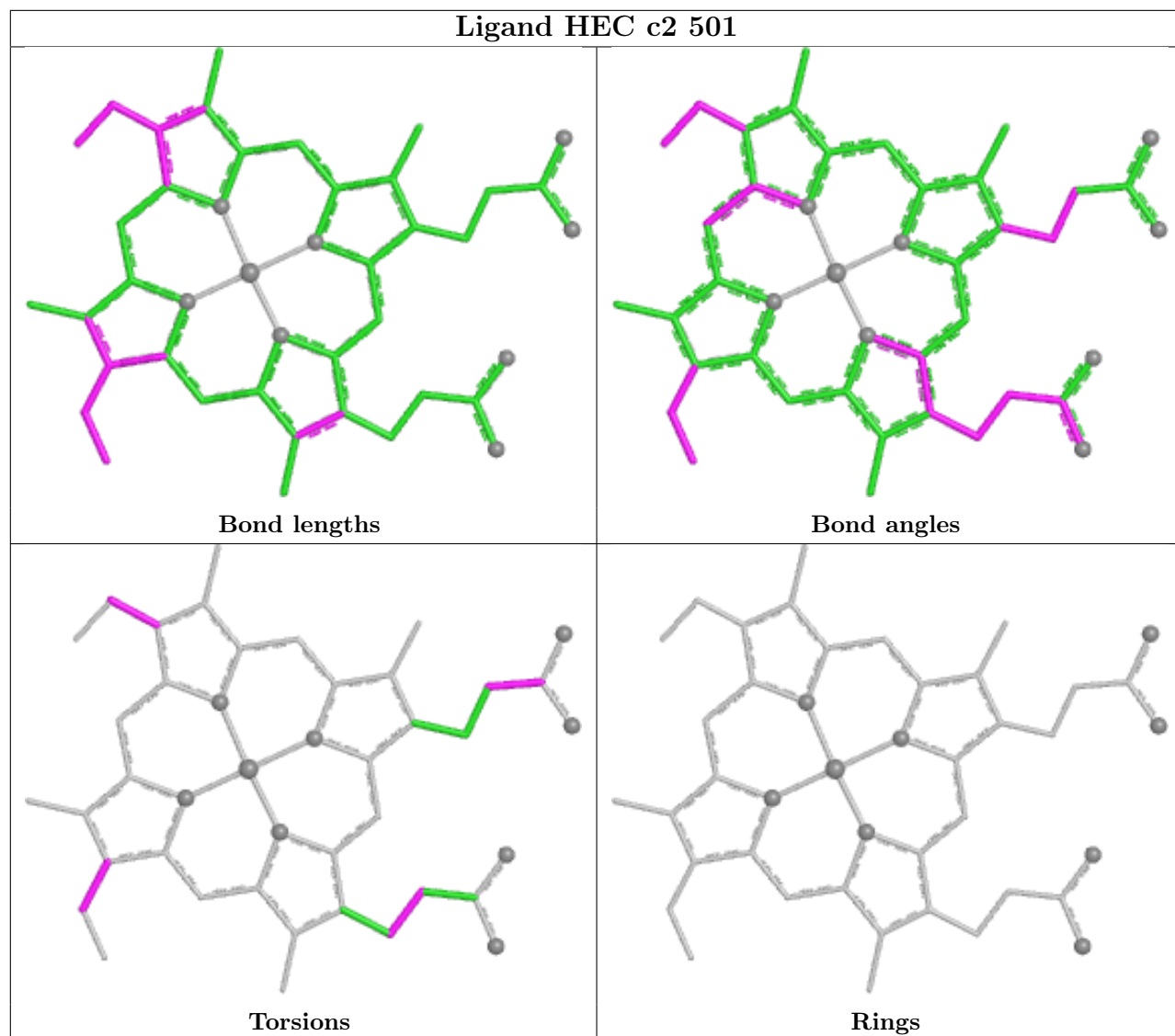
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

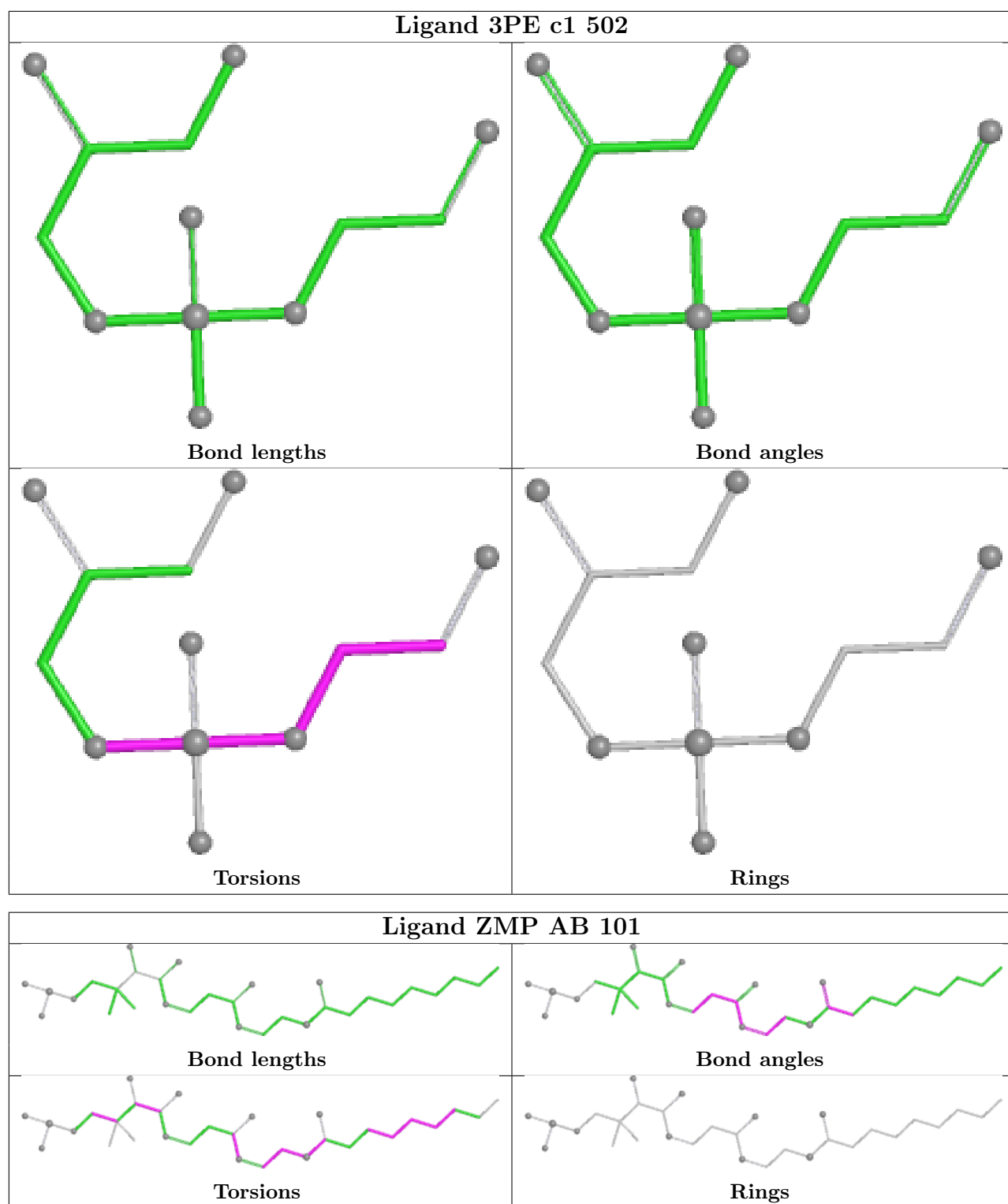
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

