



## Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 06:46 PM UTC

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

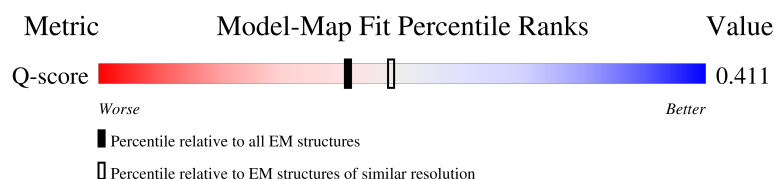
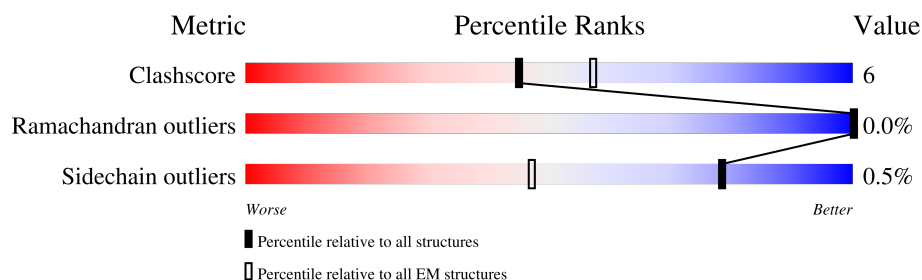
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

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

The reported resolution of this entry is 3.70 Å.

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



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

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

| Mol | Chain | Length | Quality of chain                                                                      |
|-----|-------|--------|---------------------------------------------------------------------------------------|
| 1   | 3     | 115    | <div> <div>37%</div> <div>73%</div> <div>25%</div> <div>.</div> </div>                |
| 1   | 3a    | 115    | <div> <div>55%</div> <div>79%</div> <div>17%</div> <div>.</div> </div>                |
| 2   | S3    | 263    | <div> <div>9%</div> <div>59%</div> <div>19%</div> <div>22%</div> </div>               |
| 2   | s3    | 263    | <div> <div>17%</div> <div>60%</div> <div>17%</div> <div>.</div> <div>22%</div> </div> |

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

*Continued from previous page...*

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

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 64  | SF4  | S7    | 301 | -         | -        | X       | -                |
| 64  | SF4  | s7    | 301 | -         | -        | X       | -                |
| 64  | SF4  | s8    | 301 | -         | -        | X       | -                |

## 2 Entry composition

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

*Continued on next page...*

*Continued from previous page...*

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 42 is a protein called Cytochrome b.

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

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

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

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

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

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

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

*Continued on next page...*

*Continued from previous page...*

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

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

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

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

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

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

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

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

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

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

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

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

drial.

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

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

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

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

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

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

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

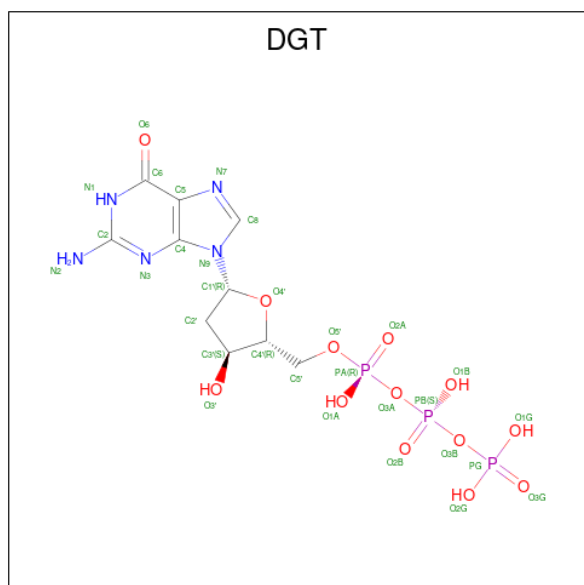
- Molecule 55 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

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

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

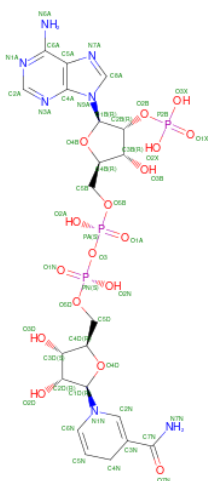
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 56  | AL    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 56  | al    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

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



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 57  | AL    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 57  | al    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |

- Molecule 58 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).

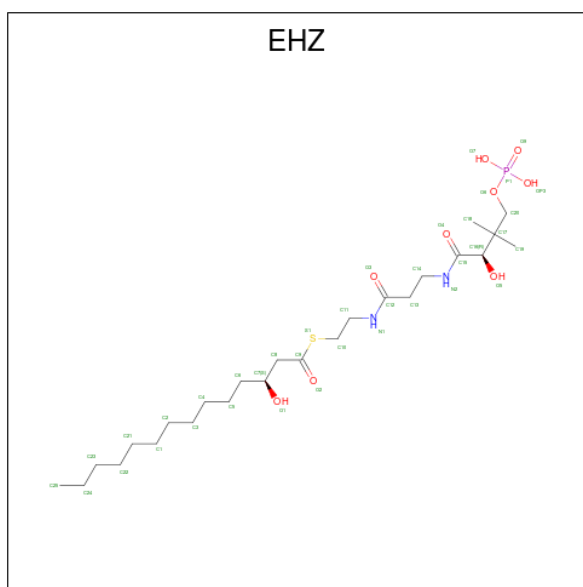


| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 58  | A9    | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       |
| 58  | a9    | 1        | Total<br>48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

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

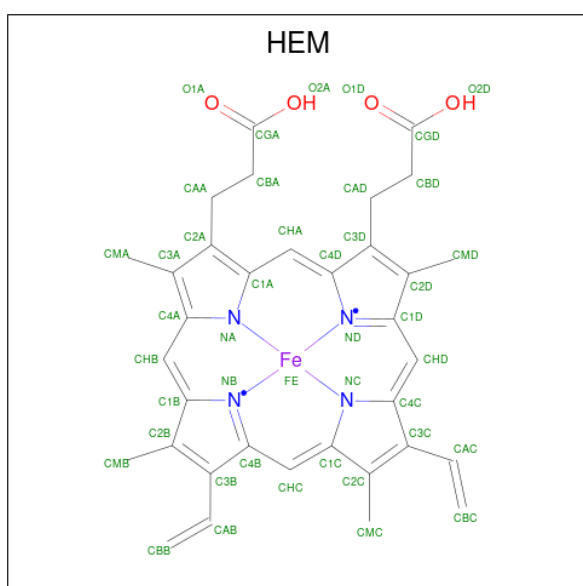
| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 59  | S6    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 59  | s6    | 1        | Total<br>1 | Zn<br>1 | 0       |

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



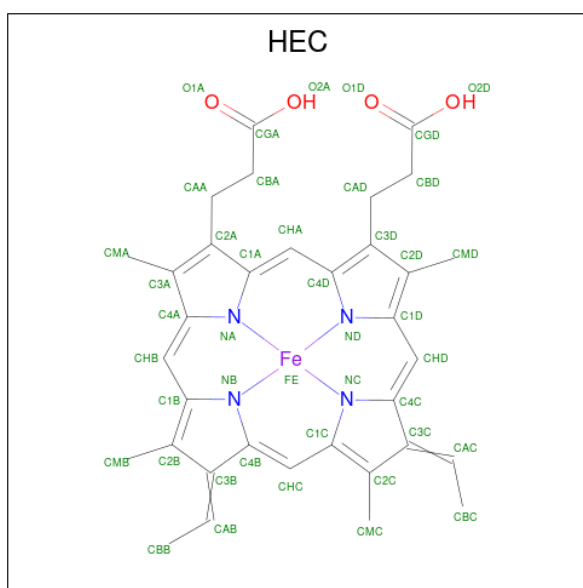
| Mol | Chain | Residues | Atoms       |         |        |        |        |        | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|--------|--------|---------|
| 60  | A6    | 1        | Total<br>37 | C<br>25 | N<br>2 | O<br>8 | P<br>1 | S<br>1 | 0       |
| 60  | B9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

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



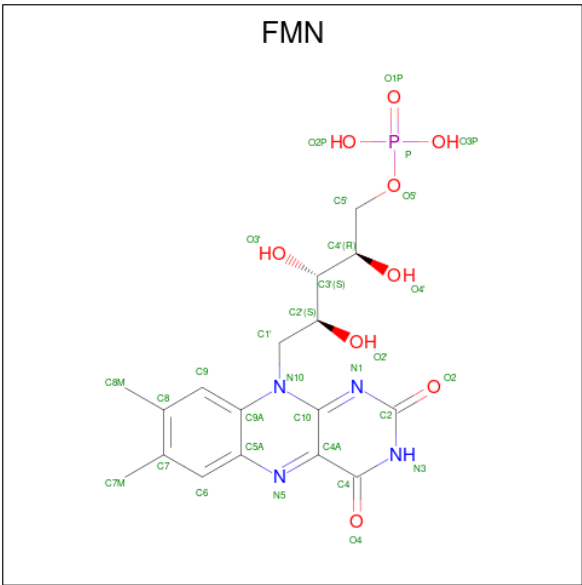
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 61  | 3C    | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 61  | 3C    | 1        | Total | C  | Fe | N |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

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



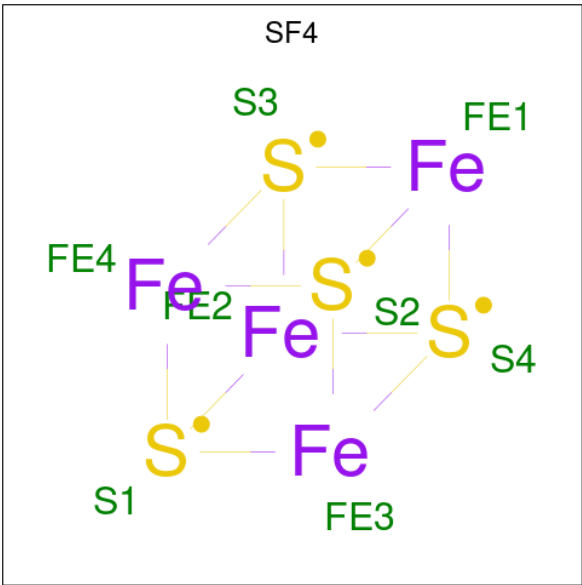
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 62  | 3D    | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |
| 62  | 3O    | 1        | Total | C  | Fe | N |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

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



| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 63  | V1    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 31    | 17 | 4 | 9 | 1 |         |
| 63  | v1    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 31    | 17 | 4 | 9 | 1 |         |

- Molecule 64 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



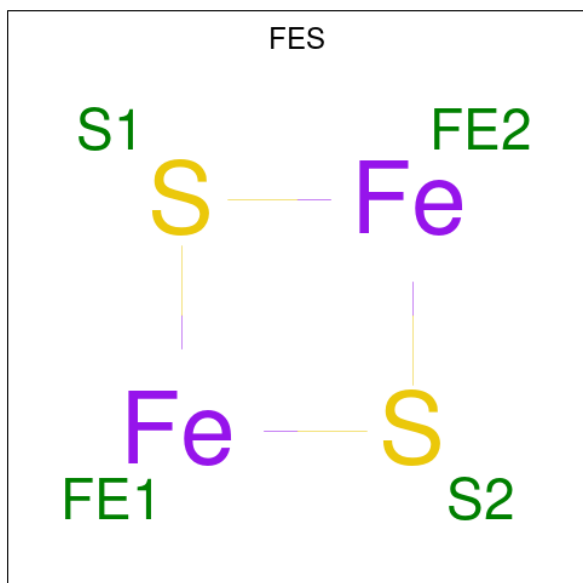
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 64  | V1    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 64  | S1    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

Continued on next page...

Continued from previous page...

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

- Molecule 65 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



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

Continued on next page...

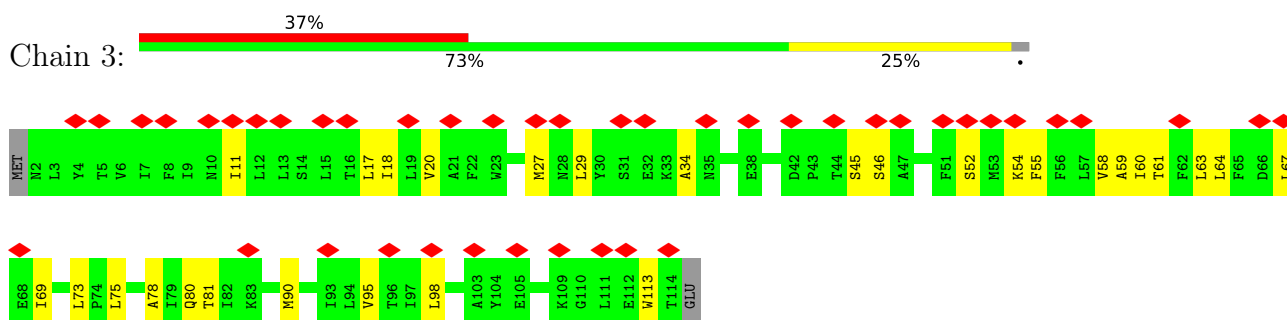
*Continued from previous page...*

| Mol | Chain | Residues | Atoms      |         |        | AltConf |
|-----|-------|----------|------------|---------|--------|---------|
| 65  | S1    | 1        | Total<br>4 | Fe<br>2 | S<br>2 | 0       |
| 65  | v2    | 1        | Total<br>4 | Fe<br>2 | S<br>2 | 0       |
| 65  | s1    | 1        | Total<br>4 | Fe<br>2 | S<br>2 | 0       |

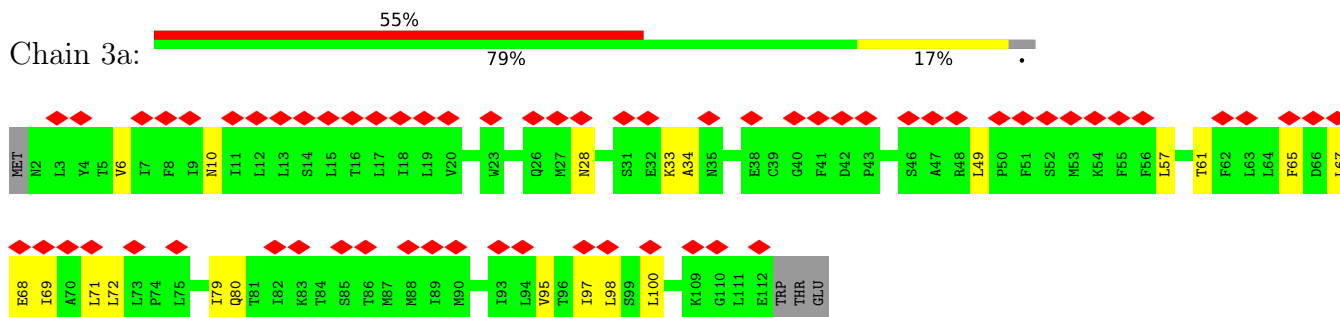
### 3 Residue-property plots

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.

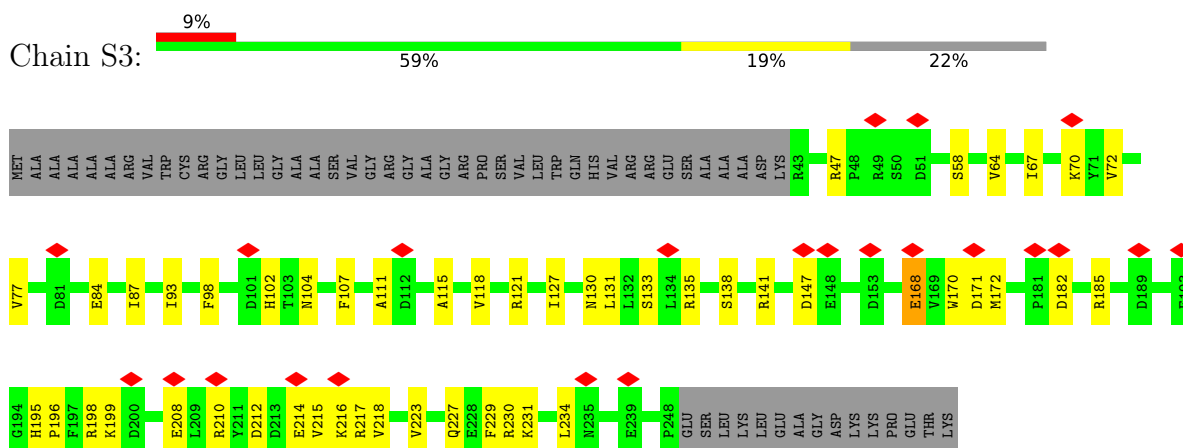
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



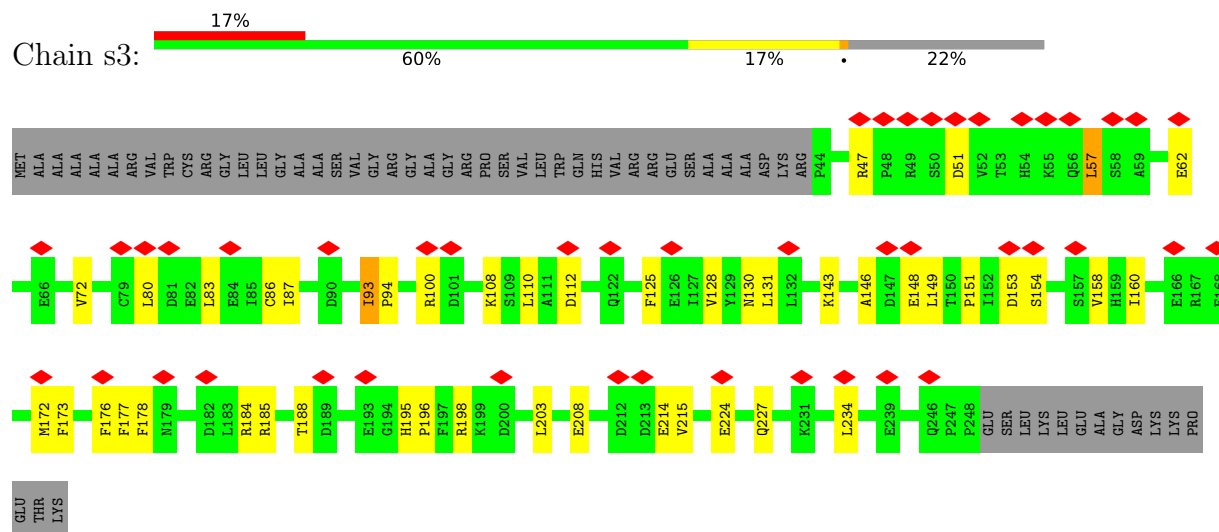
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



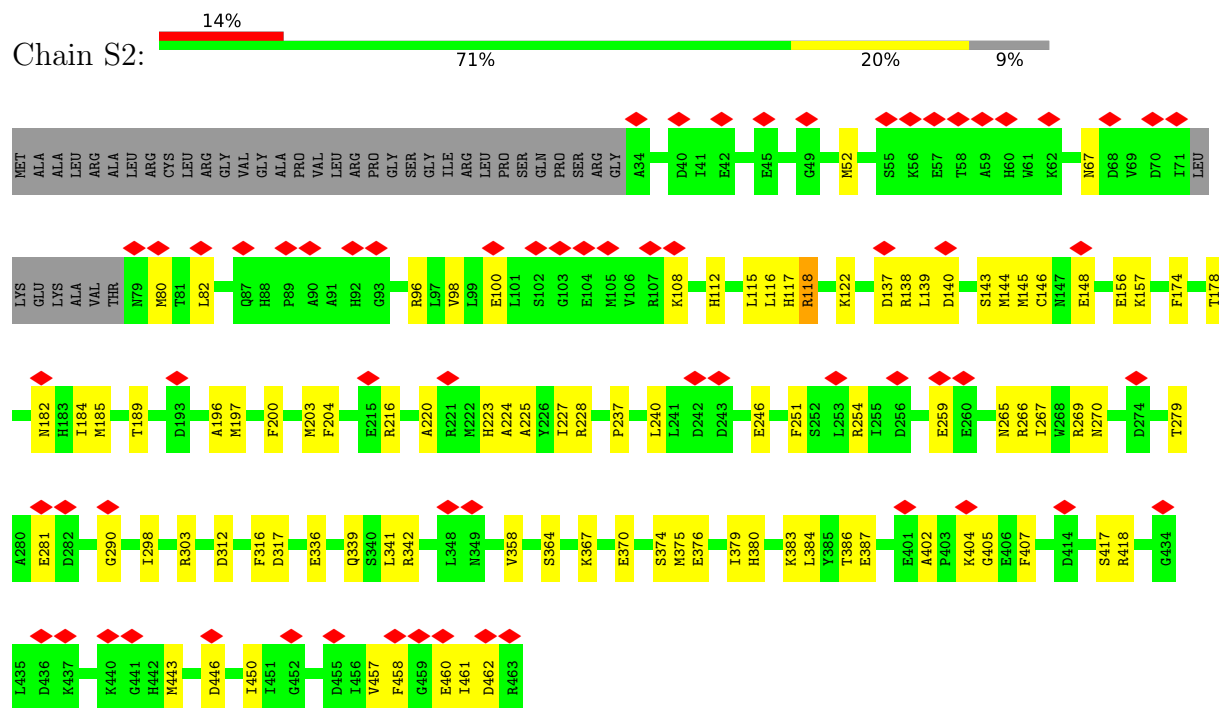
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



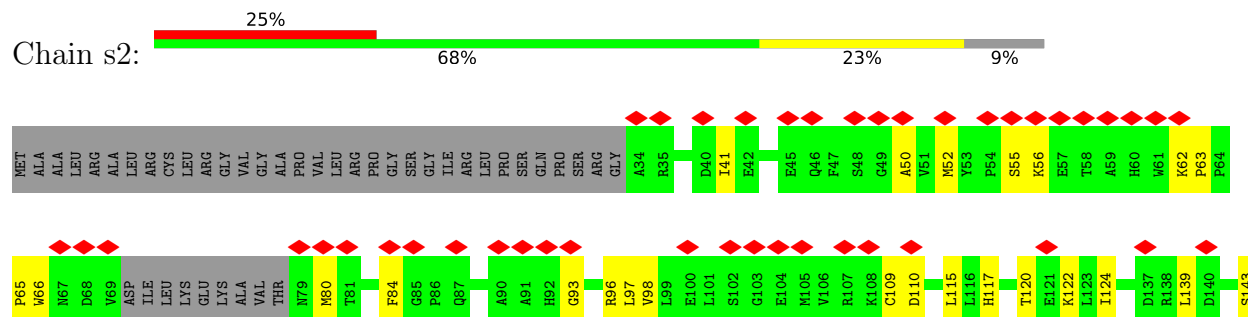
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

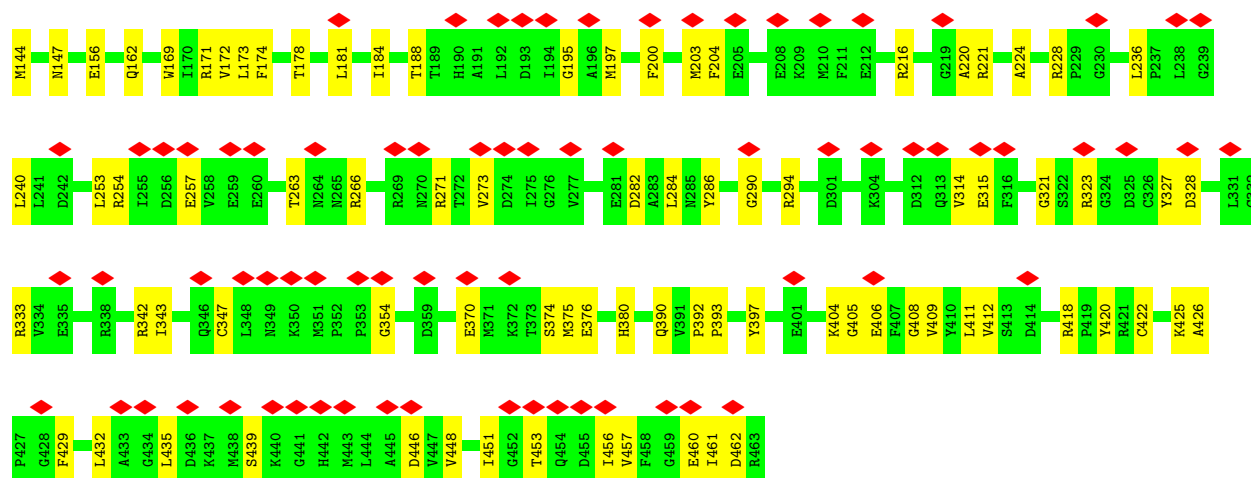


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

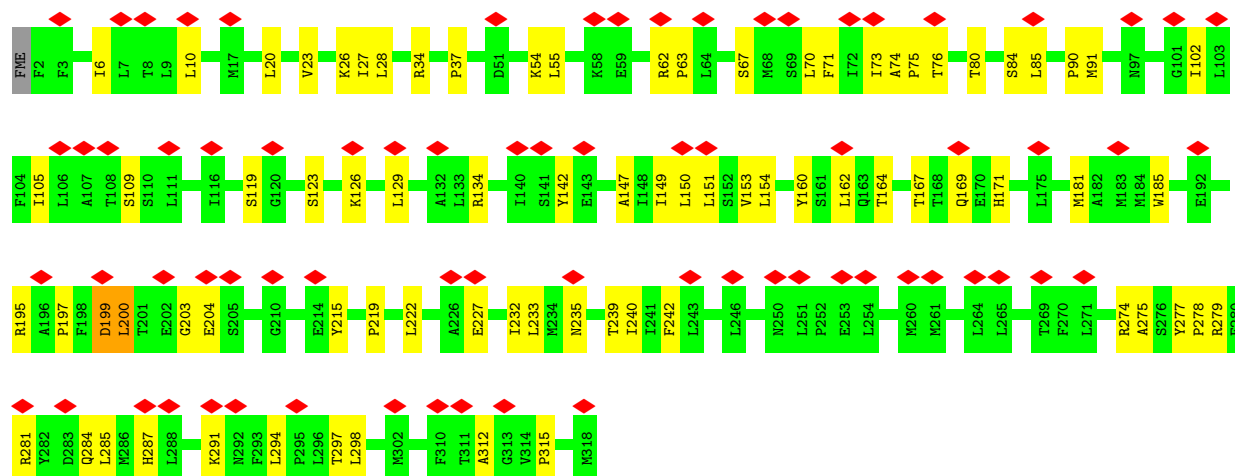
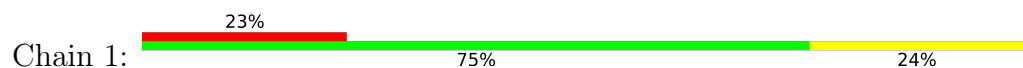


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

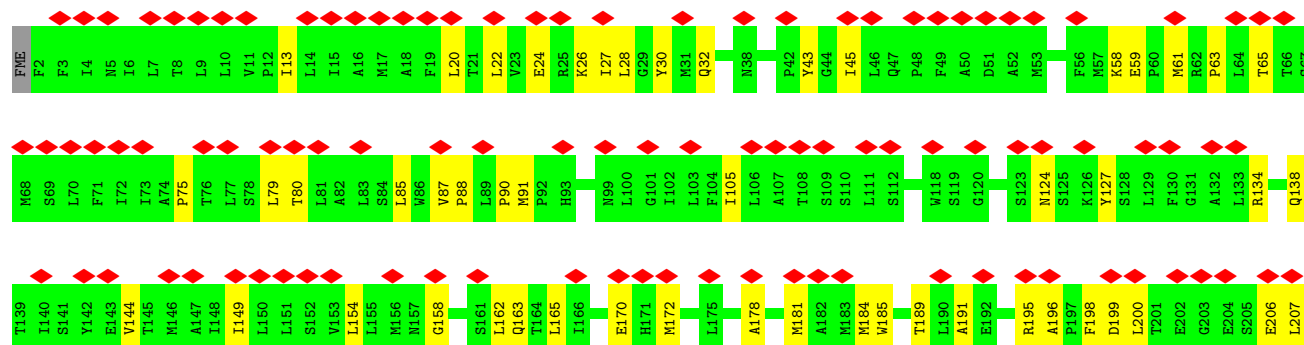
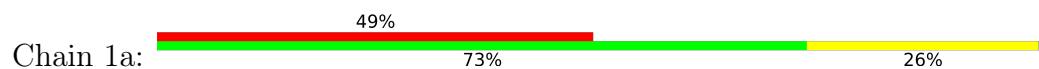


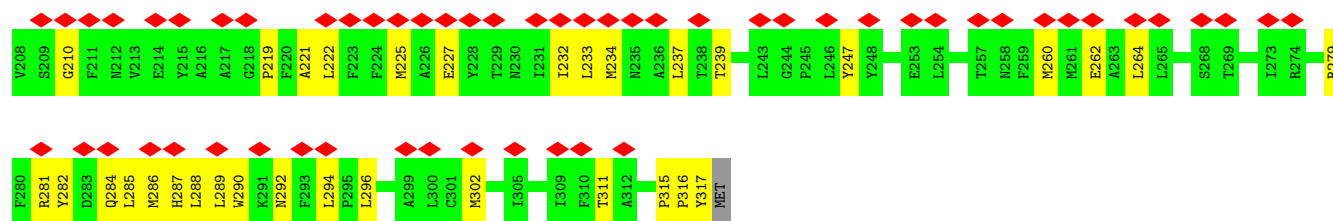


• Molecule 4: NADH-ubiquinone oxidoreductase chain 1

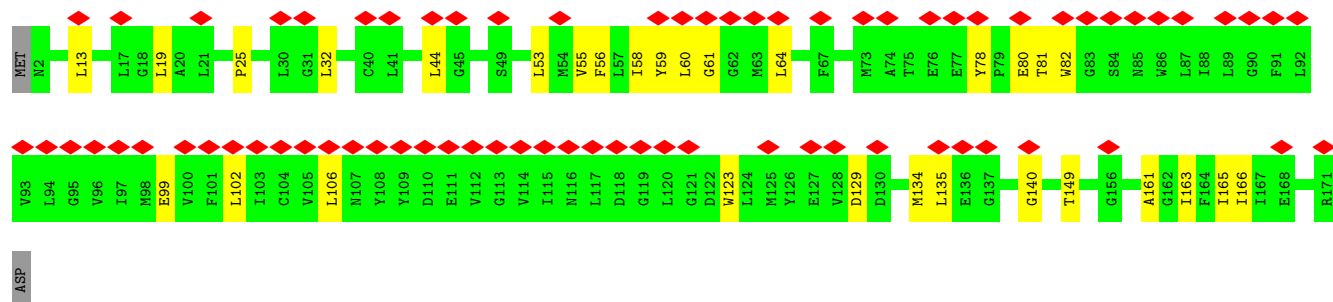
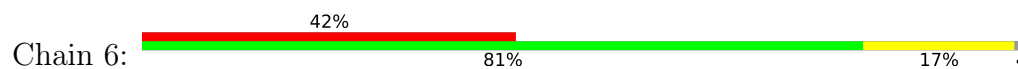


• Molecule 4: NADH-ubiquinone oxidoreductase chain 1

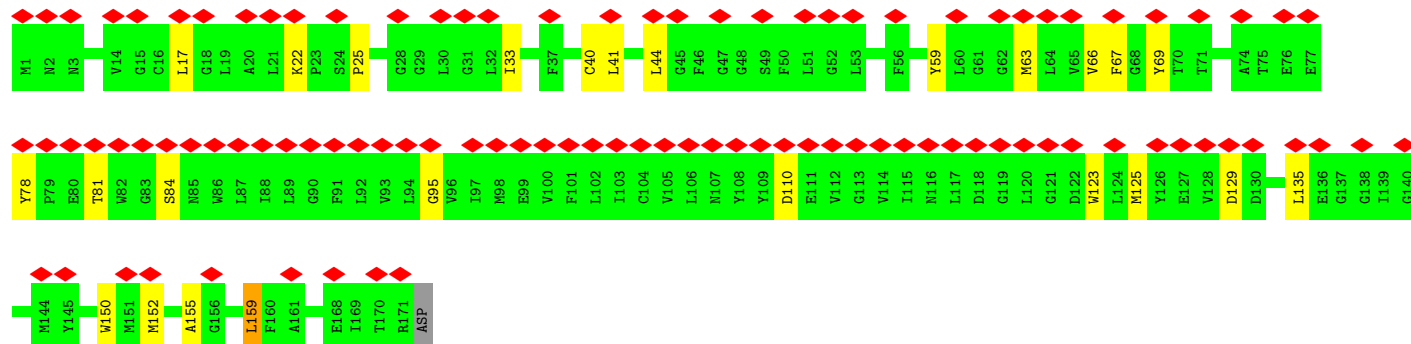
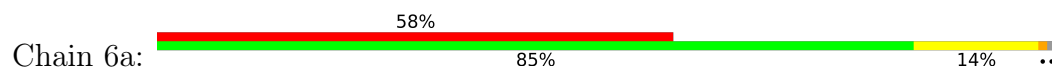