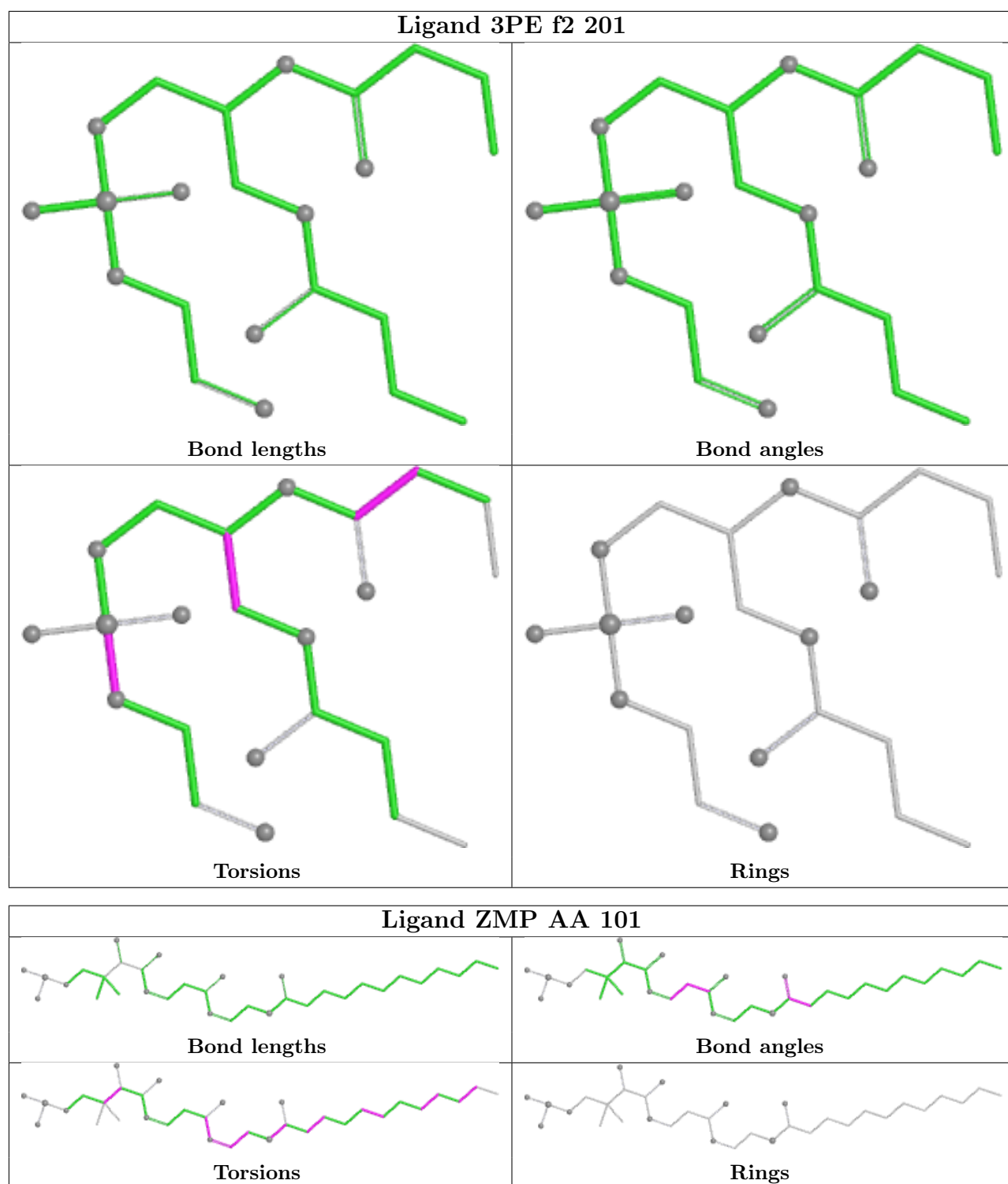




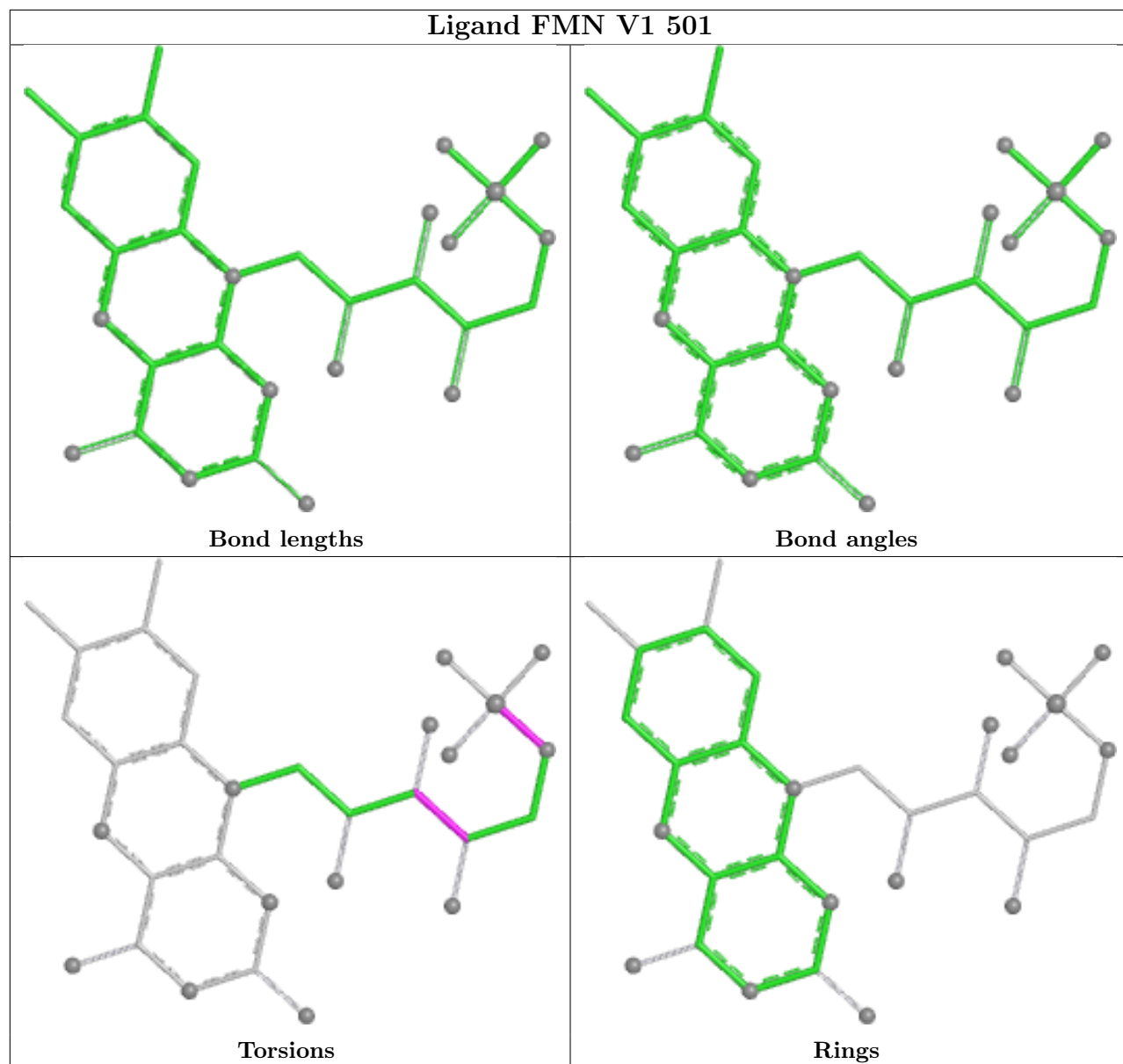


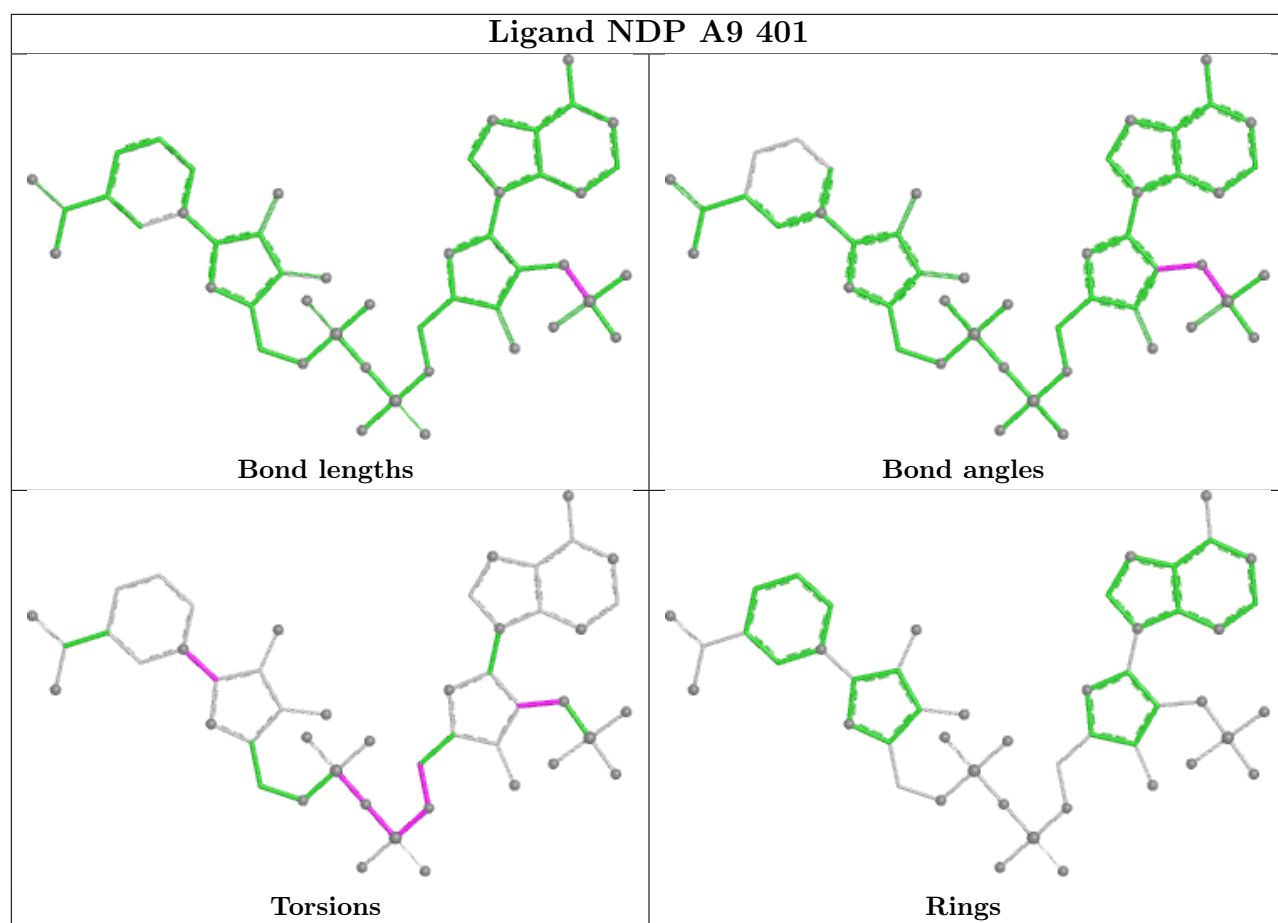