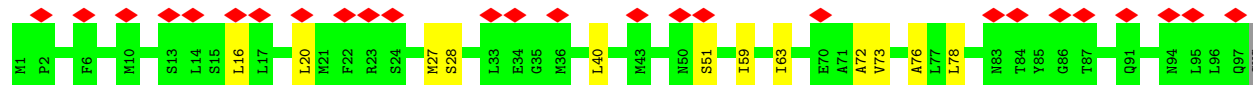
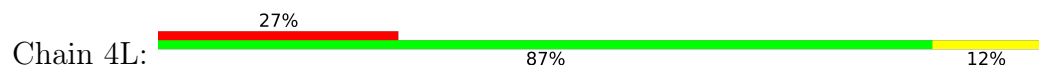
• Molecule 5: NADH-ubiquinone oxidoreductase chain 6



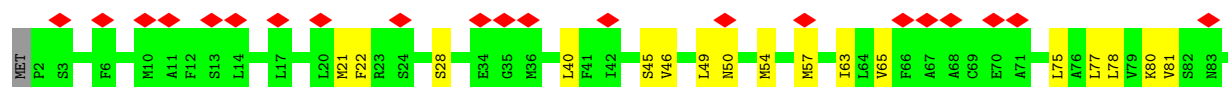
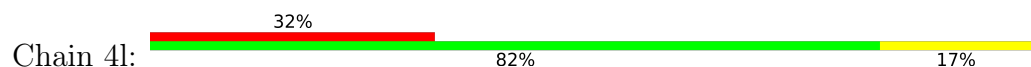
• Molecule 5: NADH-ubiquinone oxidoreductase chain 6

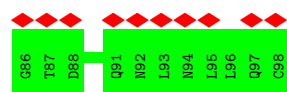


• Molecule 6: NADH-ubiquinone oxidoreductase chain 4L

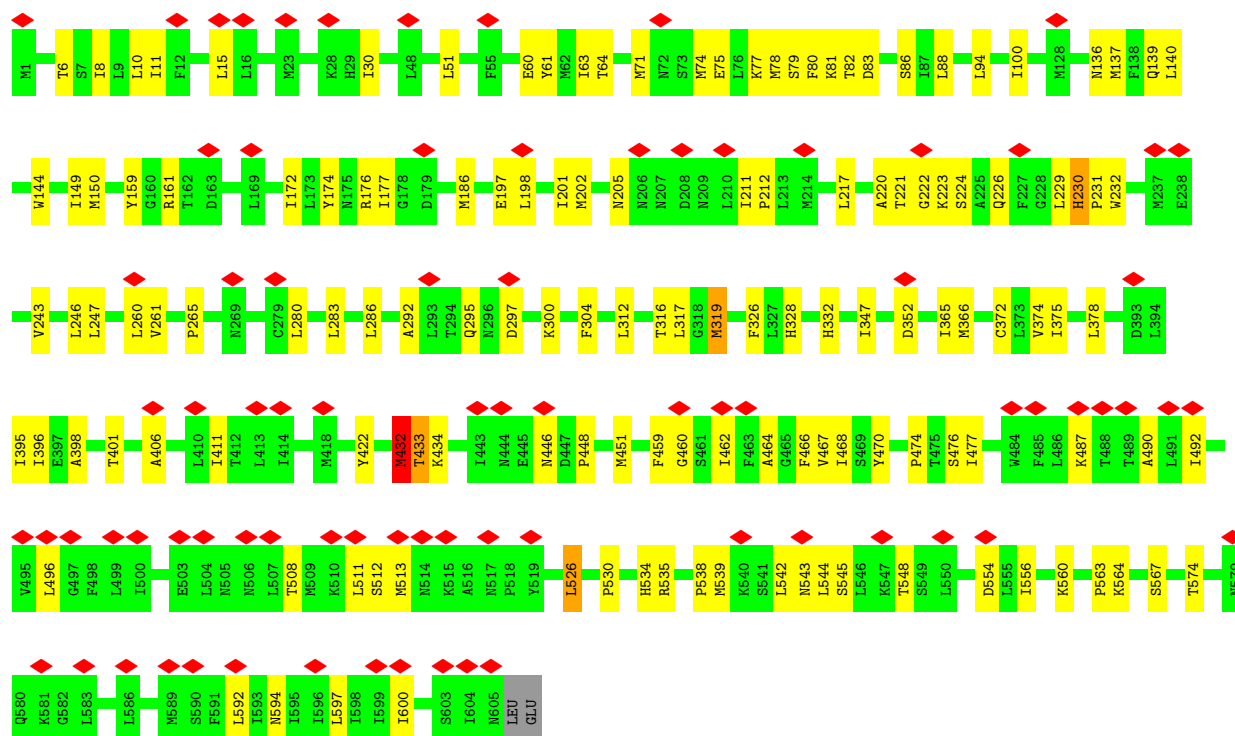
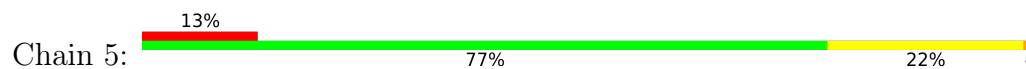


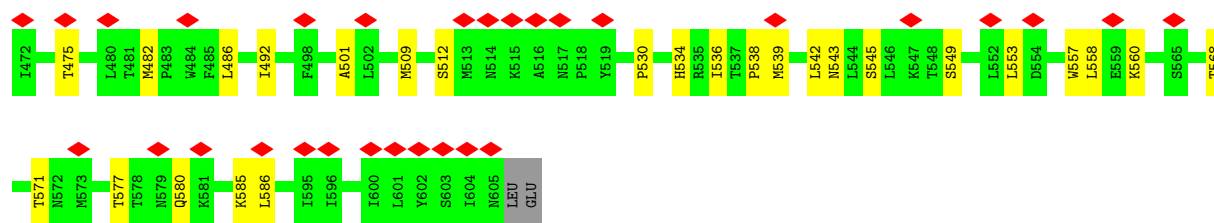
• Molecule 6: NADH-ubiquinone oxidoreductase chain 4L



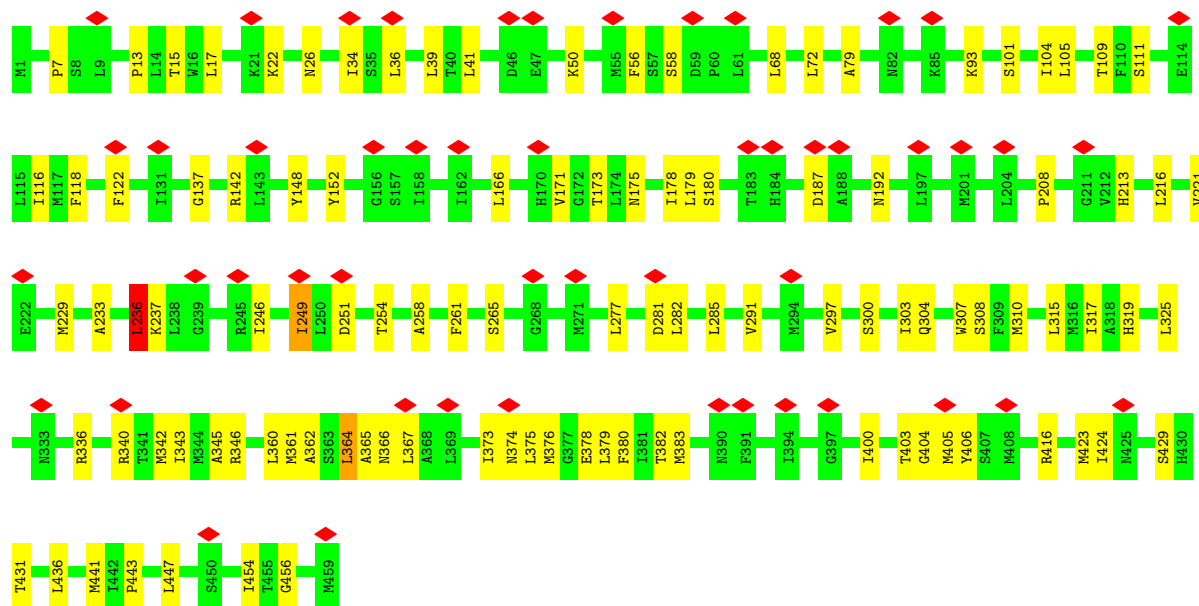
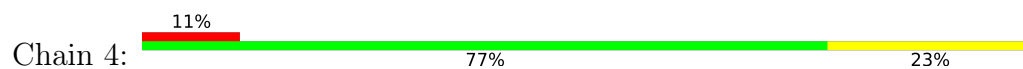


• Molecule 7: NADH-ubiquinone oxidoreductase chain 5

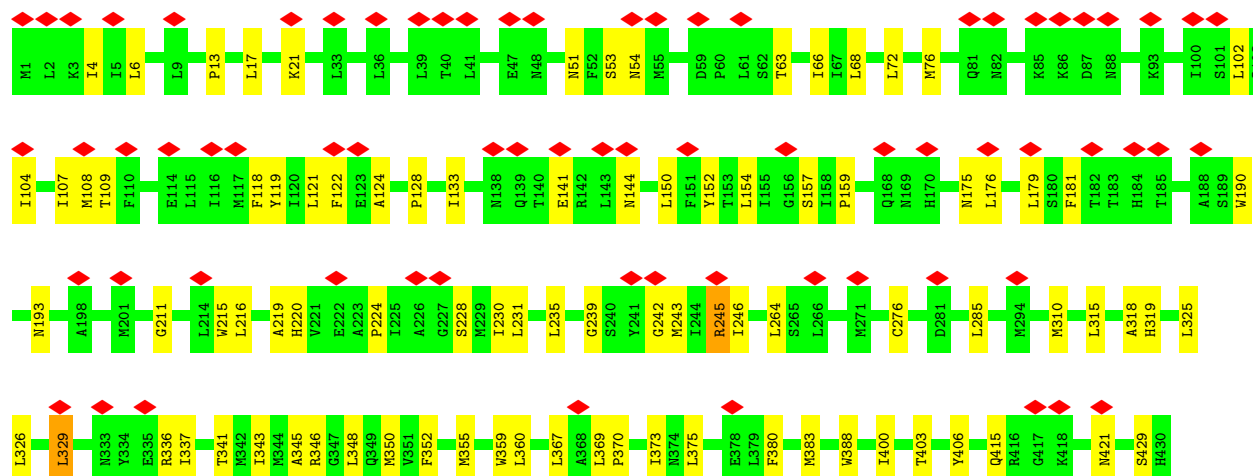
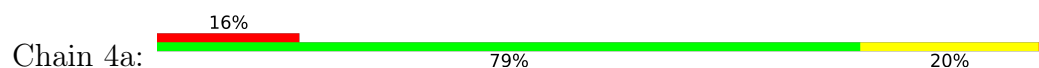


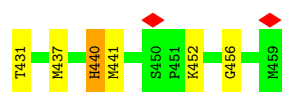


• Molecule 8: NADH-ubiquinone oxidoreductase chain 4

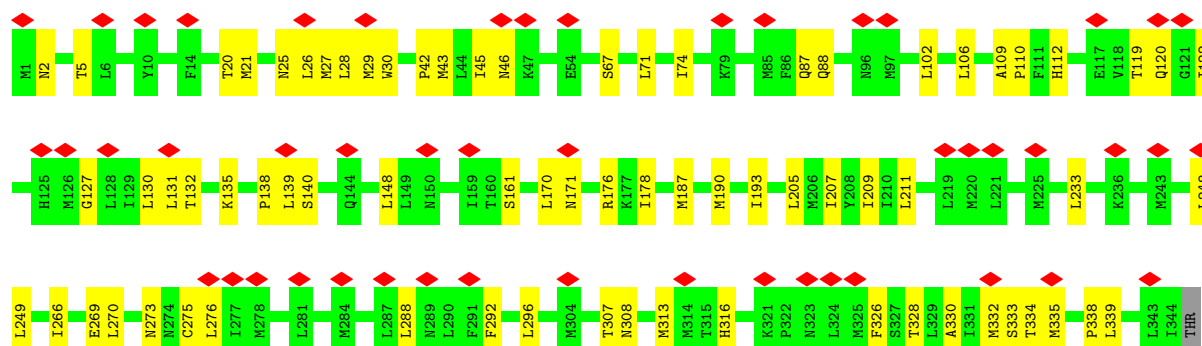
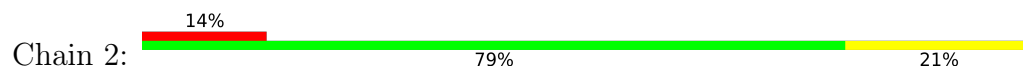


• Molecule 8: NADH-ubiquinone oxidoreductase chain 4

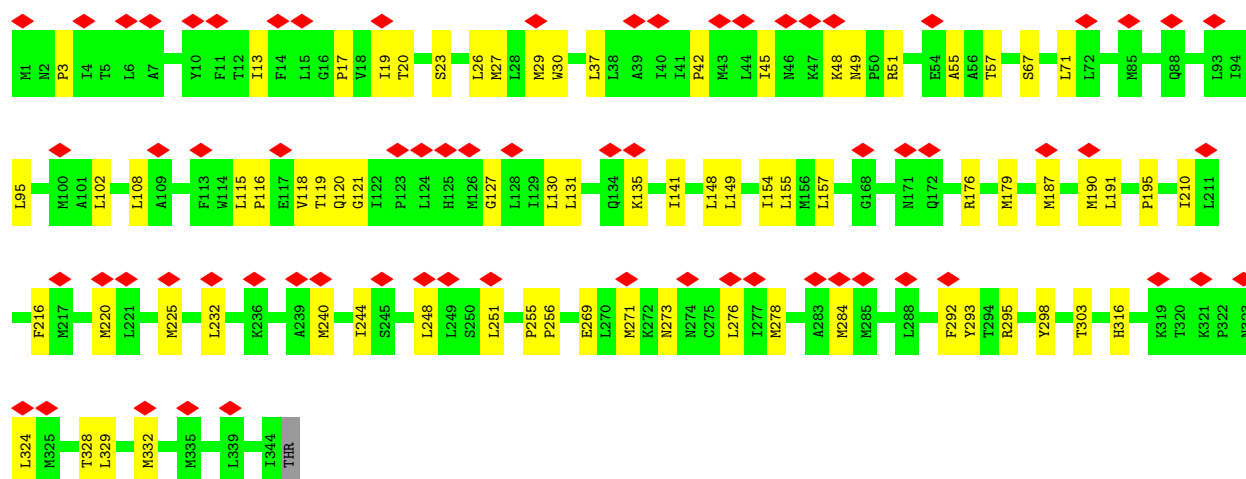
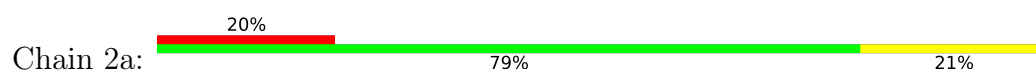




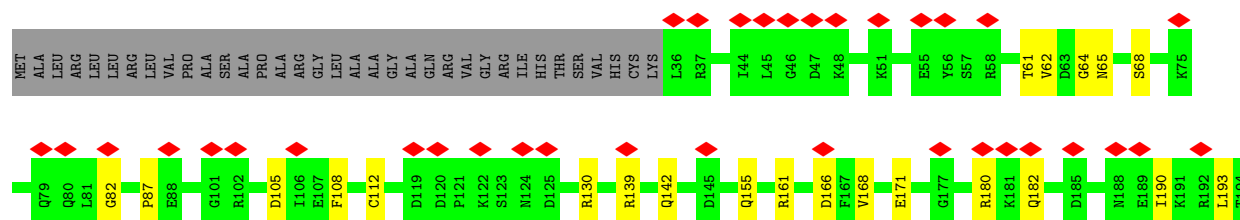
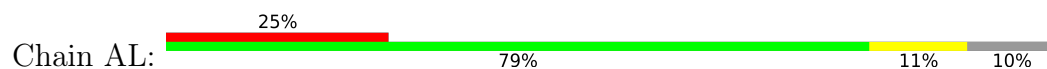
• Molecule 9: NADH-ubiquinone oxidoreductase chain 2

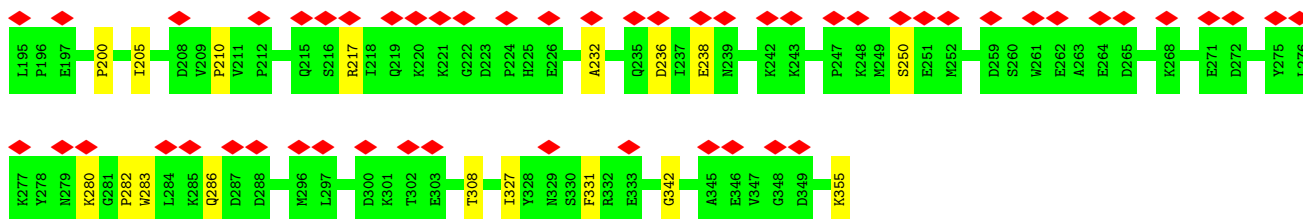


• Molecule 9: NADH-ubiquinone oxidoreductase chain 2

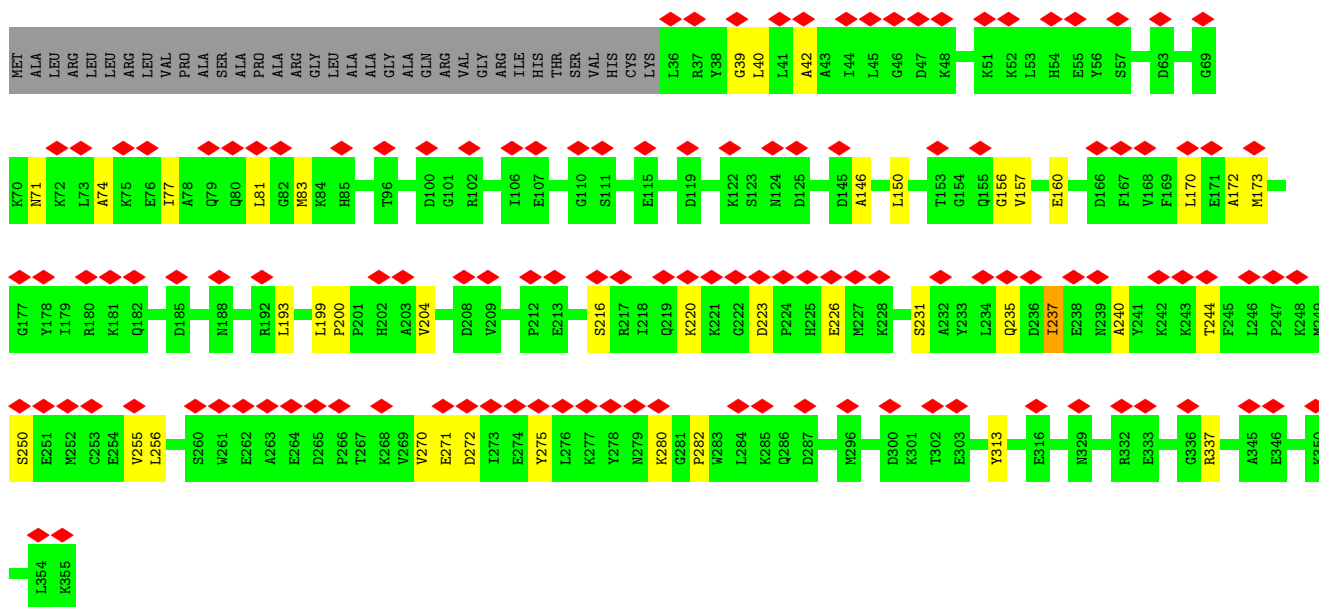
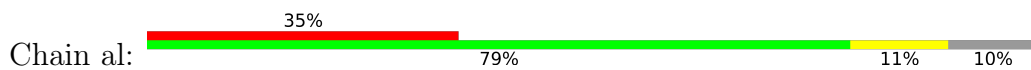


• Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

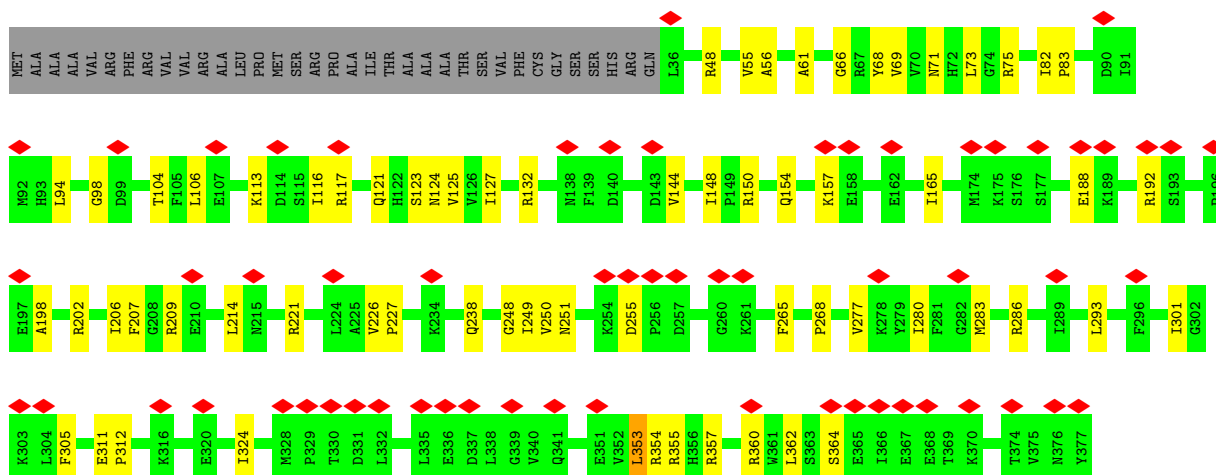
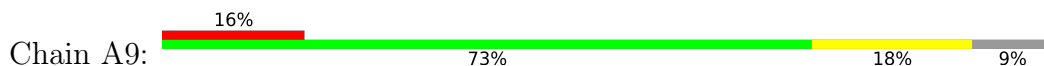




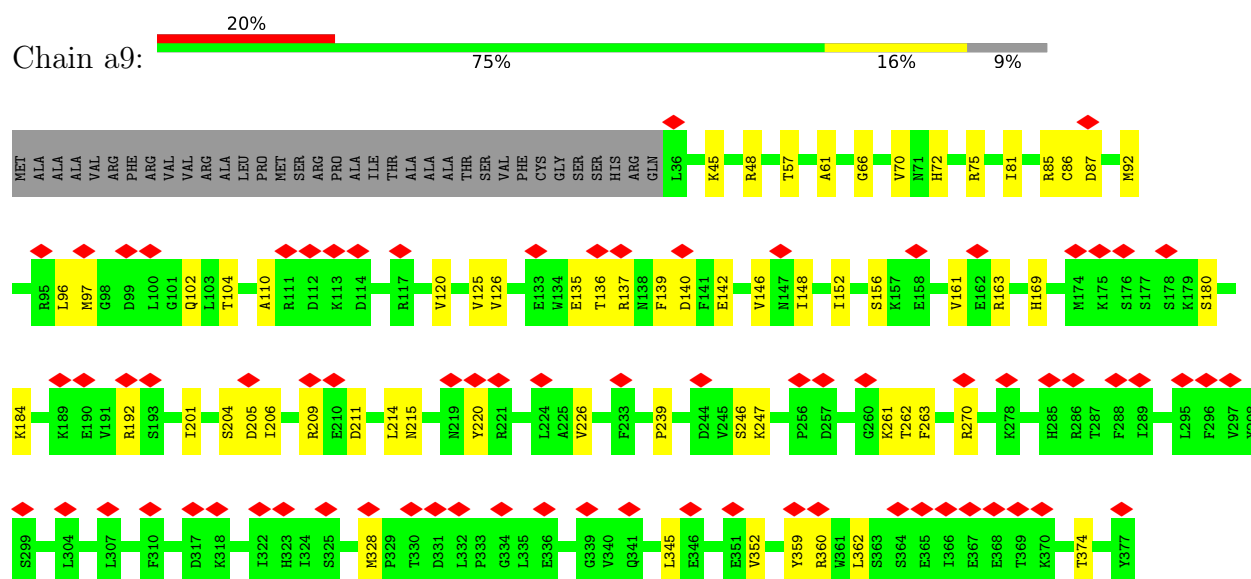
- Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



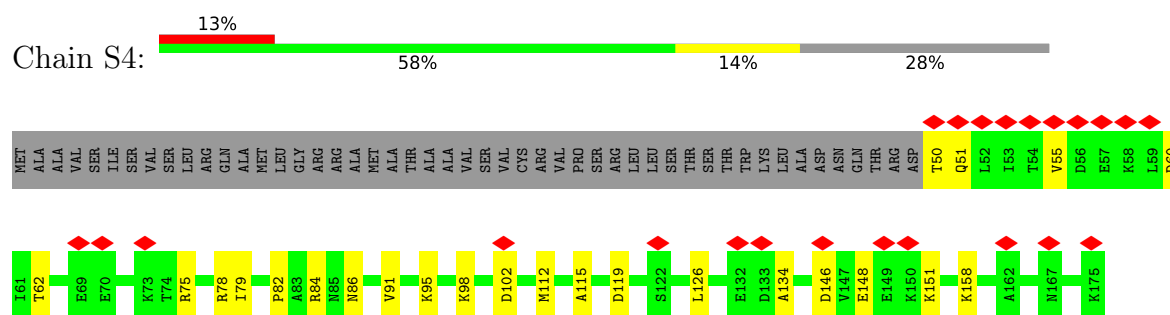
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



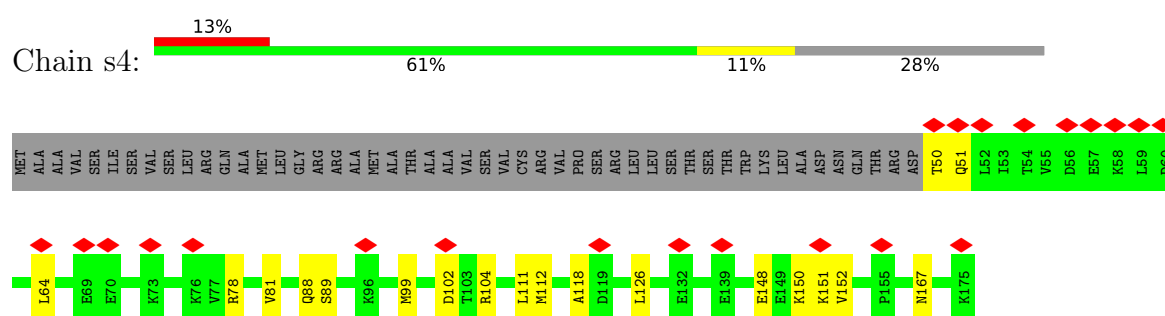
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



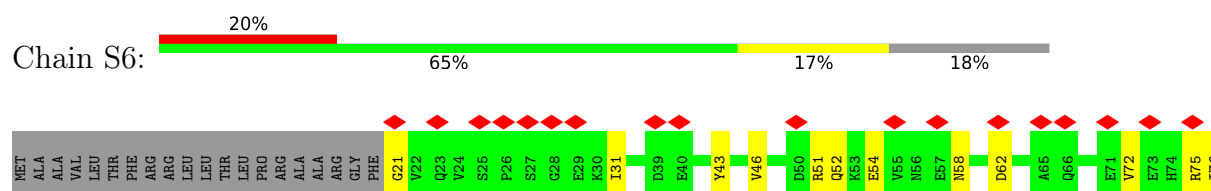
- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

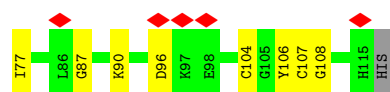


- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

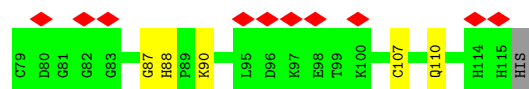
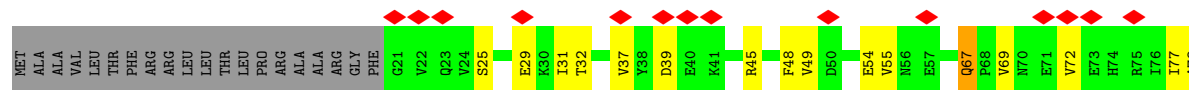


- Molecule 13: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

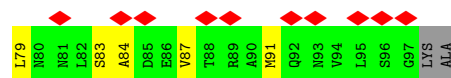
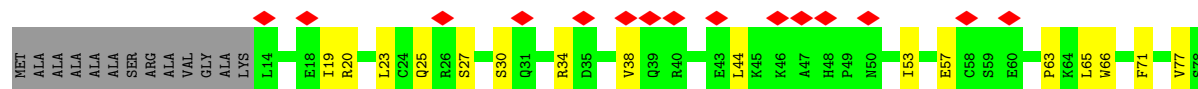




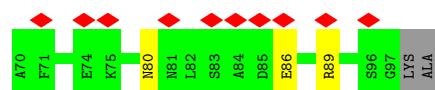
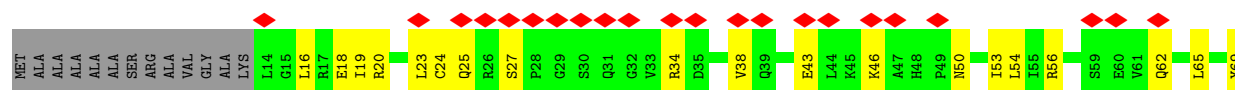
- Molecule 13: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



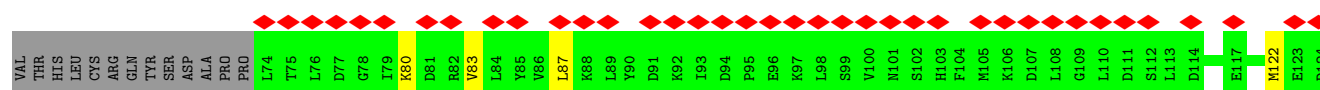
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



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



- Molecule 15: Acyl carrier protein, mitochondrial



- Molecule 15: Acyl carrier protein, mitochondrial



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

VAL THR HIS LEU CYS ARG GLN TYR S69 D70 A71 P72 L76 D77 D81 Y85 L89 D94 P95 E96 M105 K106 Q115 V116 E117 M120 E123 D124 E125 D132 A135 E136 K137 L138 P141 Q142 E143 I144 V145 D146 D150 D153 V154 Y155 E156

- Molecule 15: Acyl carrier protein, mitochondrial



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

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

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

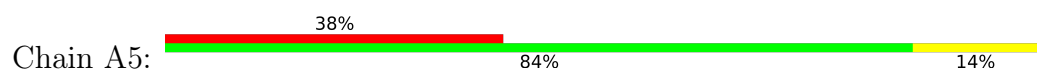
- Molecule 15: Acyl carrier protein, mitochondrial



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

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

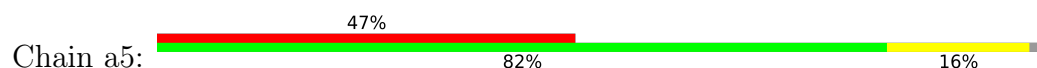
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

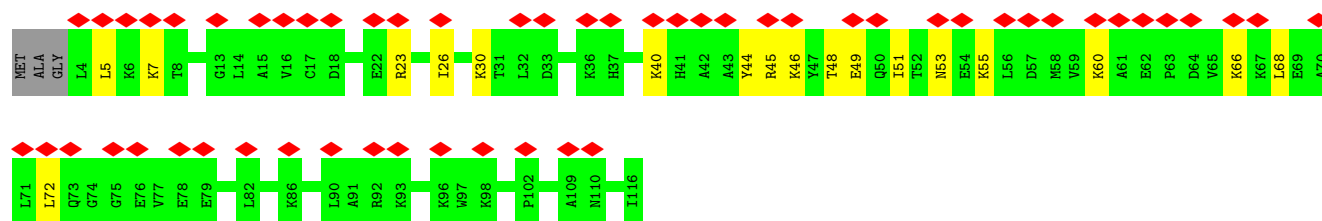


MET ALA G3 L4 L5 K6 K7 G10 G13 C17 D18 R23 L26 D33 K36 H37 F38 P39 K40 H41 A42 A43 Y44 R45 T48 E49 T52 N53 E54 K55 L56 D57 A61 E62 P63 P64 V65 K66 K67 K68 L68 L71 L72 Q73 G74 G75 E78 L82