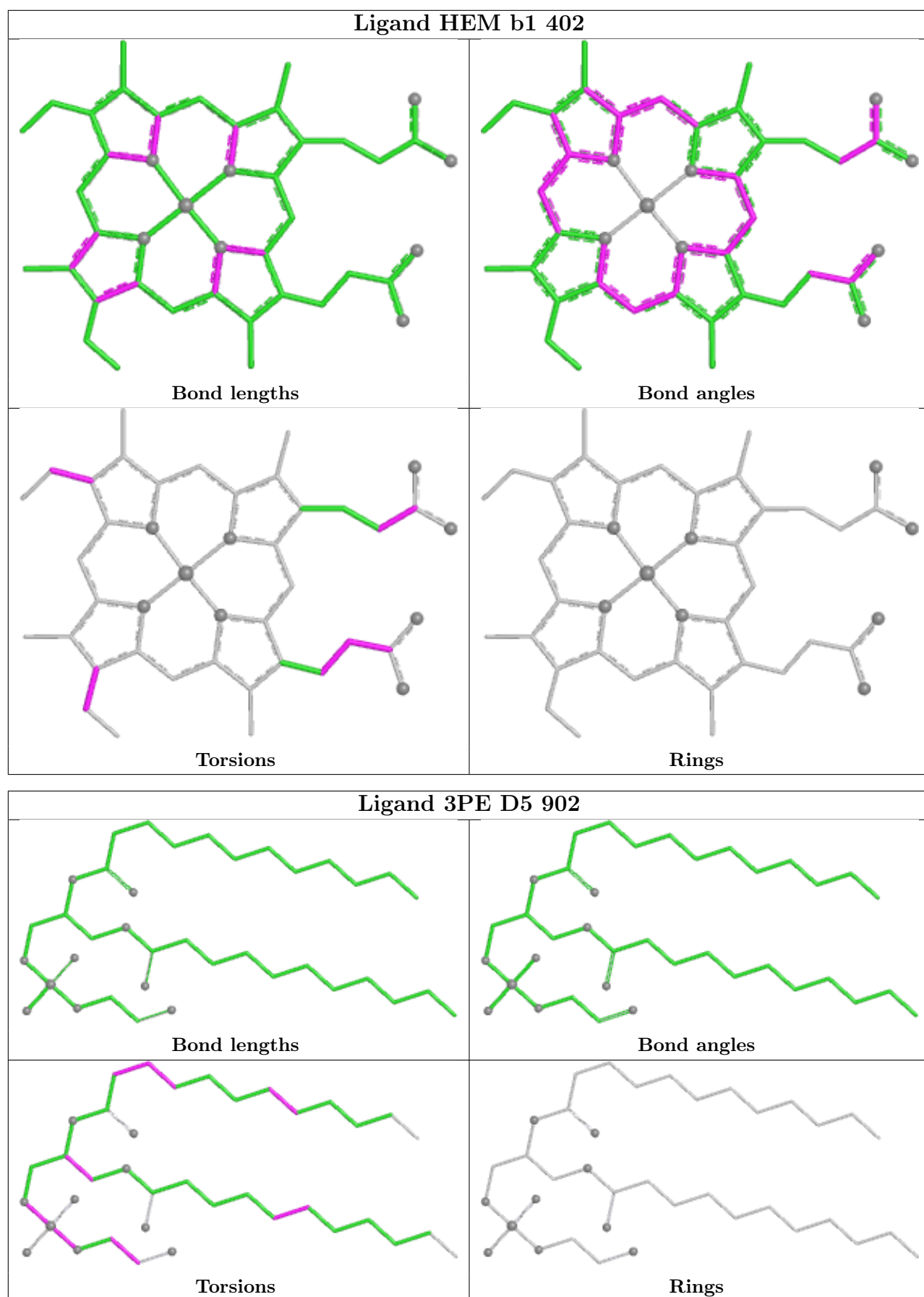


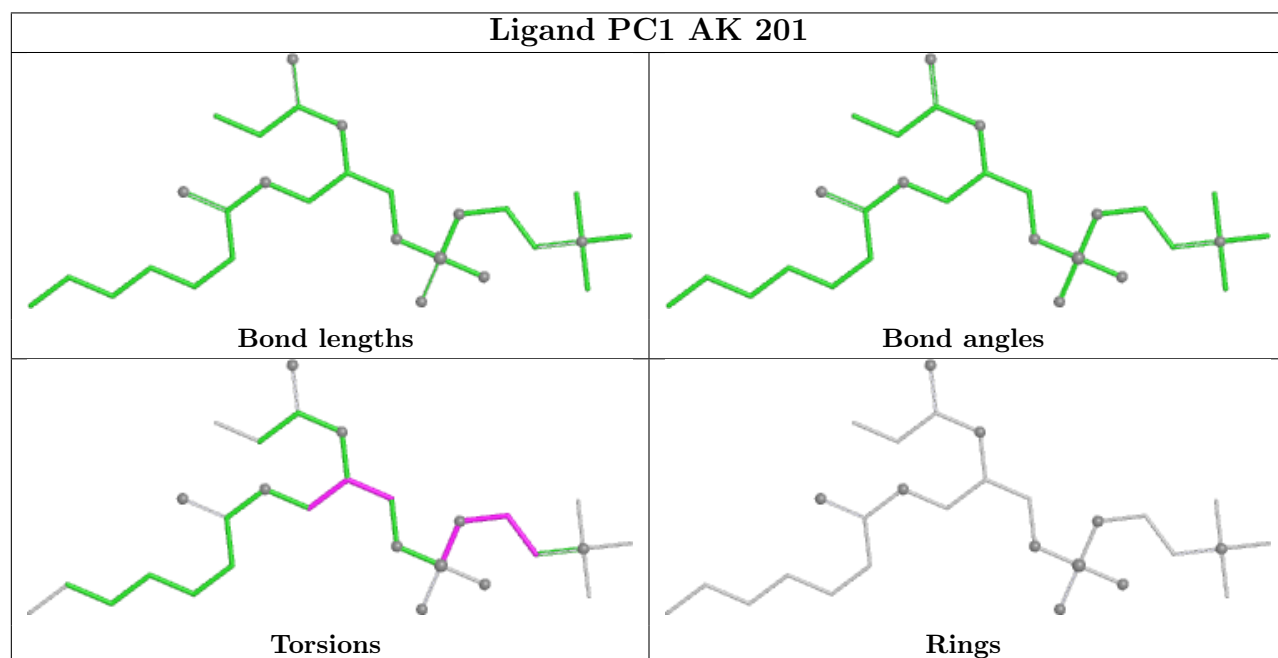
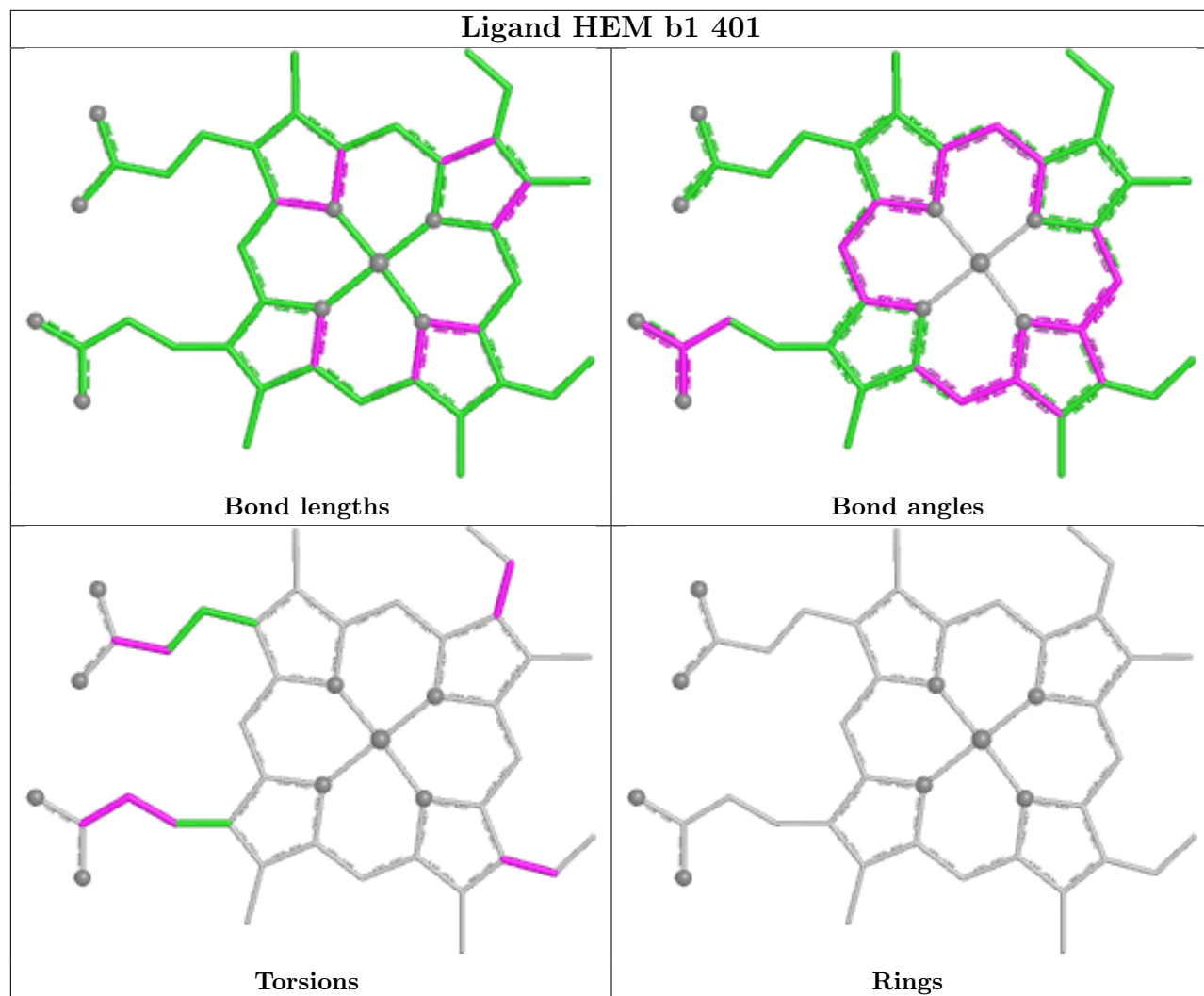