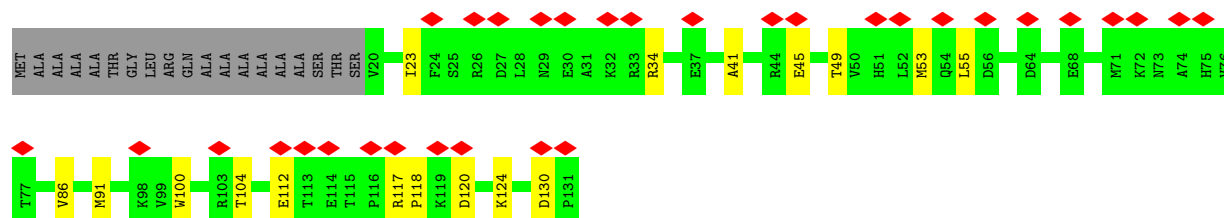
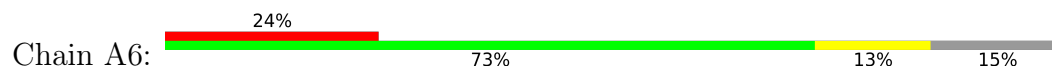
E85 K86 R82 K93 M94 L95 H97 K98 E101 P102 L103 V104 E105 E106 A109 M110 P115 I116

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

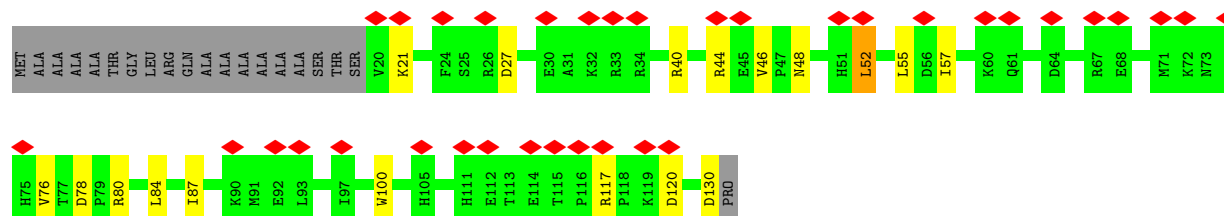
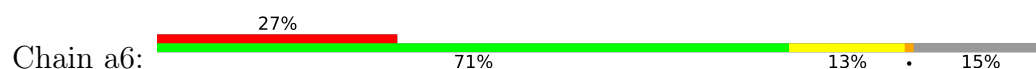




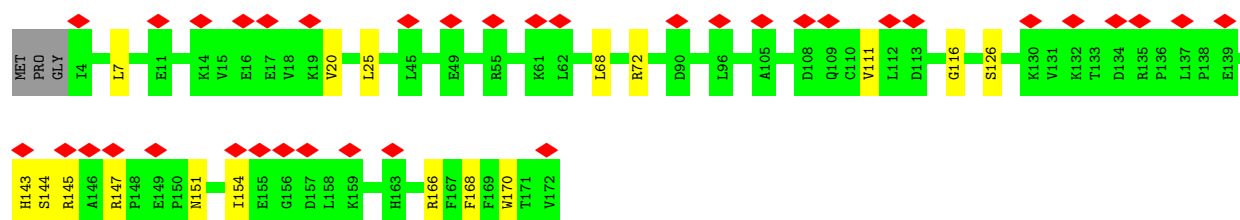
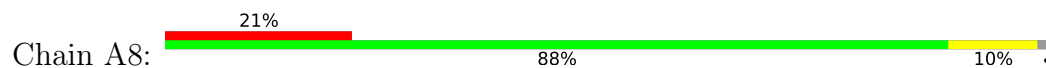
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



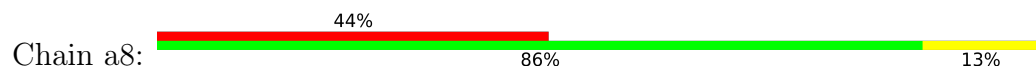
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

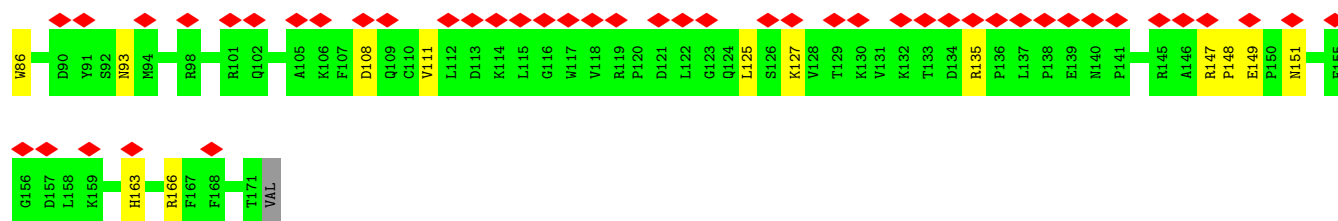


- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

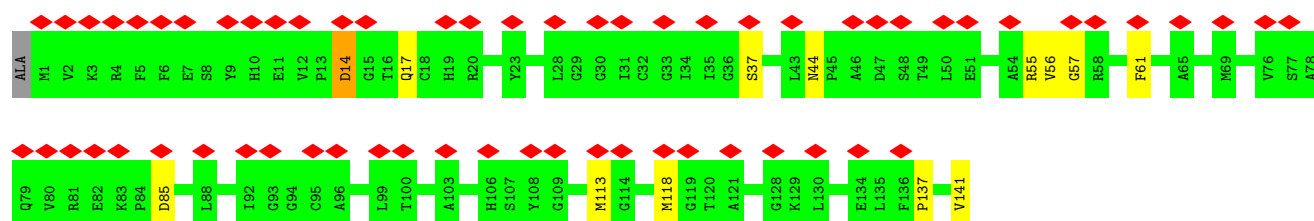
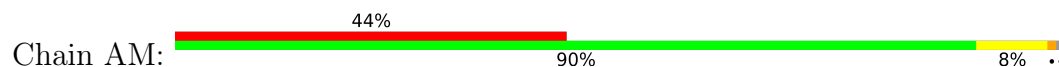


- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

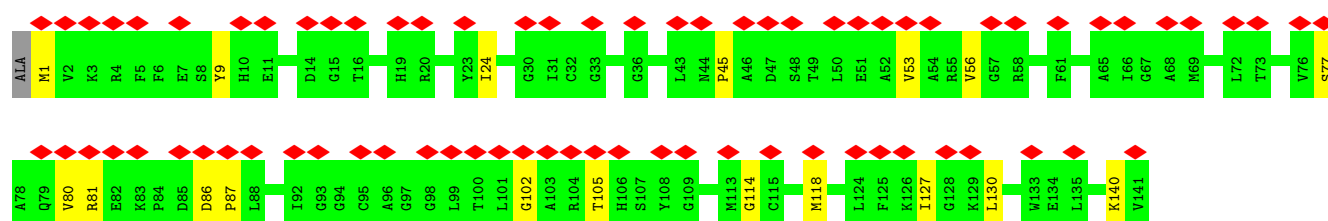
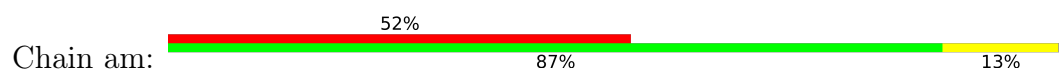




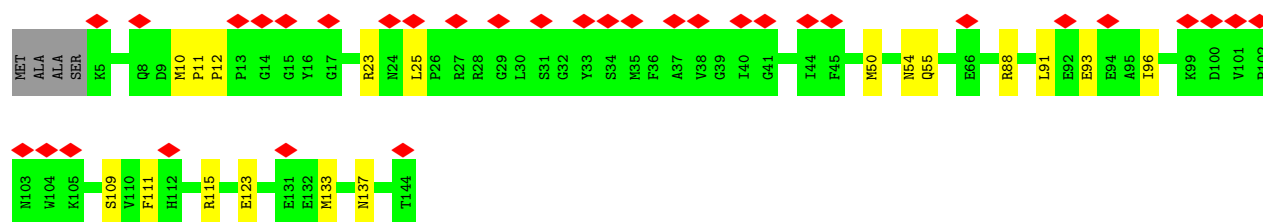
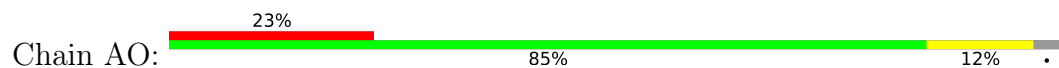
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



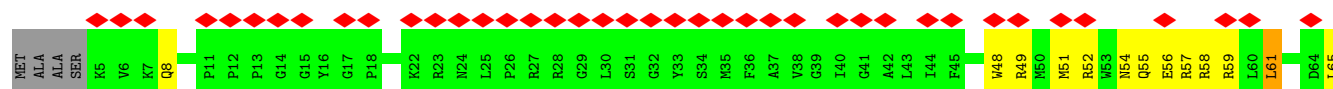
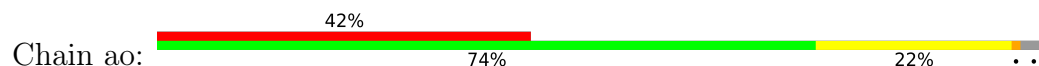
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

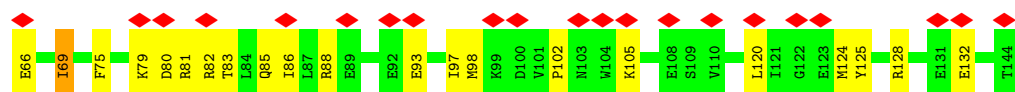


- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

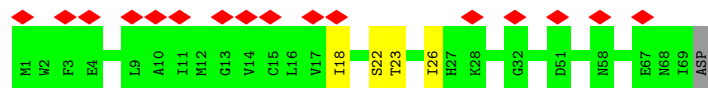


- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

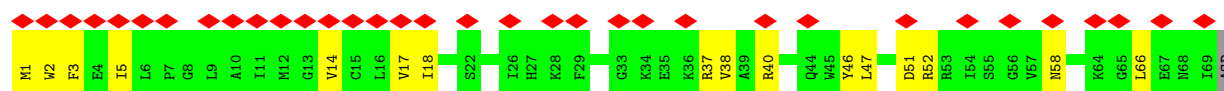
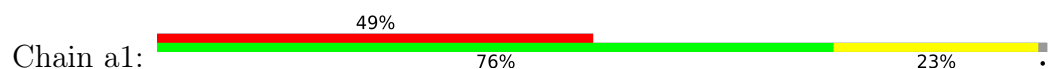




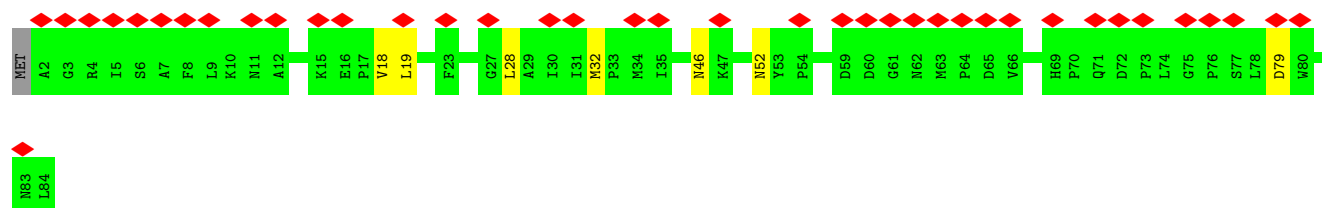
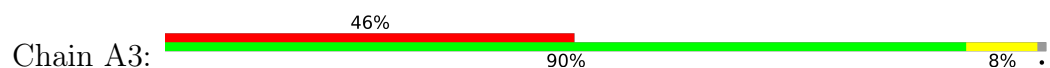
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



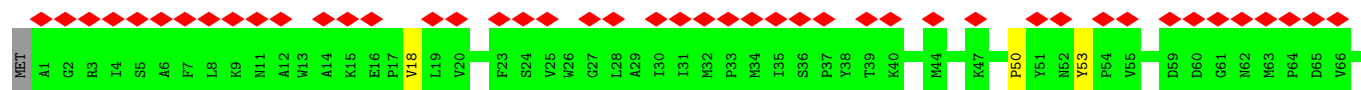
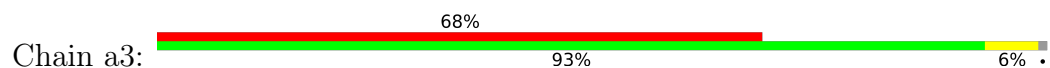
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



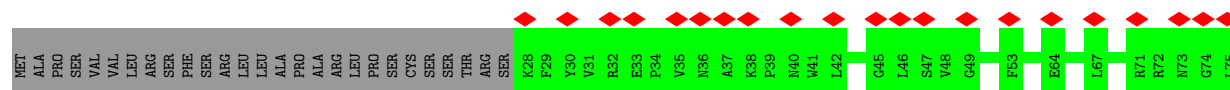
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



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

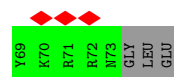
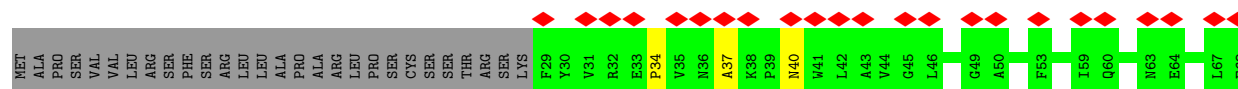


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

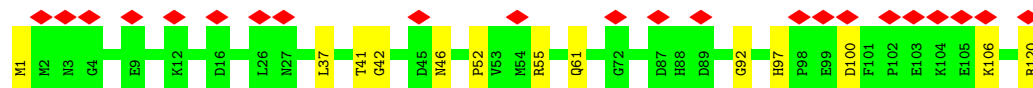
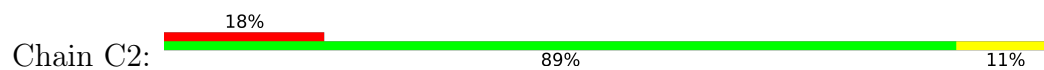




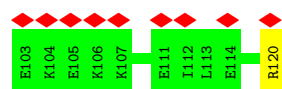
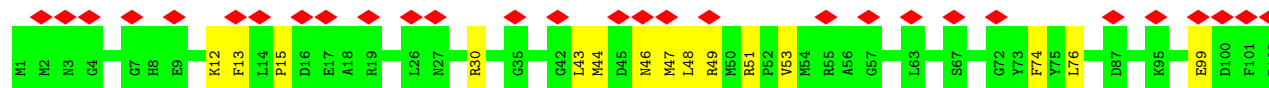
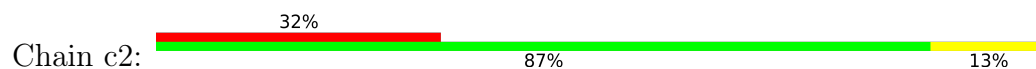
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



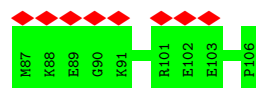
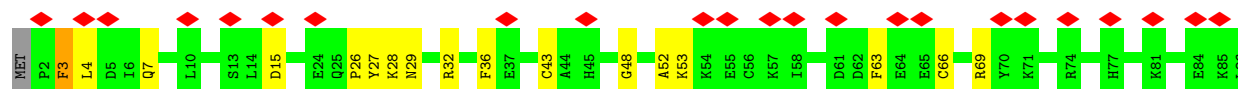
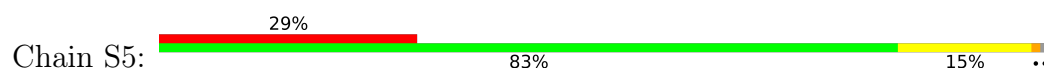
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 subunit C2



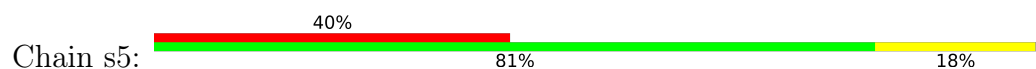
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 subunit C2

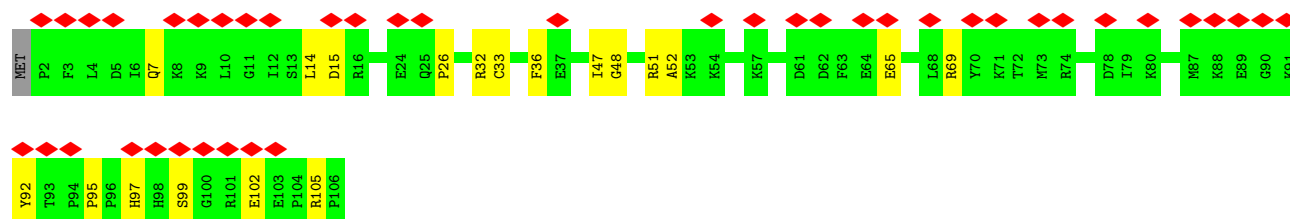


- Molecule 25: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

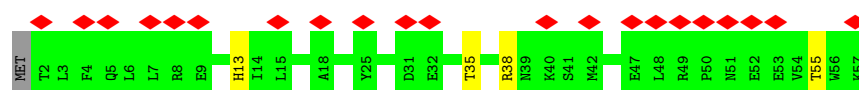
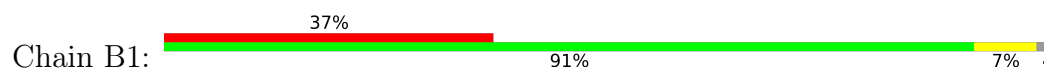


- Molecule 25: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

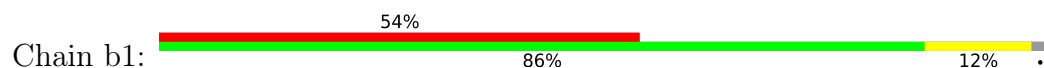




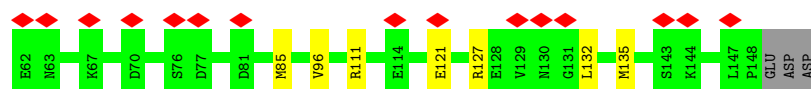
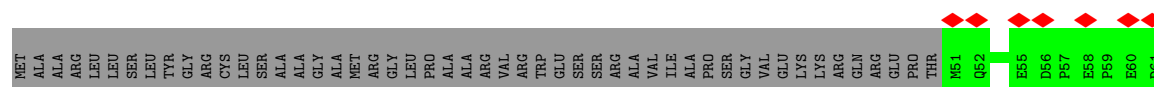
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



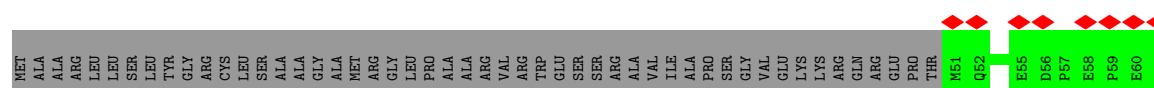
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



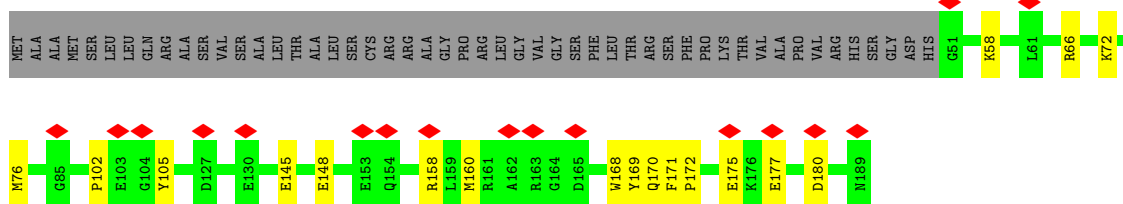
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



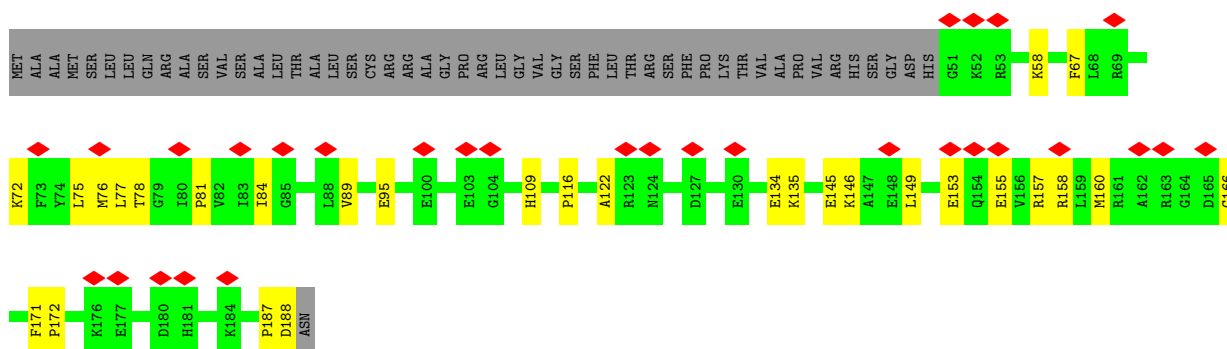
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



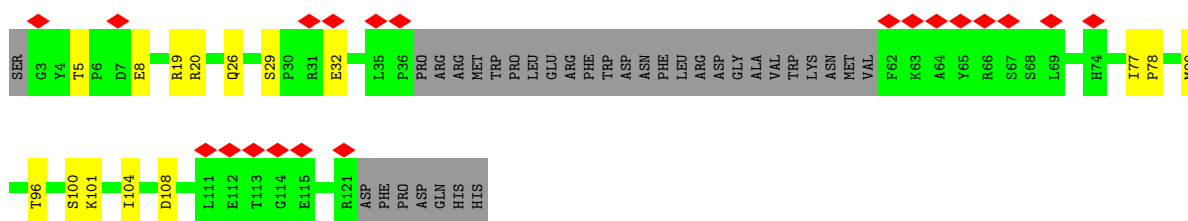
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



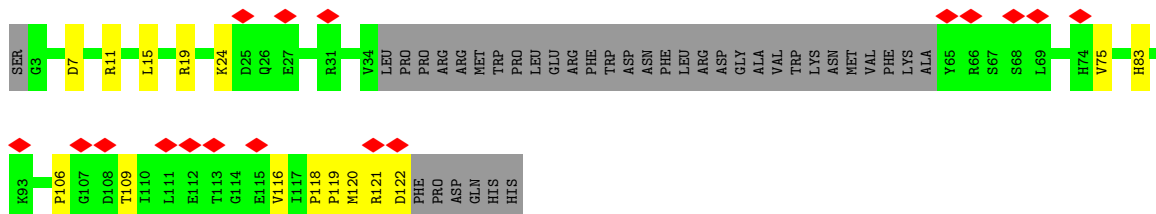
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



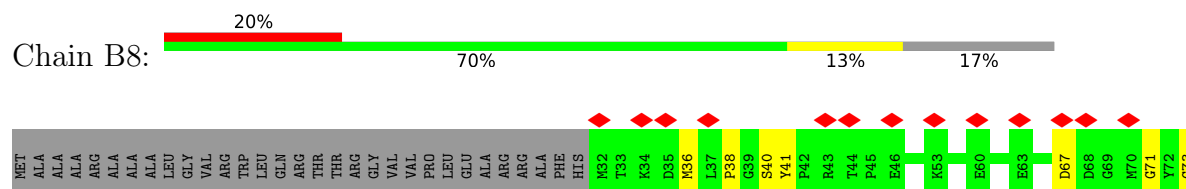
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

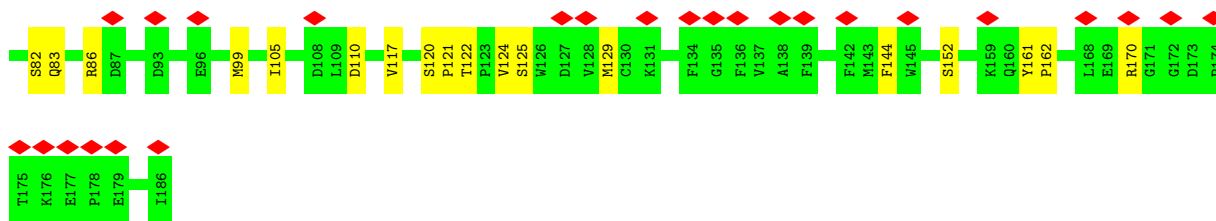


- Molecule 29: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

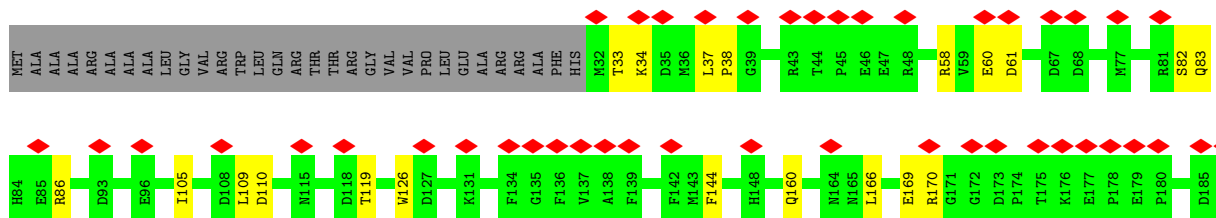
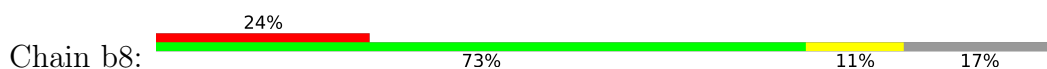


- Molecule 30: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

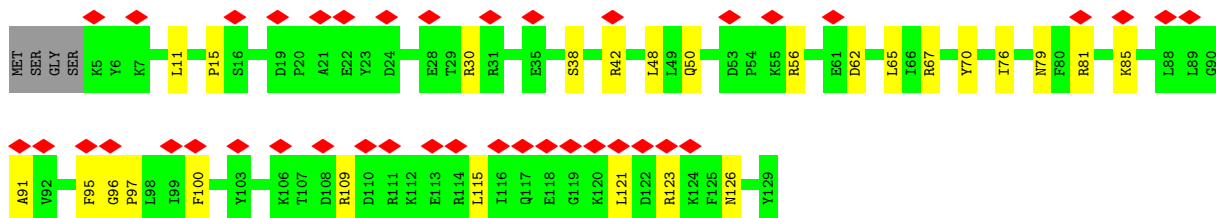
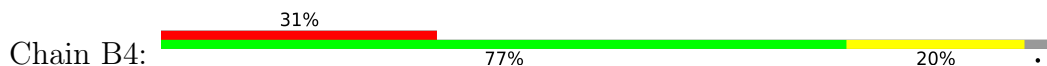




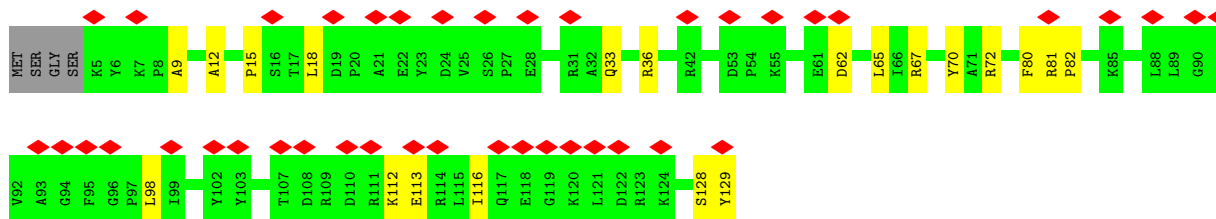
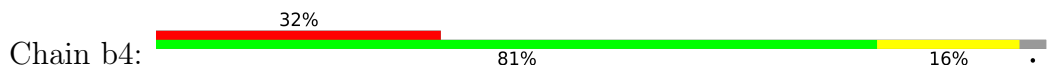
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



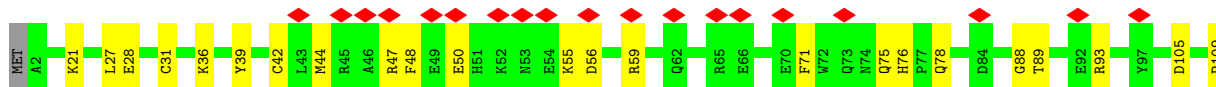
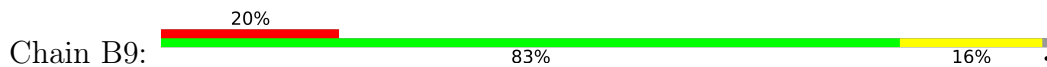
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

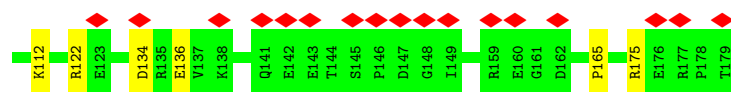


- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

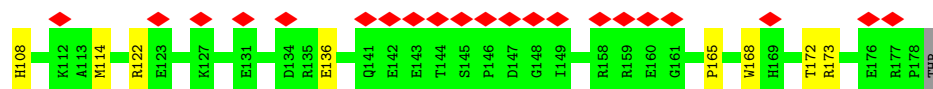
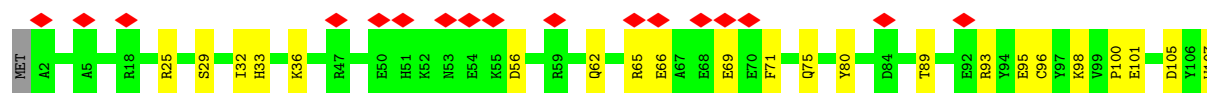
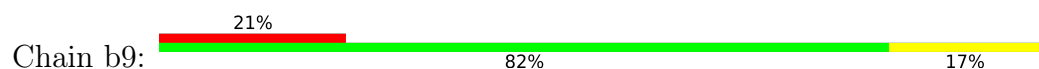


- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

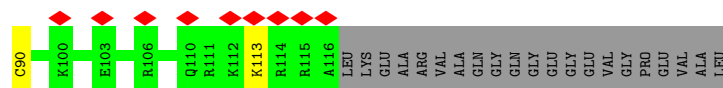
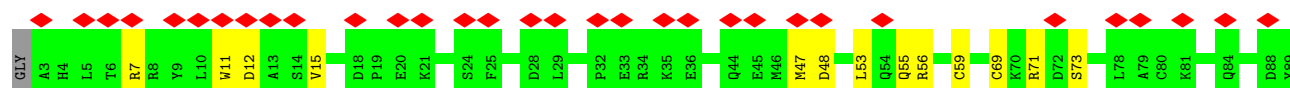
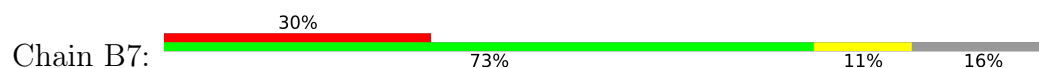




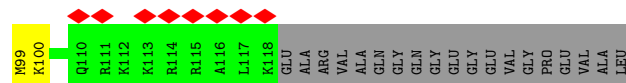
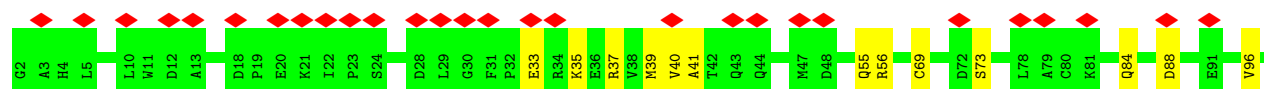
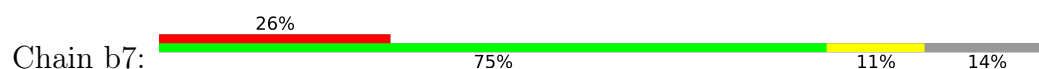
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



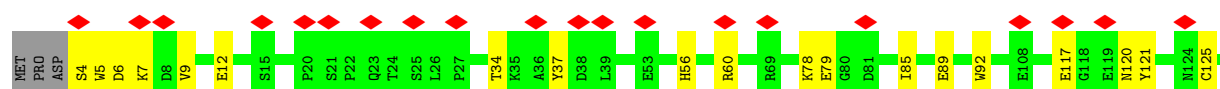
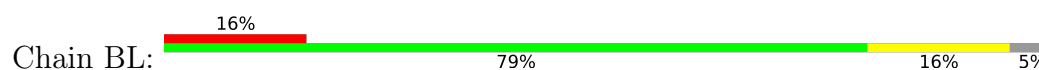
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