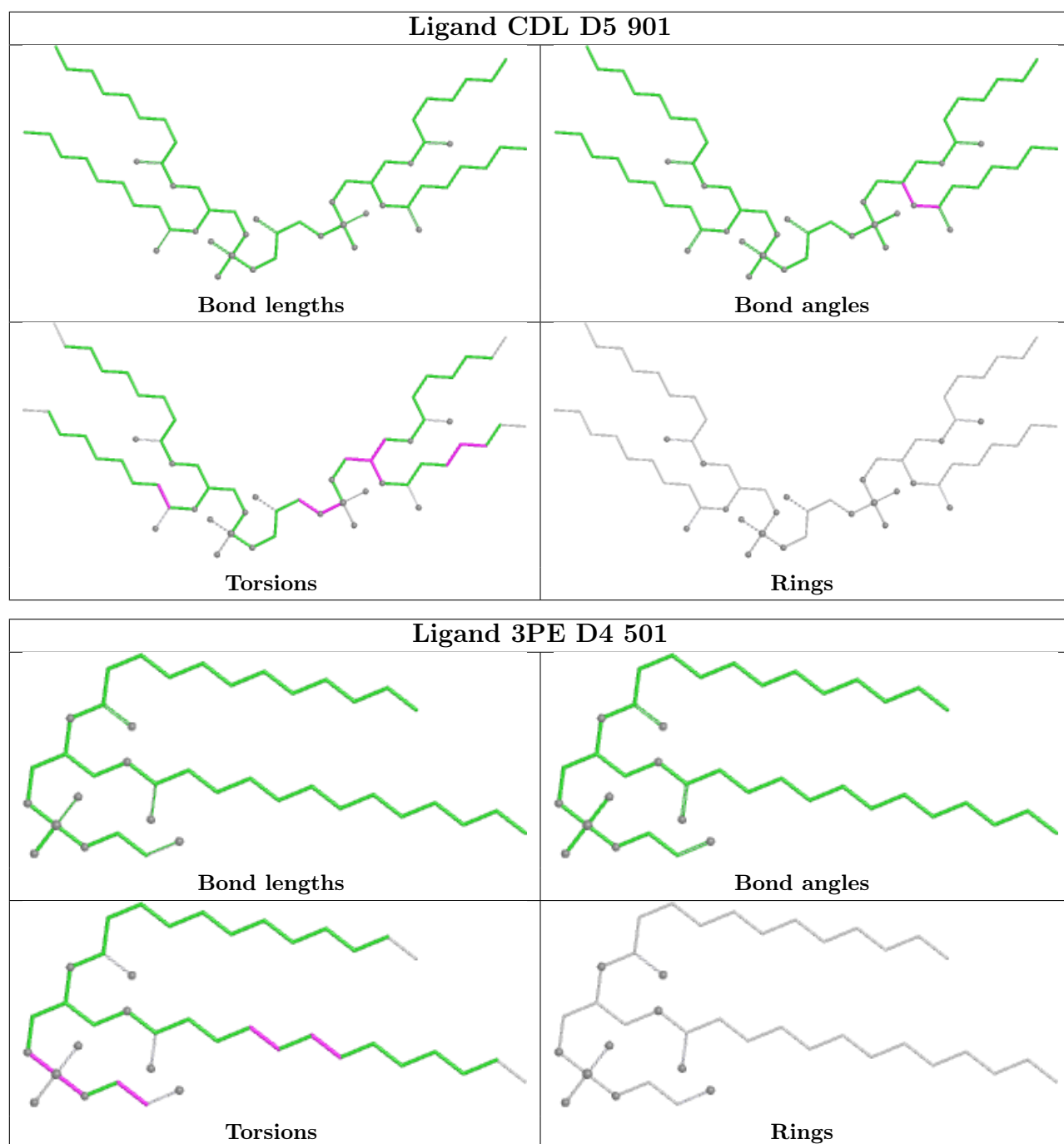
## Ligand FMN V1 501

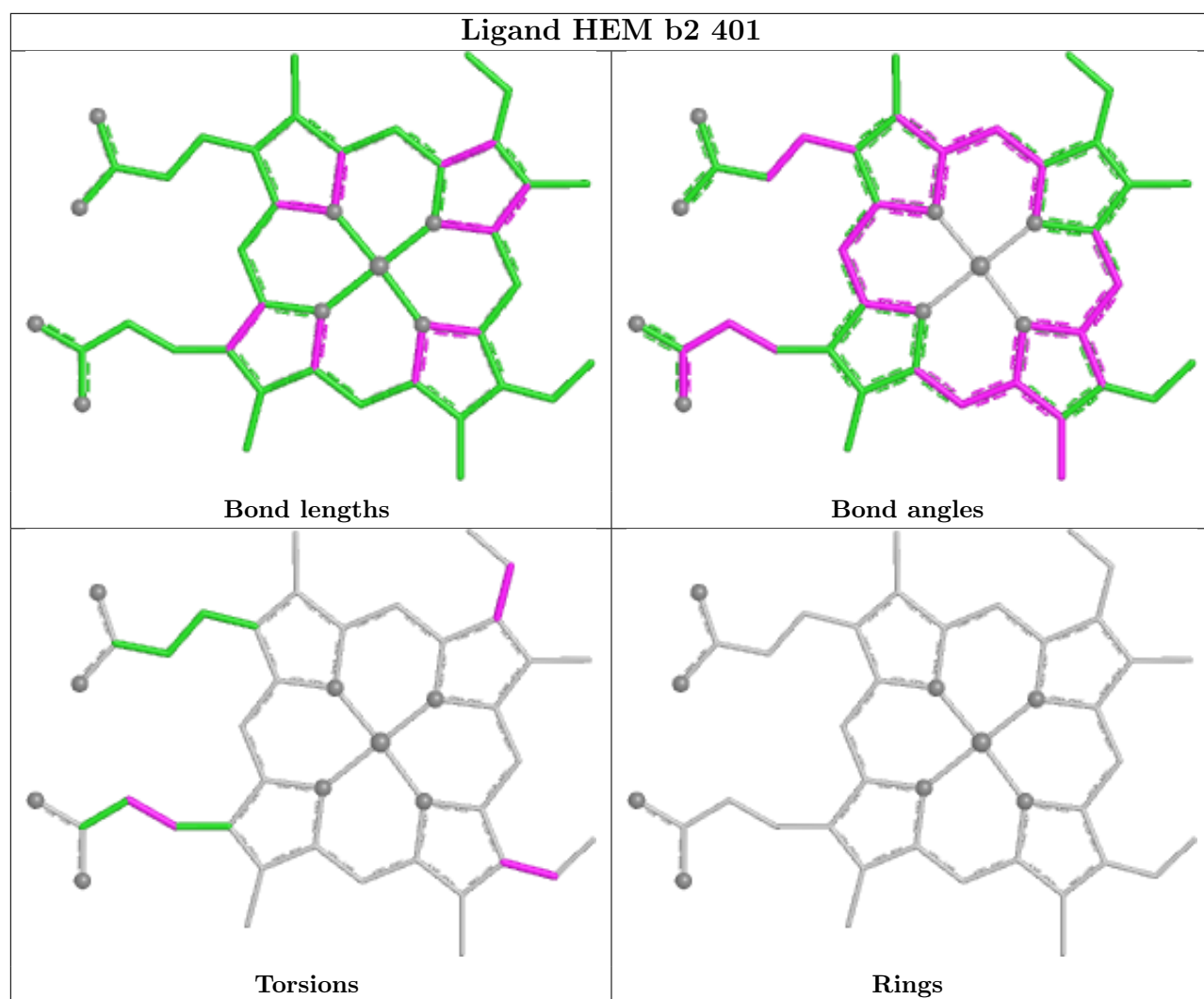












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

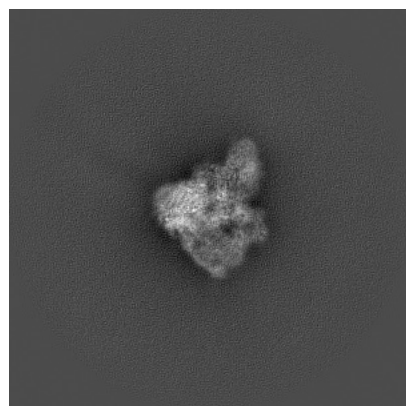
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4495. These allow visual inspection of the internal detail of the map and identification of artifacts.

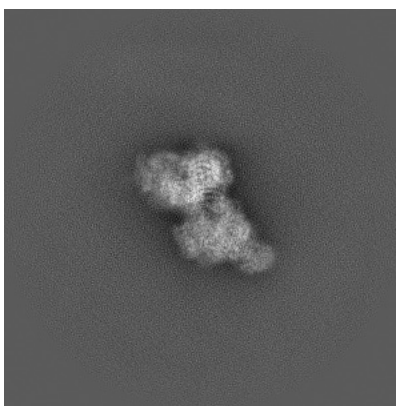
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

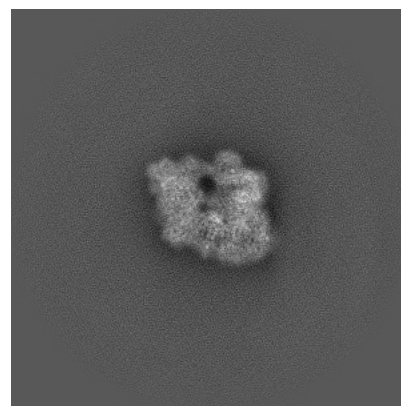
#### 6.1.1 Primary map



X

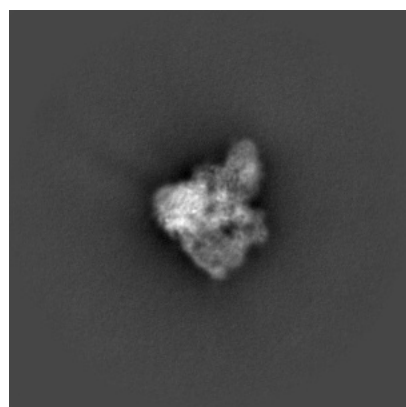


Y

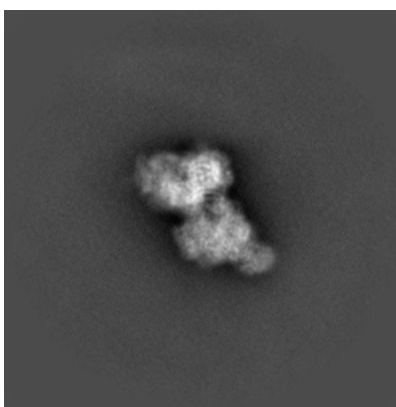


Z

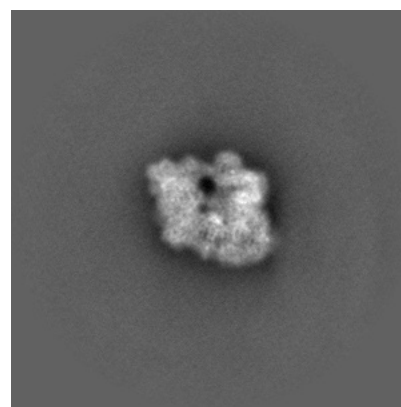
#### 6.1.2 Raw map



X



Y

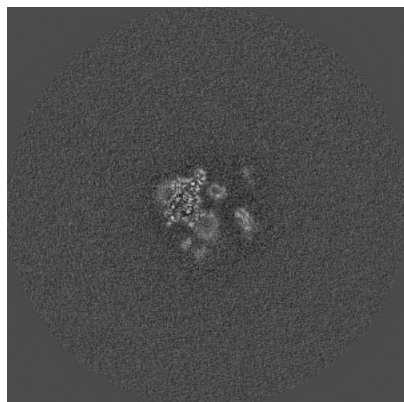


Z

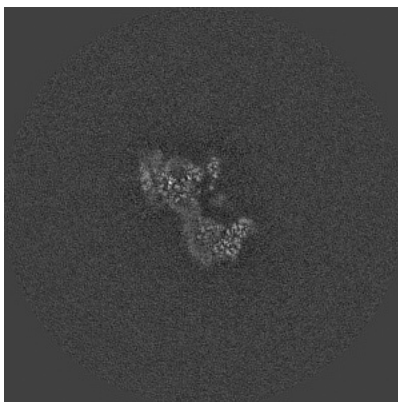
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

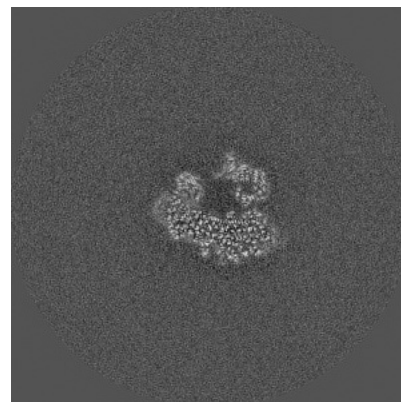
### 6.2.1 Primary map



X Index: 256

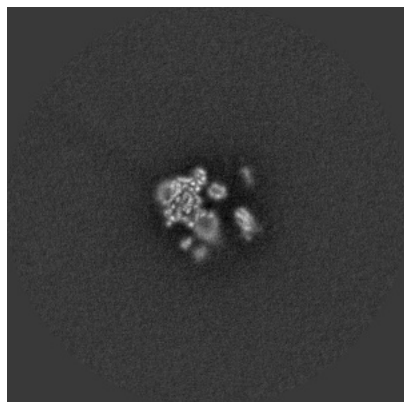


Y Index: 256

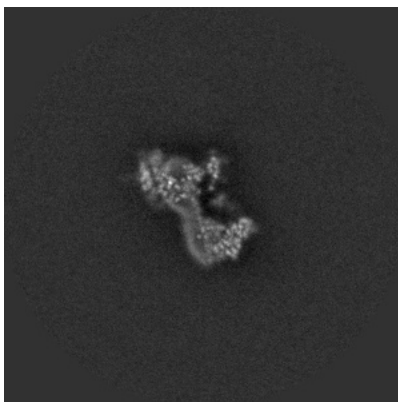


Z Index: 256

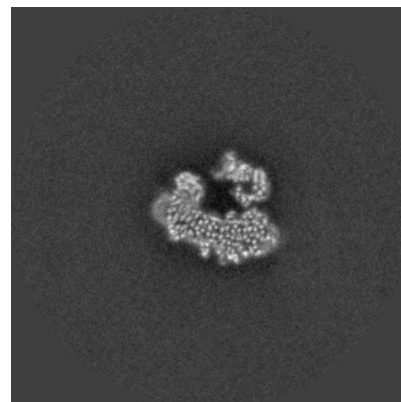
### 6.2.2 Raw map



X Index: 256



Y Index: 256

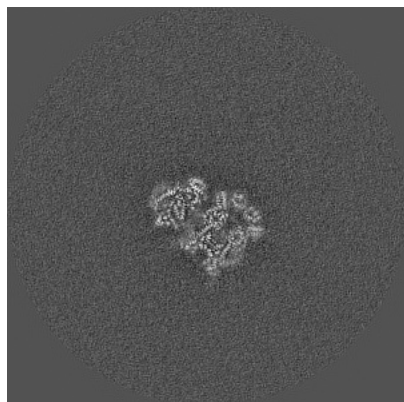


Z Index: 256

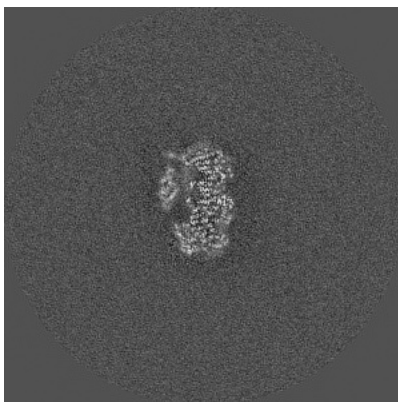
The images above show central slices of the map in three orthogonal directions.

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

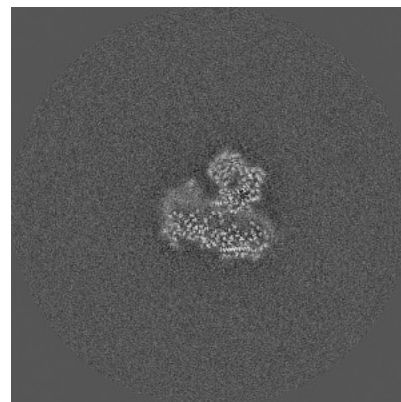
### 6.3.1 Primary map



X Index: 290

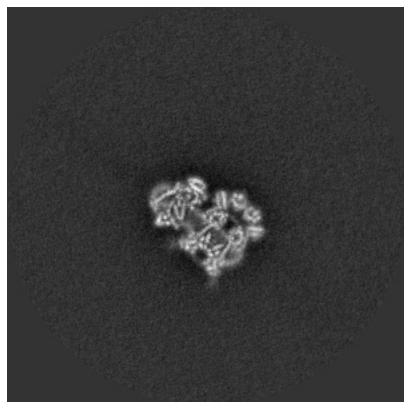


Y Index: 229

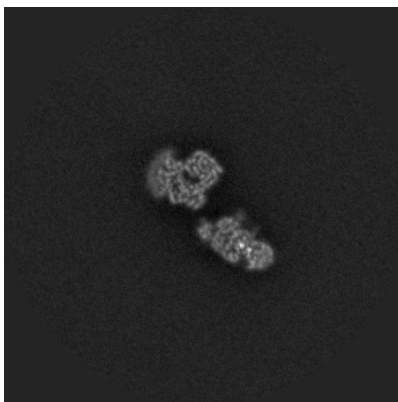


Z Index: 243

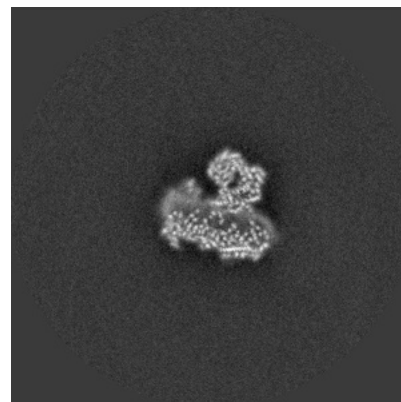
### 6.3.2 Raw map



X Index: 290



Y Index: 295

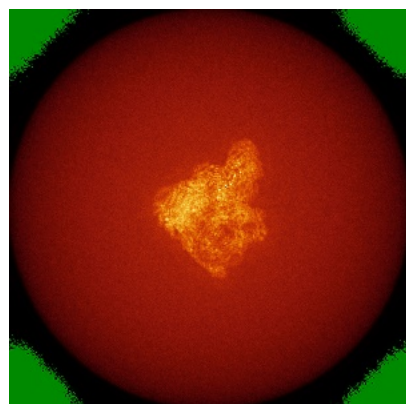


Z Index: 243

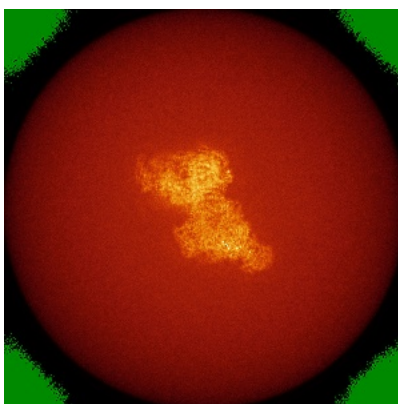
The images above show the largest variance slices of the map in three orthogonal directions.

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

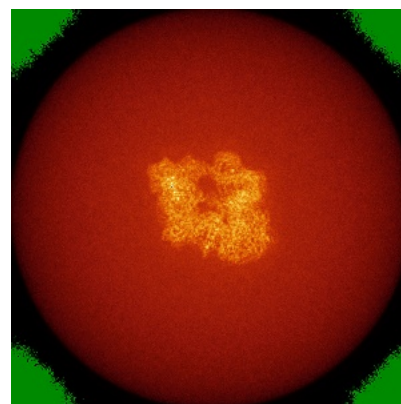
### 6.4.1 Primary map



X

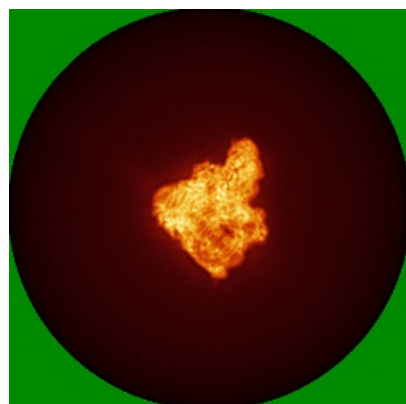


Y

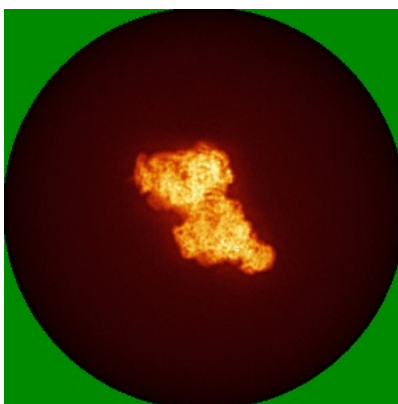


Z

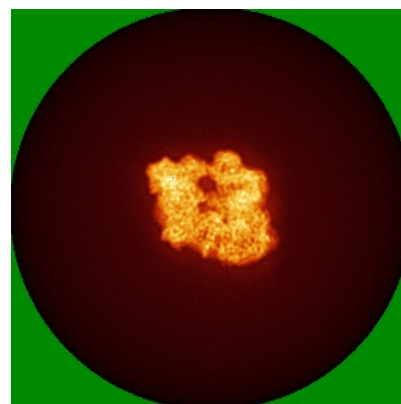
### 6.4.2 Raw map



X



Y



Z

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

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

This section was not generated.