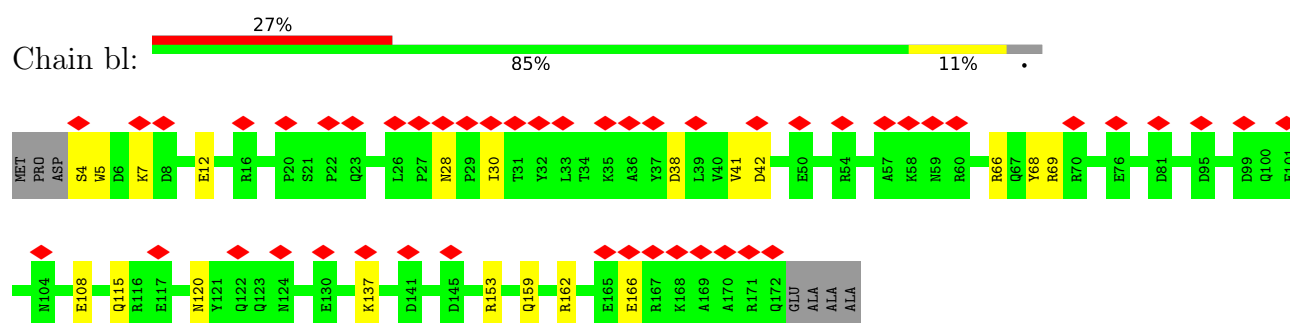
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



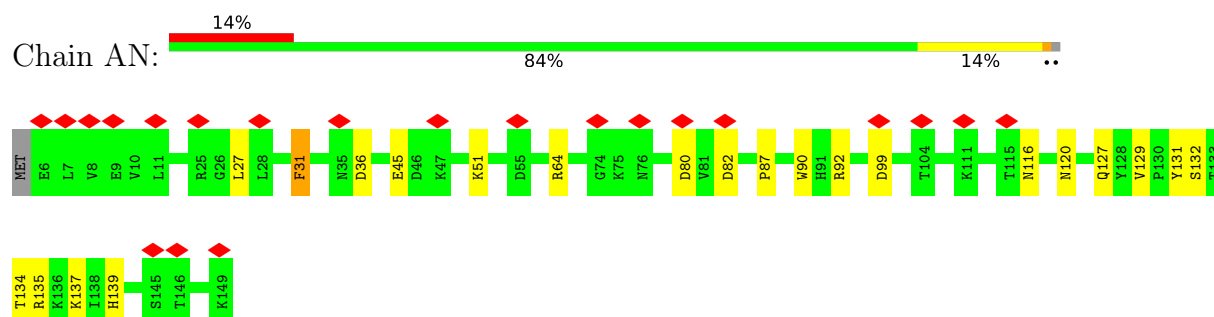
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



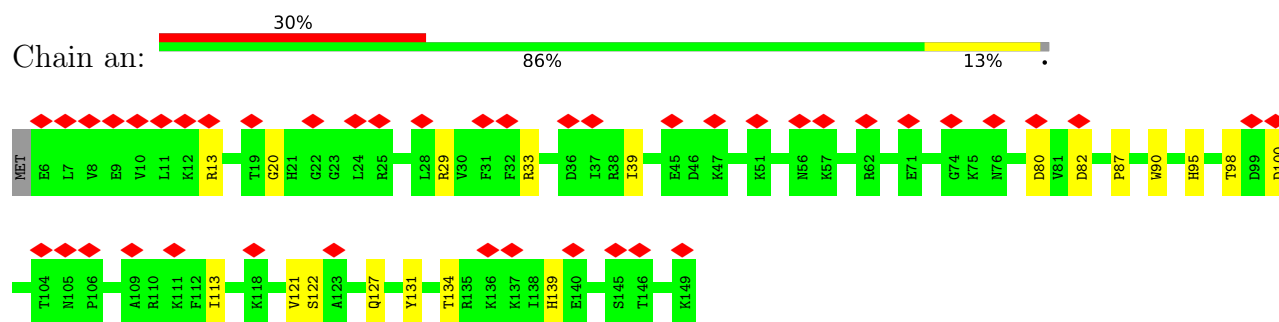
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



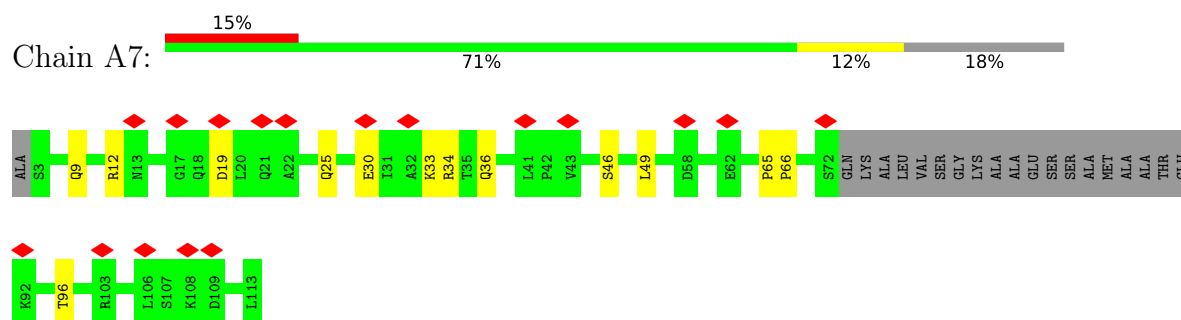
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



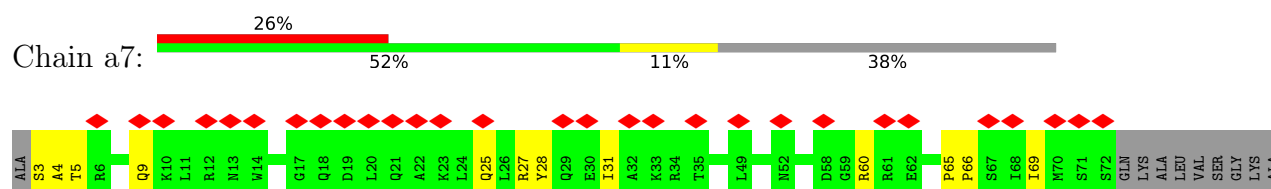
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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



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



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

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



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

PRO  
THR  
ASP  
THR  
T65  
T66  
L70  
L71  
H72  
H73  
L81  
L85  
D86  
L87  
S88  
K89  
P90  
R91  
L92  
P93  
Q94  
P95  
S96  
S97  
G98  
R99  
E100  
E103  
H104

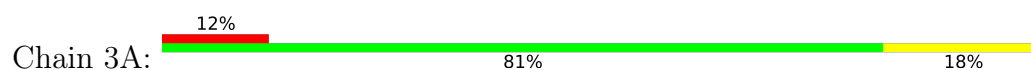
- Molecule 39: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



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

PRO  
THR  
ASP  
THR  
THR  
THR  
TYR  
K68  
N69  
L70  
H73  
D74  
L81  
D82  
L83  
N84  
D86  
K89  
F90  
R91  
R99  
E100  
R103  
HIS

- Molecule 40: Cytochrome b-c1 complex subunit 1, mitochondrial



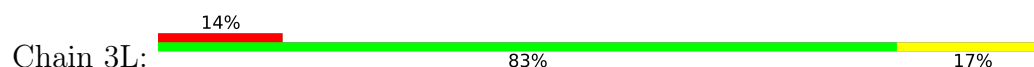
THR  
A36  
T37  
F38  
A39  
Q40  
A41  
L42  
Q43  
S44  
E47  
L53  
D54  
R53  
S64  
S65  
T70  
V71  
W74  
R80  
E84  
K85  
N86  
N87  
G88  
F92  
L93  
E94  
A97  
F98  
K99  
G100  
T101  
K102  
N103  
V113  
L120  
A122  
R126  
L132  
I133  
K138  
D139

V144  
D149  
I150  
D158  
E162  
R165  
D166  
E174  
N175  
D176  
A177  
S178  
Q199  
S205  
E206  
R210  
L211  
T214  
D215  
L216  
T217  
D218  
R222  
V230  
L231  
A232  
Q240  
L245  
A246  
S252  
E258  
E259  
D260  
A261  
V263  
G264  
L265  
T266  
E274  
I275  
R276  
R277  
R278

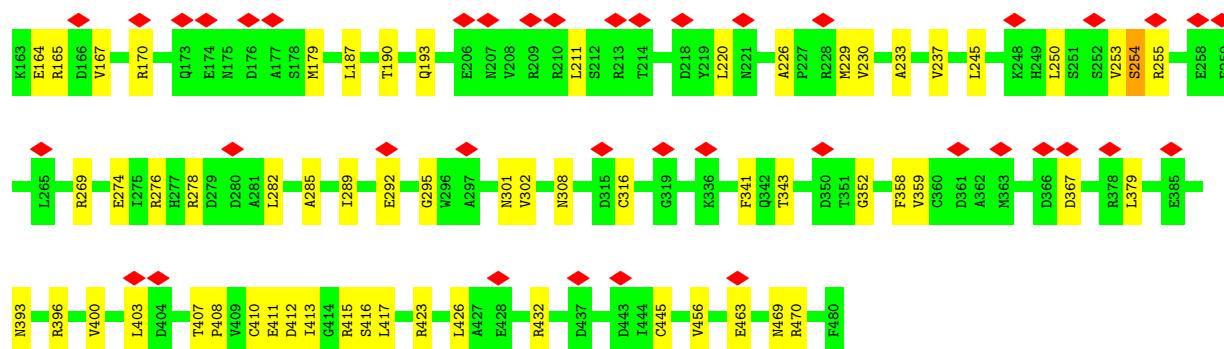
D279  
D280  
A281  
E292  
N298  
P299  
D300  
N301  
V302  
T303  
Q305  
V306  
I310  
D315  
A332  
N335  
K336  
L337  
S349  
D350  
T351  
G352  
C360  
D361  
A362  
M363  
S364  
M368  
L372  
E385  
V388  
K392  
L395  
R396  
N397  
A398  
L399  
T406  
E411  
D412  
L417

L426  
W429  
I433  
Q434  
E435  
V436  
D437  
A438  
Q439  
D443  
I444  
C445  
S446  
F449  
Y450  
D451  
Q452  
C453  
E463  
Q464  
L465  
M469  
R472  
S473  
G474  
E479  
F480

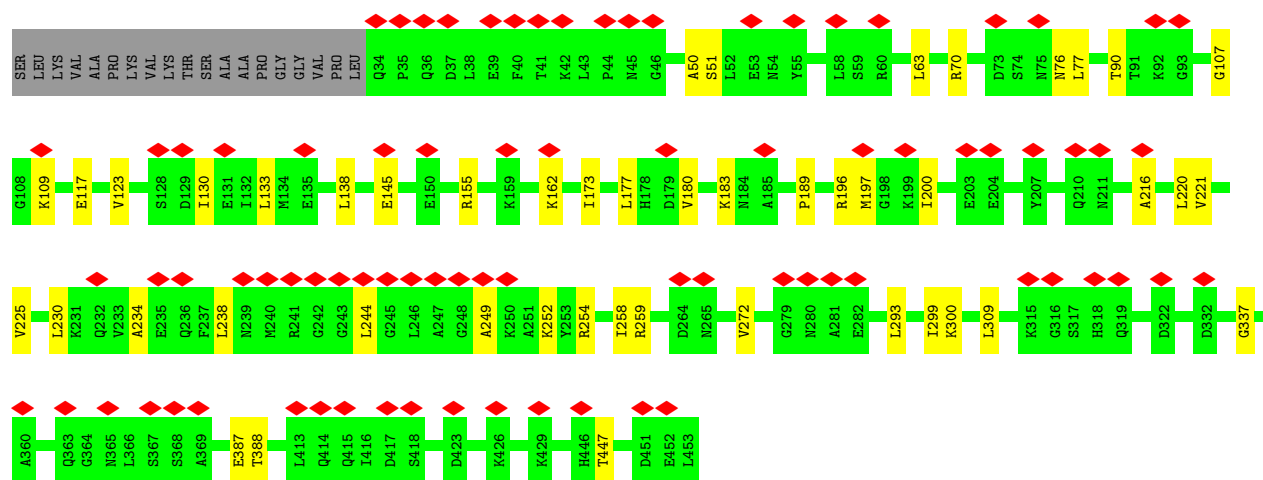
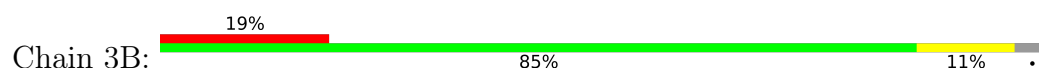
- Molecule 40: Cytochrome b-c1 complex subunit 1, mitochondrial



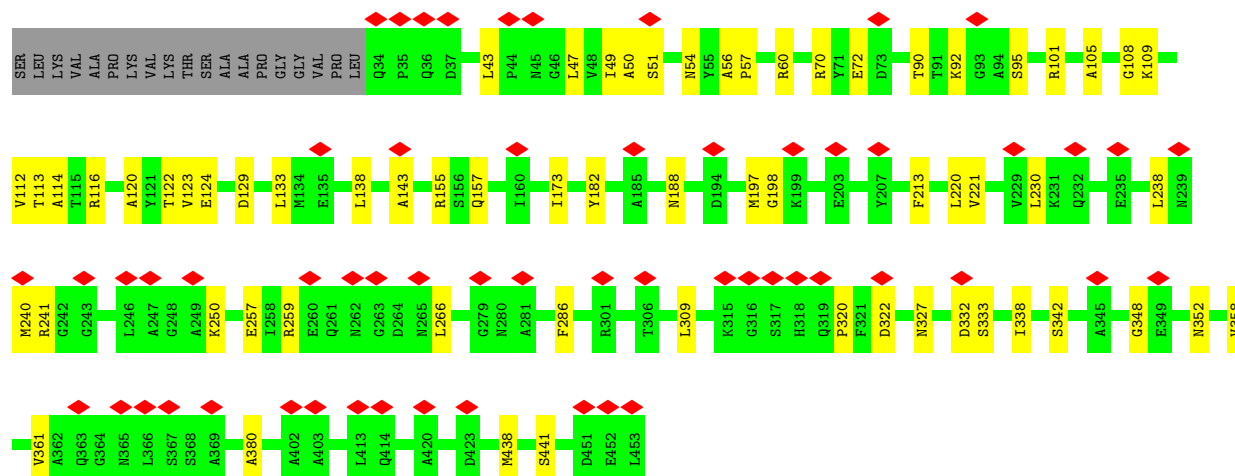
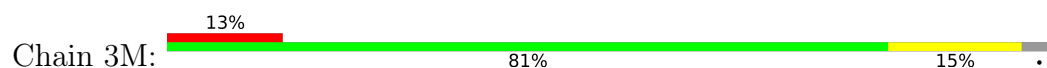
THR  
A36  
T37  
F38  
A39  
Q40  
Q43  
S44  
E47  
T48  
D54  
N55  
R58  
E62  
S65  
T70  
D76  
T83  
E84  
K85  
L93  
E94  
K102  
N103  
N107  
E110  
E114  
A118  
I133  
K134  
A135  
L136  
S137  
K138  
D139  
L140  
P141  
K142  
V143  
D158  
S159  
E162



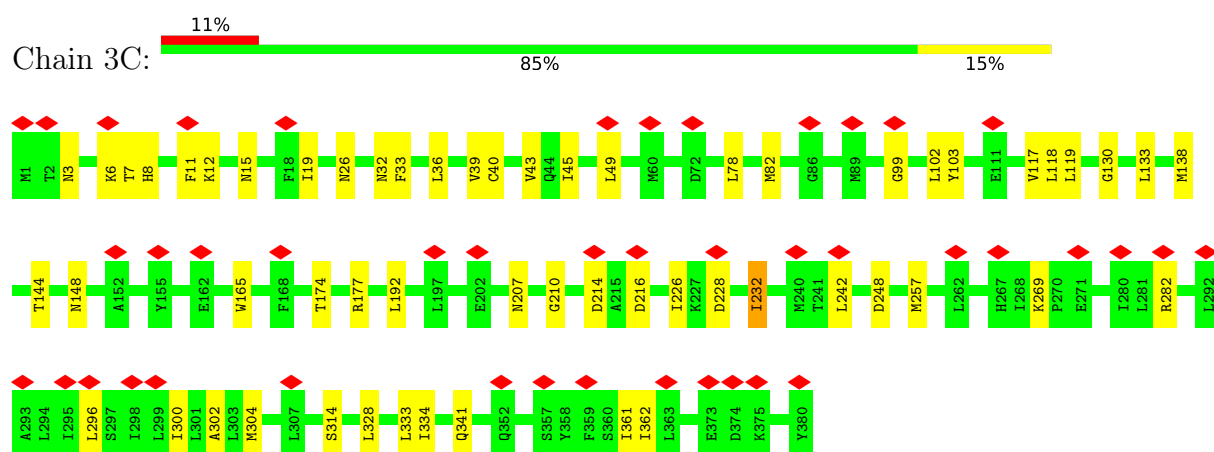
- Molecule 41: Cytochrome b-c1 complex subunit 2, mitochondrial