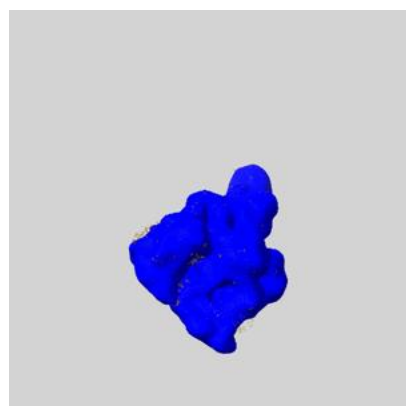
## 6.6 Mask visualisation [i](#)

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

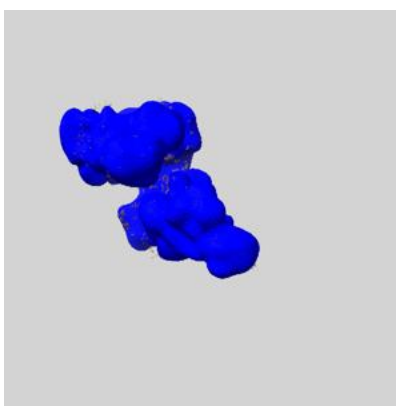
A mask typically either:

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

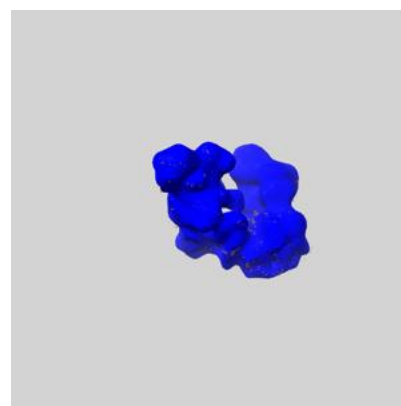
### 6.6.1 emd\_4495\_msk\_1.map [i](#)



X



Y

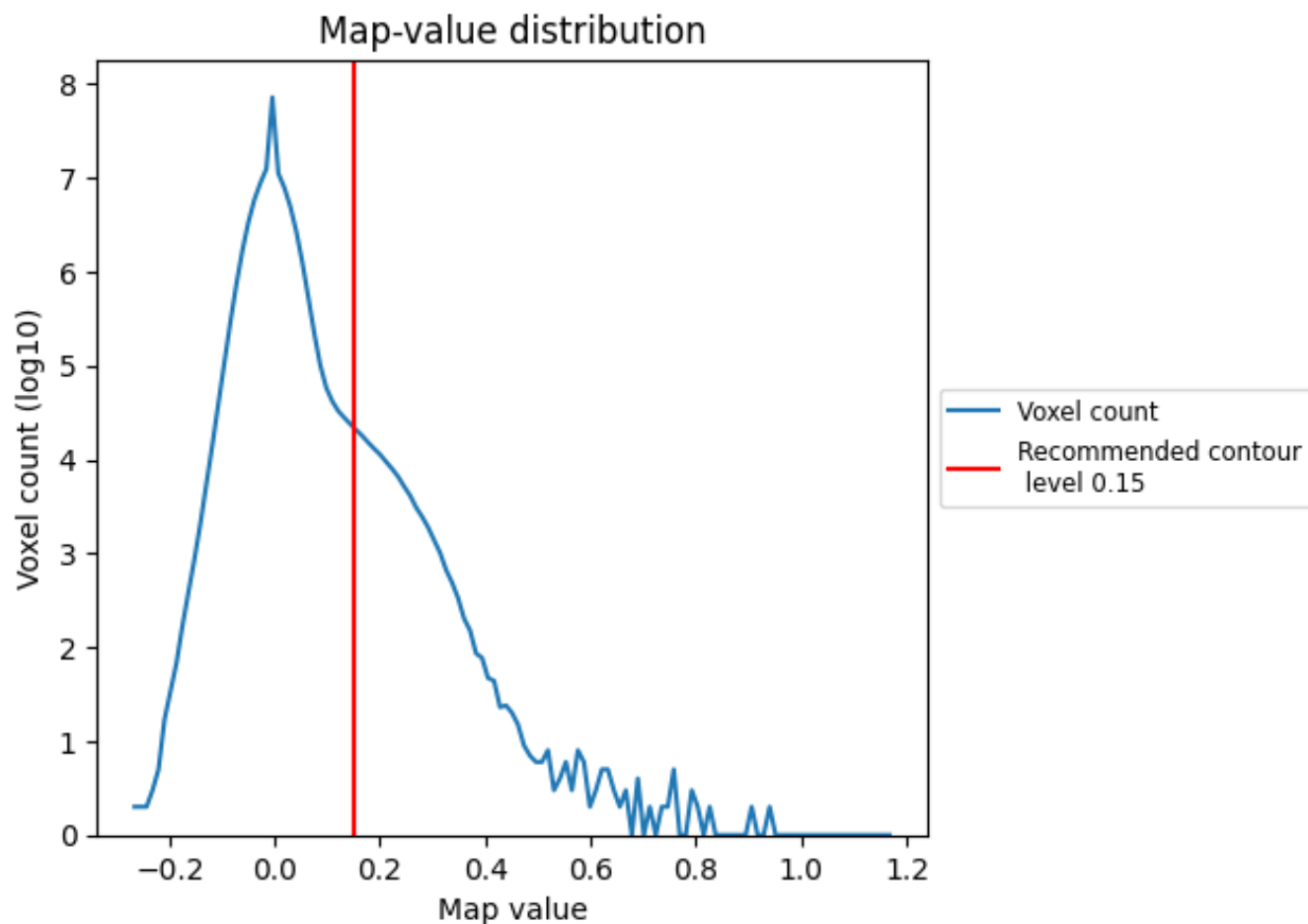


Z

## 7 Map analysis [i](#)

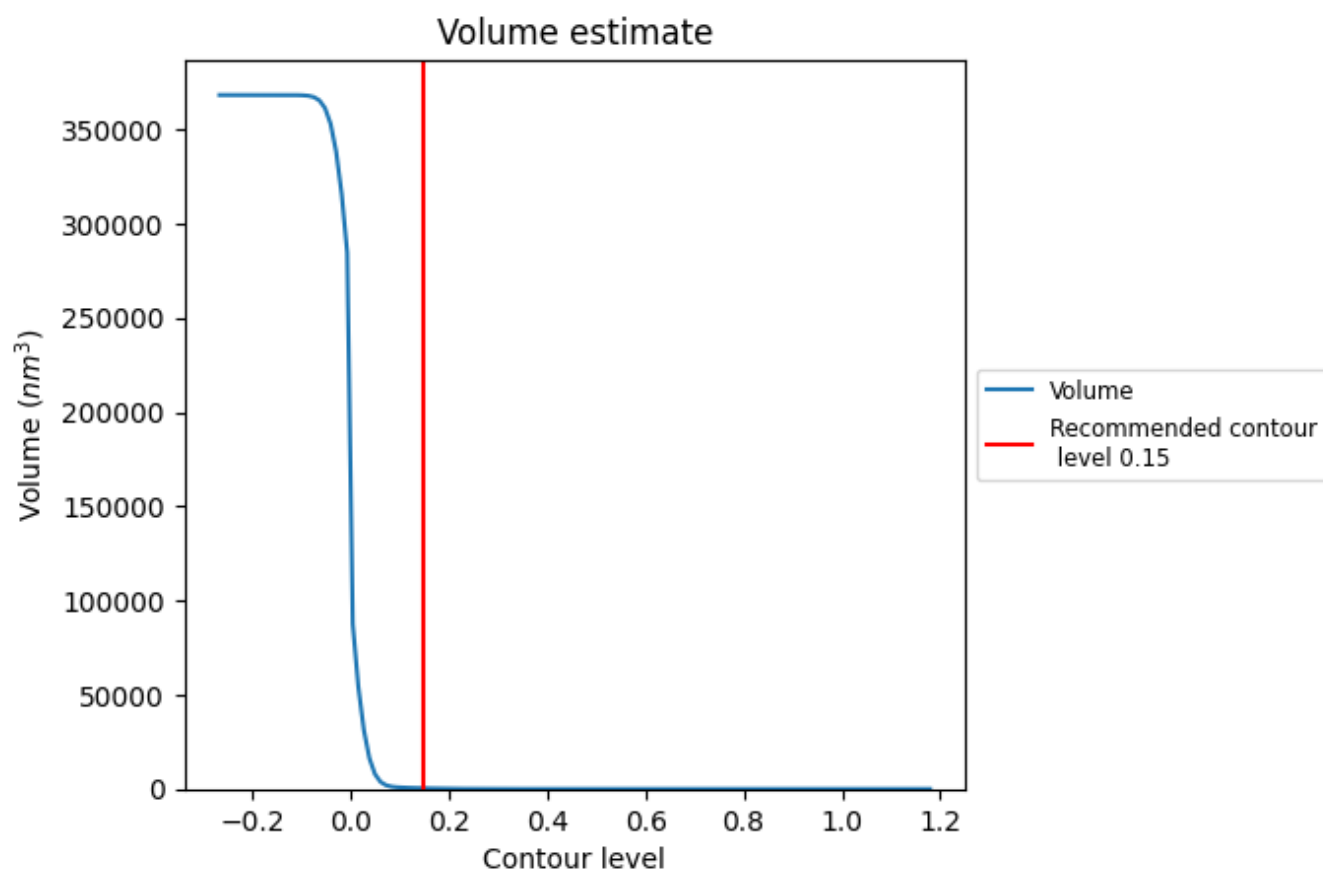
This section contains the results of statistical analysis of the map.

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



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

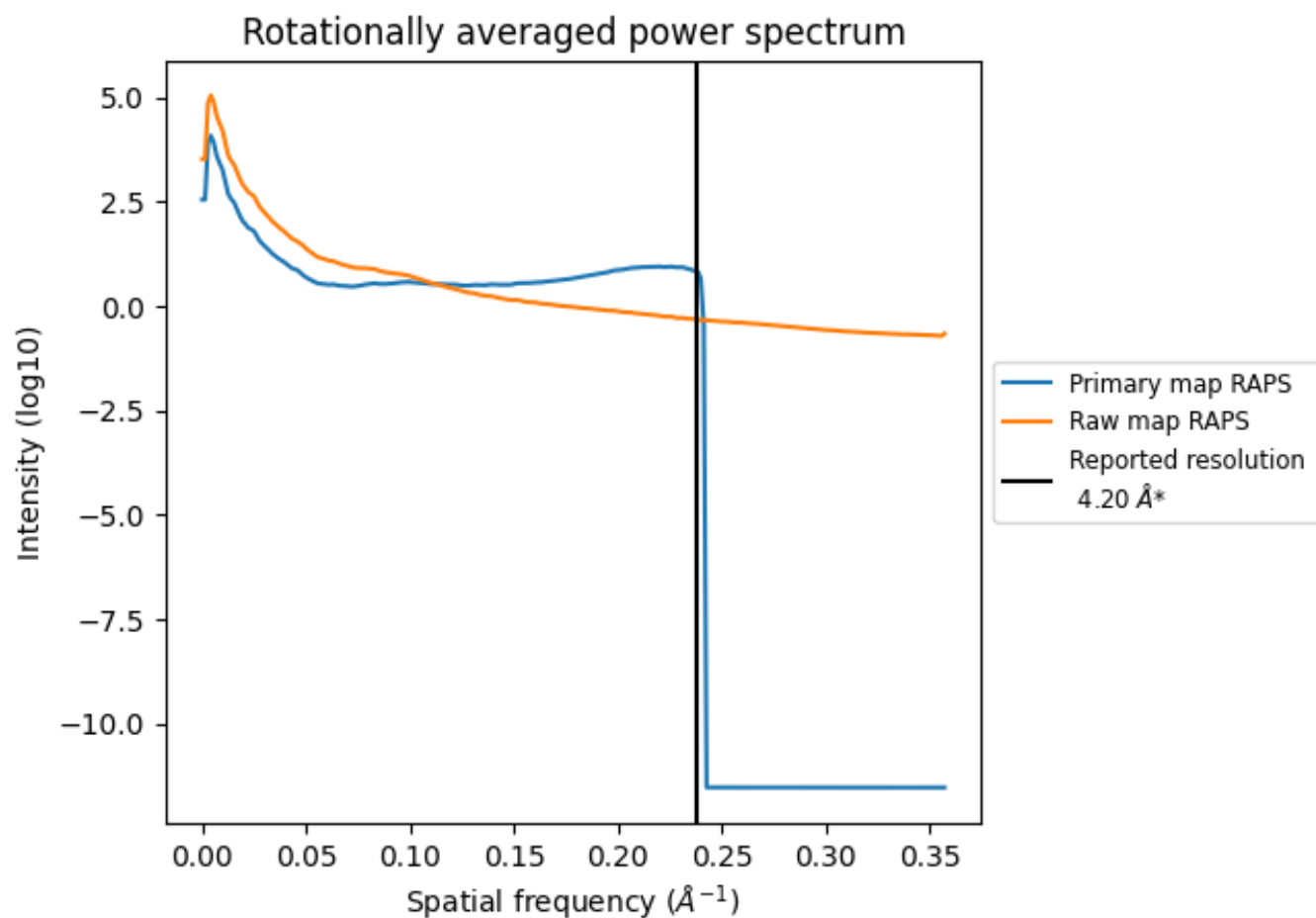
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 365  $\text{nm}^3$ ; this corresponds to an approximate mass of 330 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

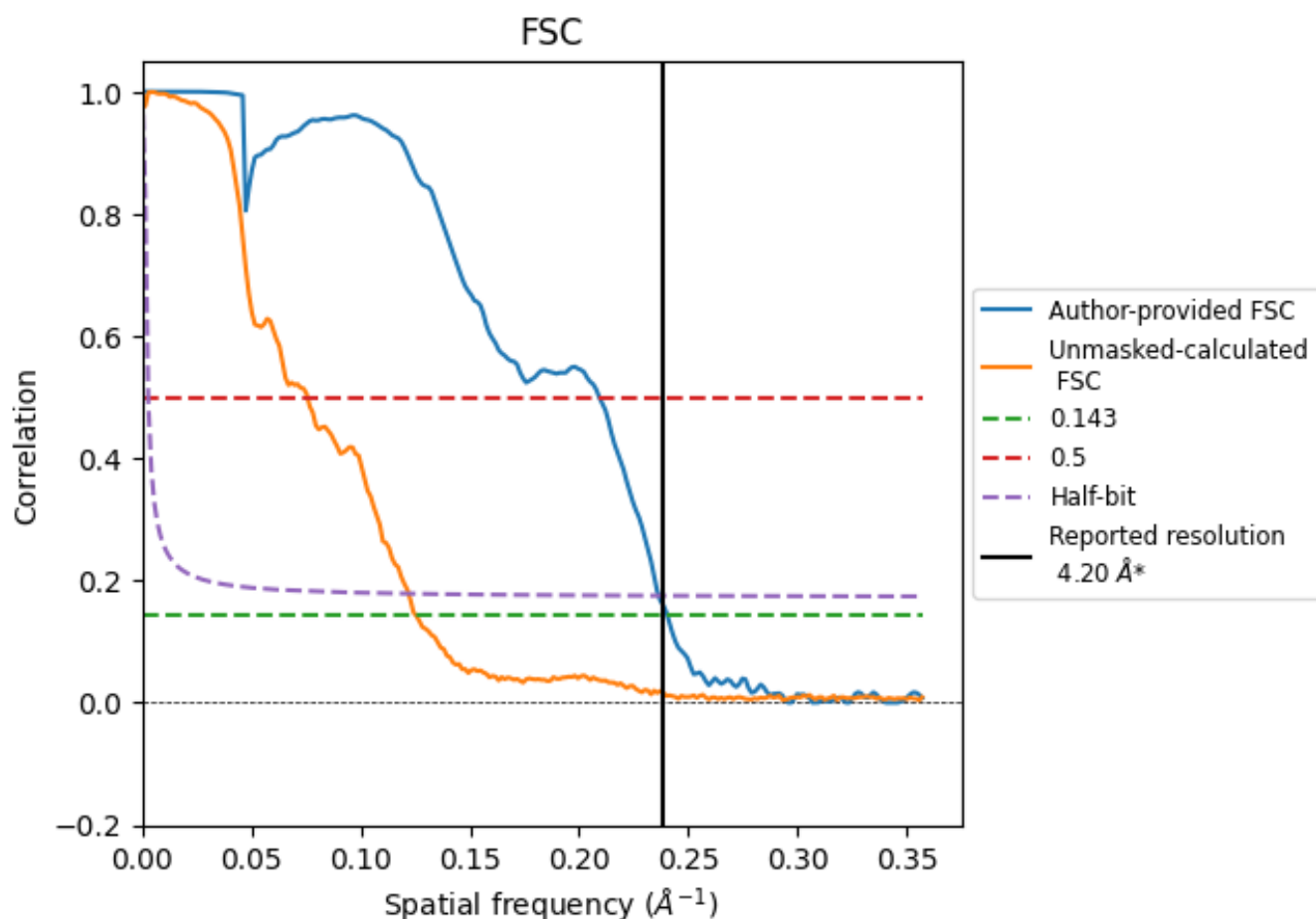


\*Reported resolution corresponds to spatial frequency of 0.238 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.238 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

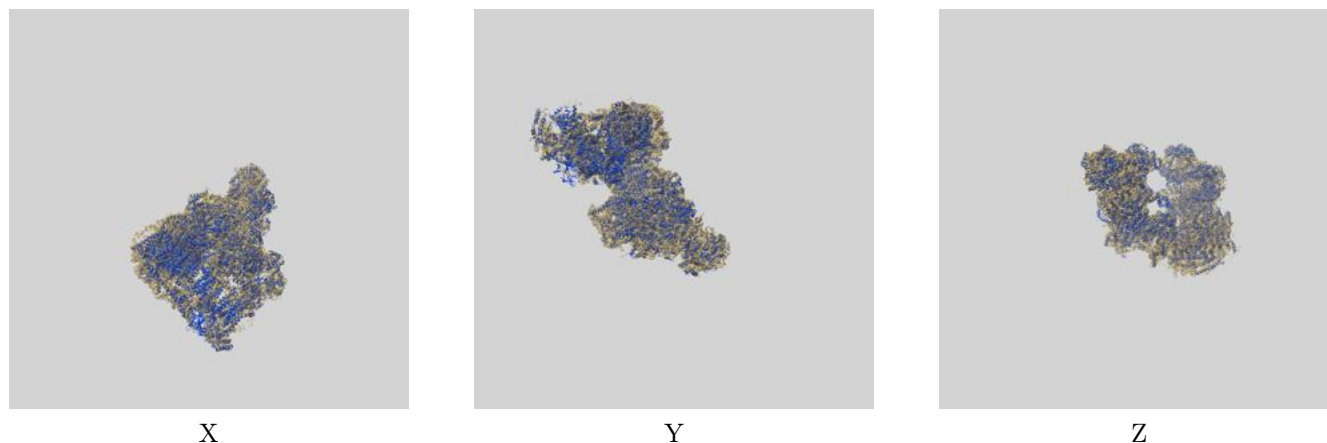
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |       |          |
|---------------------------|------------------------------------|-------|----------|
|                           | 0.143                              | 0.5   | Half-bit |
| Reported by author        | 4.20                               | -     | -        |
| Author-provided FSC curve | 4.16                               | 4.78  | 4.23     |
| Unmasked-calculated*      | 7.99                               | 13.21 | 8.20     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.99 differs from the reported value 4.2 by more than 10 %

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

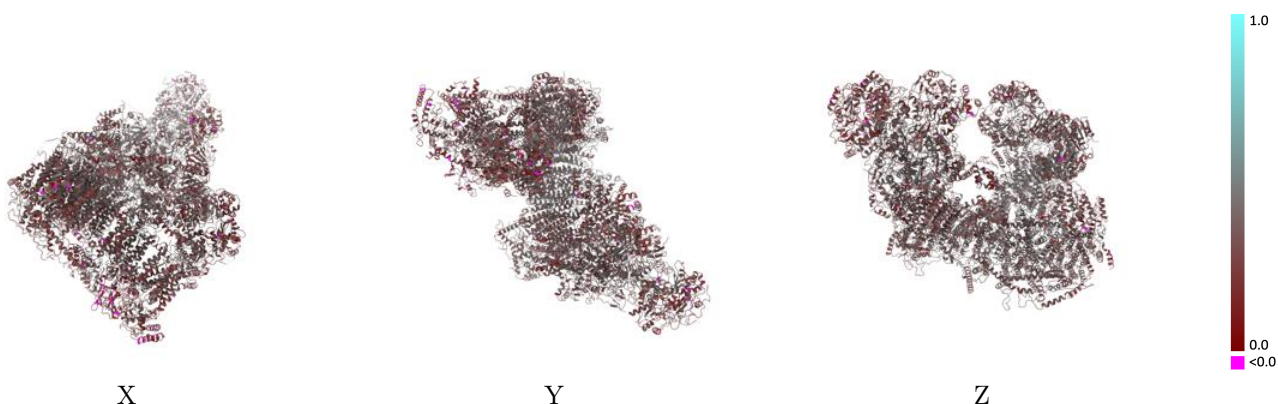
This section contains information regarding the fit between EMDB map EMD-4495 and PDB model 6QC3. Per-residue inclusion information can be found in section [3](#) on page [21](#).

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



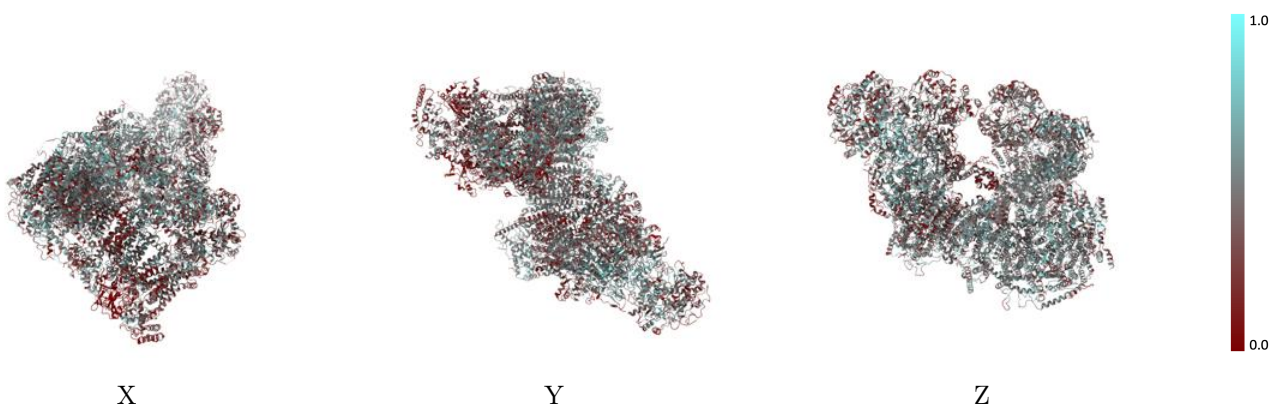
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



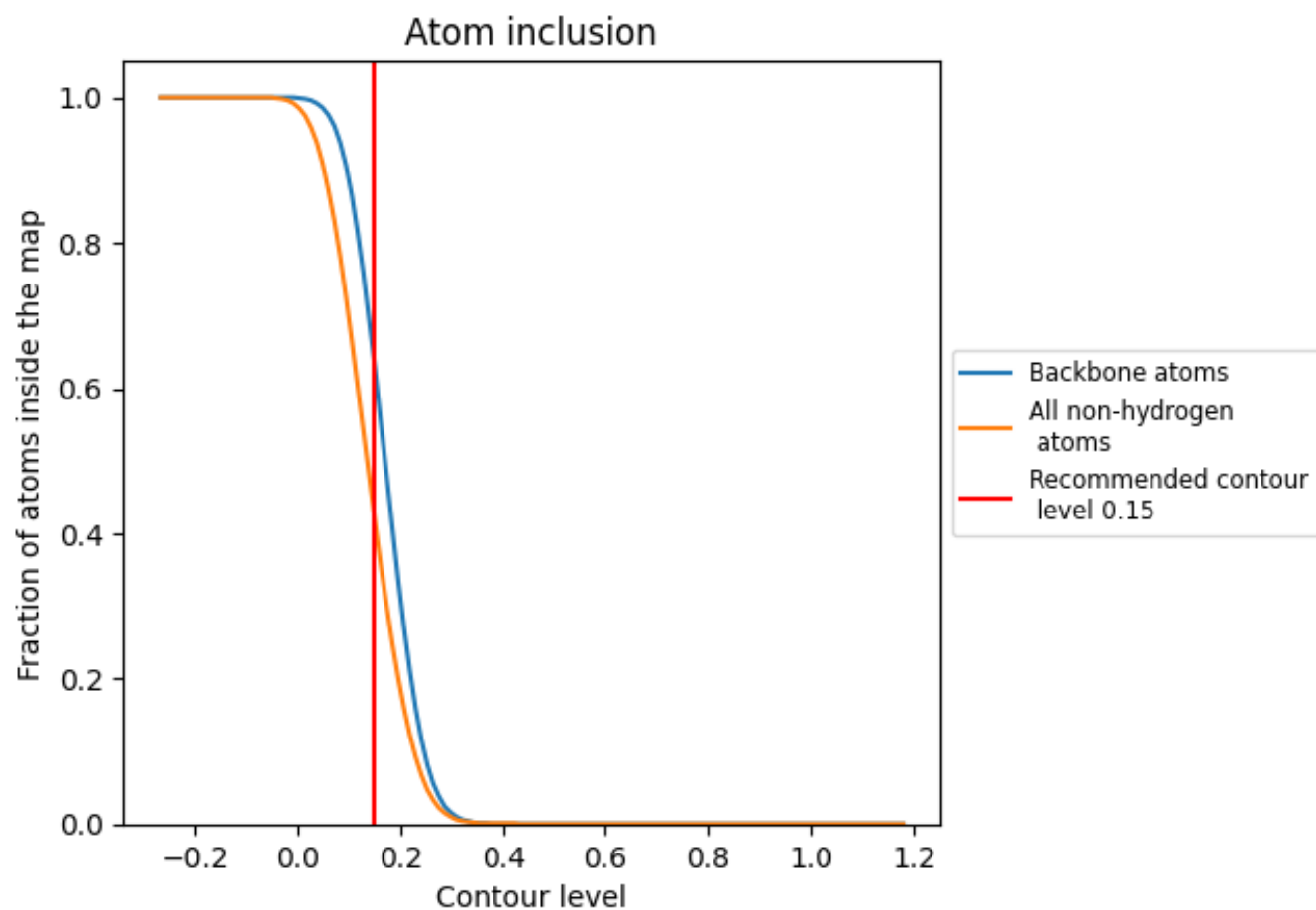
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 64% of all backbone atoms, 42% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|----------------|---------|
| All   | 0.4230         | 0.3540  |
| 4L    | 0.4160         | 0.3700  |
| A1    | 0.4660         | 0.3710  |
| A2    | 0.3140         | 0.2760  |
| A3    | 0.4170         | 0.3490  |
| A5    | 0.4010         | 0.3400  |
| A6    | 0.3640         | 0.3520  |
| A7    | 0.3320         | 0.3480  |
| A8    | 0.4610         | 0.3420  |
| A9    | 0.3330         | 0.3300  |
| AA    | 0.1990         | 0.2840  |
| AB    | 0.4620         | 0.3350  |
| AJ    | 0.4950         | 0.3710  |
| AK    | 0.4050         | 0.3780  |
| AL    | 0.3000         | 0.3580  |
| AM    | 0.4660         | 0.3500  |
| B1    | 0.4060         | 0.3760  |
| B2    | 0.4230         | 0.3280  |
| B3    | 0.4400         | 0.3180  |
| B4    | 0.4940         | 0.3850  |
| B5    | 0.5330         | 0.3720  |
| B6    | 0.4530         | 0.3460  |
| B7    | 0.4400         | 0.3040  |
| B8    | 0.5030         | 0.3840  |
| B9    | 0.5660         | 0.3800  |
| BJ    | 0.5100         | 0.3570  |
| BK    | 0.4560         | 0.3700  |
| C1    | 0.4580         | 0.3520  |
| C2    | 0.4930         | 0.3920  |
| D1    | 0.4210         | 0.3780  |
| D2    | 0.4970         | 0.3980  |
| D3    | 0.3680         | 0.3780  |
| D4    | 0.4860         | 0.3970  |
| D5    | 0.4420         | 0.3640  |
| D6    | 0.3330         | 0.3560  |



*Continued on next page...*

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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| S1    |  0.4170   |  0.3430   |
| S2    |  0.4960   |  0.3800   |
| S3    |  0.5020   |  0.3990   |
| S4    |  0.4440   |  0.3890   |
| S5    |  0.4780   |  0.3540   |
| S6    |  0.4160   |  0.3720   |
| S7    |  0.5130   |  0.3790   |
| S8    |  0.5730   |  0.3970   |
| V1    |  0.4180   |  0.3130   |
| V2    |  0.3950   |  0.3090   |
| V3    |  0.3420   |  0.3270   |
| a1    |  0.3890   |  0.3280   |
| a2    |  0.3650   |  0.3260   |
| a3    |  0.5050   |  0.3810   |
| a4    |  0.4610   |  0.3530   |
| b1    |  0.3900   |  0.3570   |
| b2    |  0.4720   |  0.3910   |
| c1    |  0.3560   |  0.3280   |
| c2    |  0.4320   |  0.3670   |
| d1    |  0.4020  |  0.3300  |
| d2    |  0.4360 |  0.3630 |
| f1    |  0.0800 |  0.2870 |
| f2    |  0.0910 |  0.2590 |
| h1    |  0.2130 |  0.2530 |
| h2    |  0.2900 |  0.2710 |
| i1    |  0.2600 |  0.2770 |
| i2    |  0.2410 |  0.2970 |
| q1    |  0.3400 |  0.3290 |
| q2    |  0.4310 |  0.3880 |
| x1    |  0.2720 |  0.3730 |
| x2    |  0.2770 |  0.4020 |