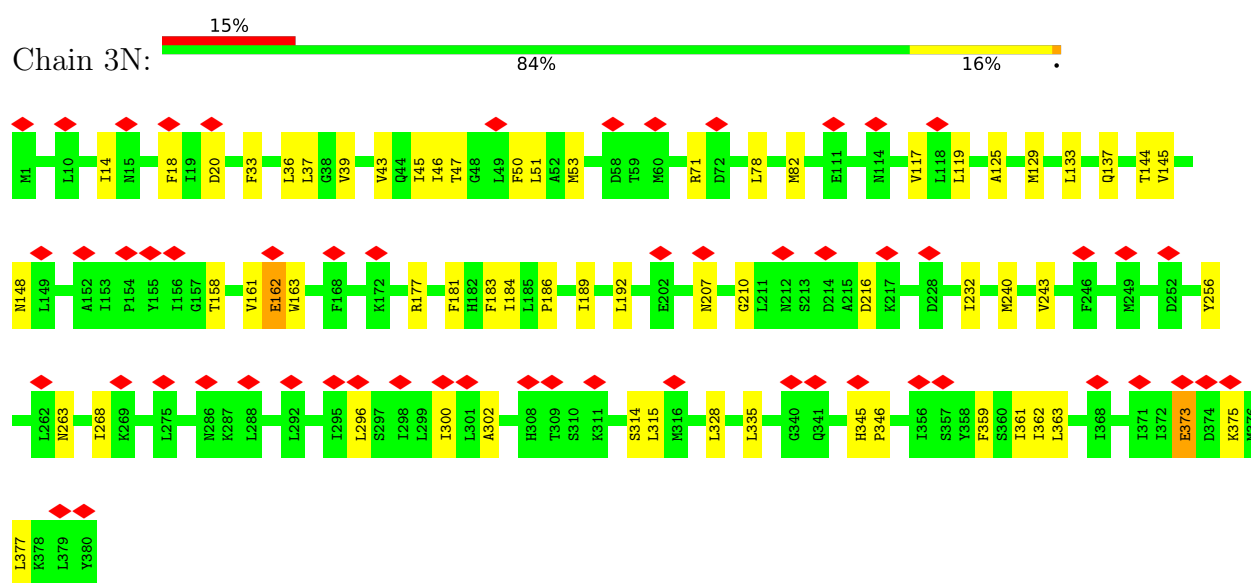
- Molecule 41: Cytochrome b-c1 complex subunit 2, mitochondrial



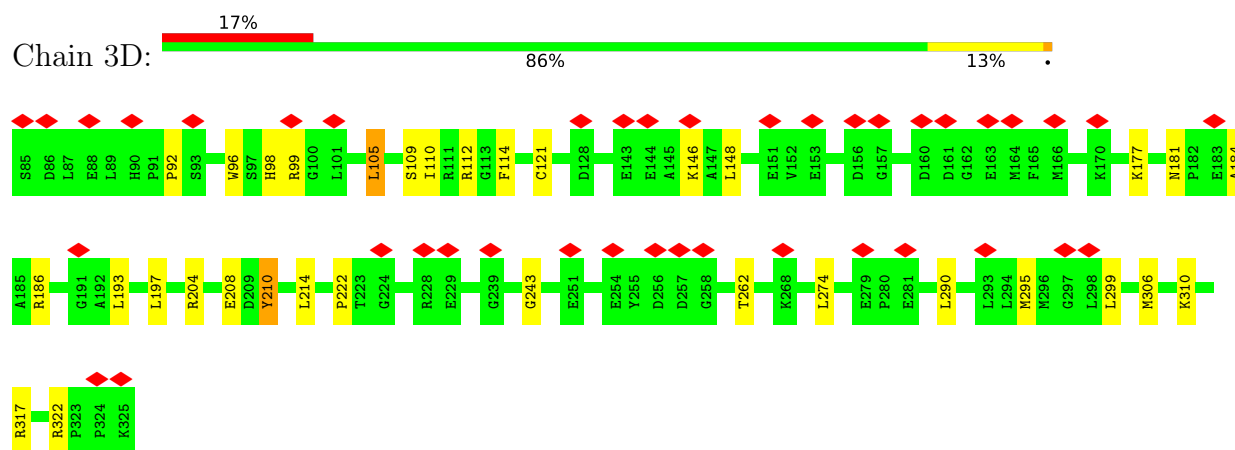
- Molecule 42: Cytochrome b



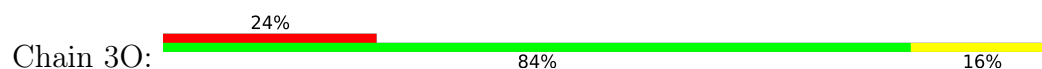
• Molecule 42: Cytochrome b

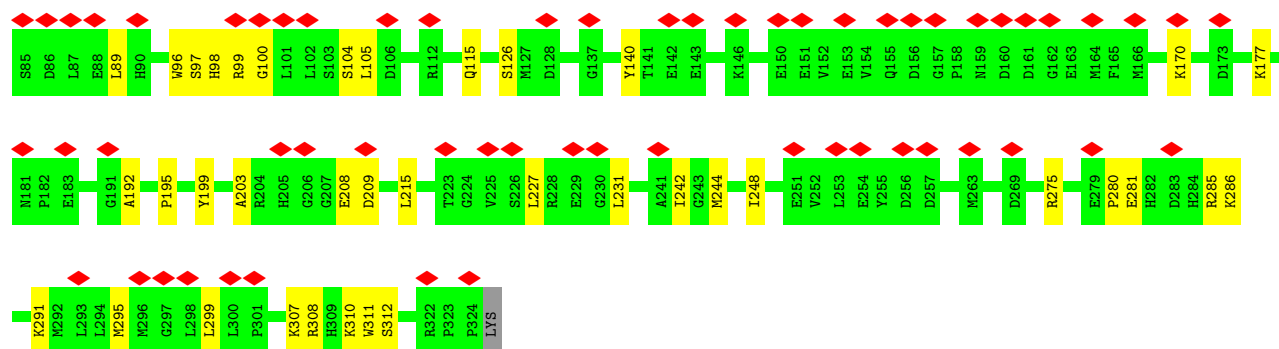


• Molecule 43: Cytochrome c1, heme protein, mitochondrial

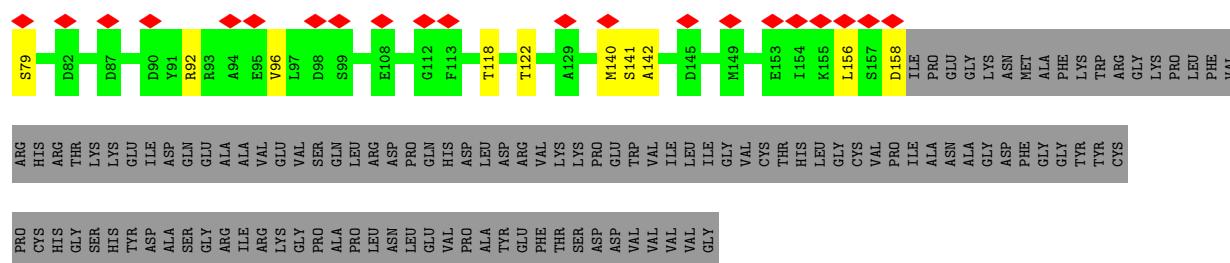
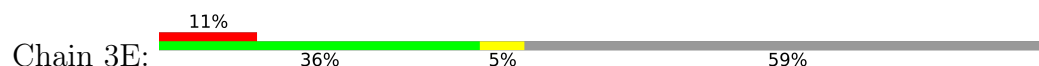


• Molecule 43: Cytochrome c1, heme protein, mitochondrial

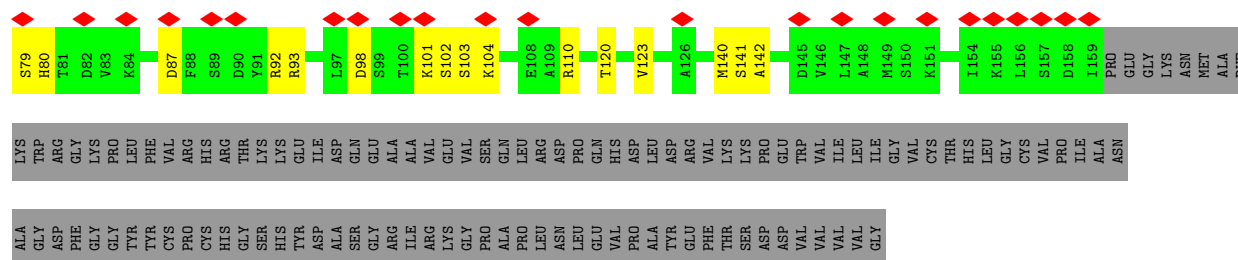
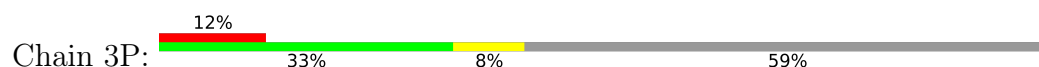




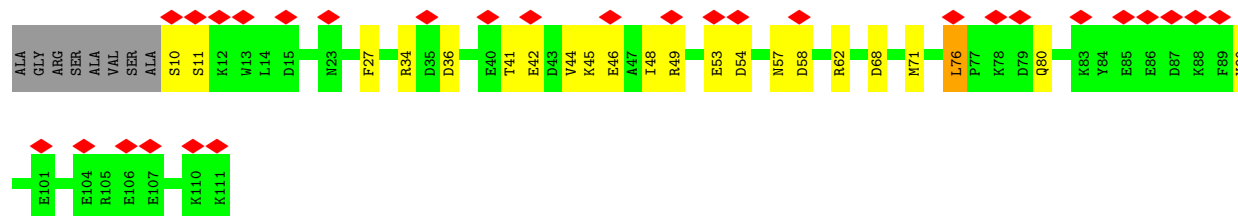
• Molecule 44: Cytochrome b-c1 complex subunit 9



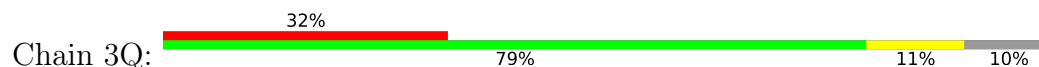
• Molecule 44: Cytochrome b-c1 complex subunit 9

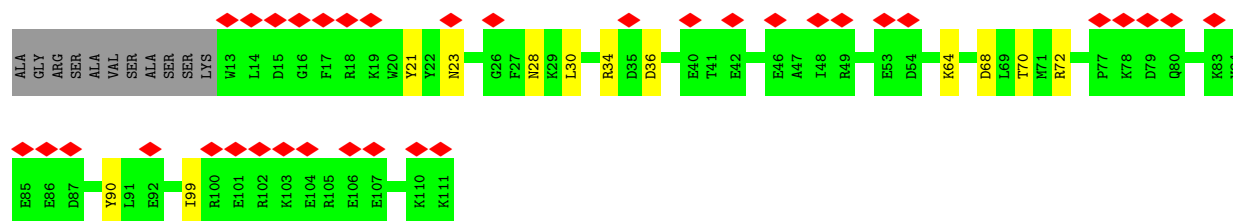


• Molecule 45: Cytochrome b-c1 complex subunit 7

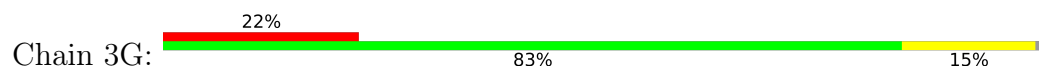


• Molecule 45: Cytochrome b-c1 complex subunit 7

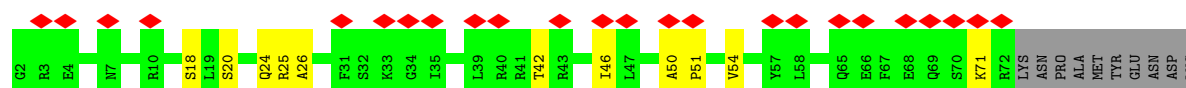
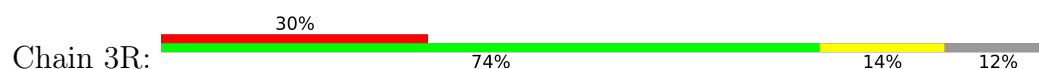




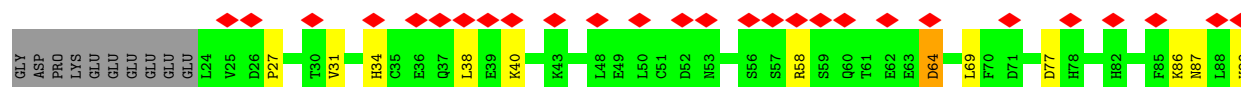
- Molecule 46: Cytochrome b-c1 complex subunit 8



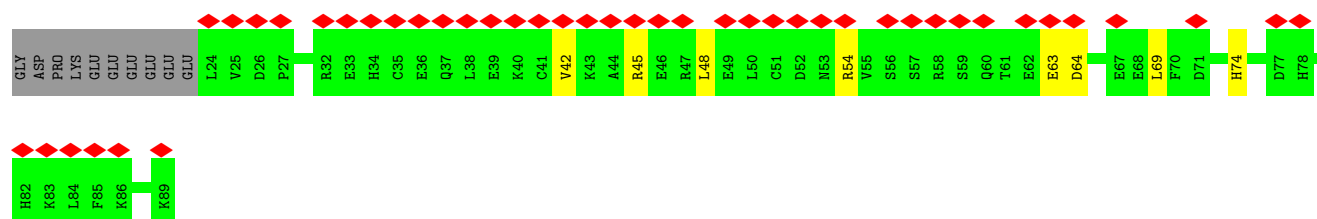
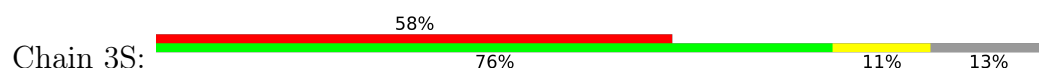
- Molecule 46: Cytochrome b-c1 complex subunit 8



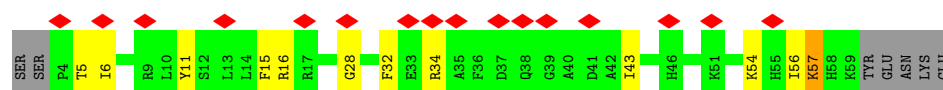
- Molecule 47: Cytochrome b-c1 complex subunit 6, mitochondrial



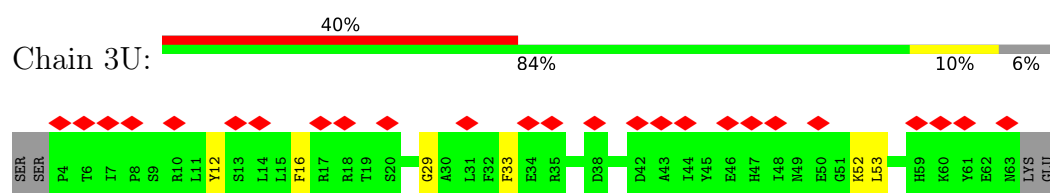
- Molecule 47: Cytochrome b-c1 complex subunit 6, mitochondrial



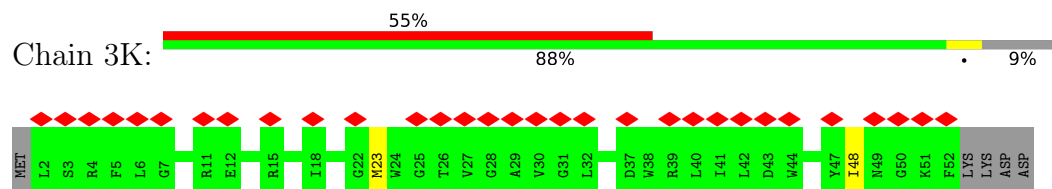
- Molecule 48: Cytochrome b-c1 complex subunit 9



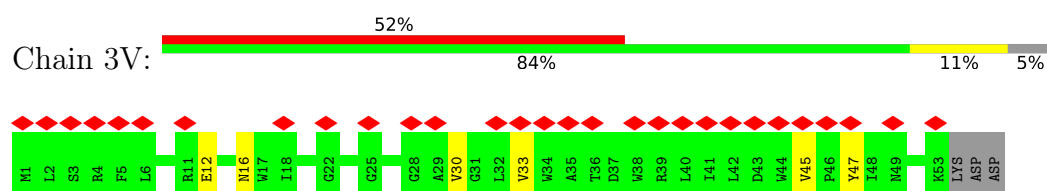
- Molecule 48: Cytochrome b-c1 complex subunit 9



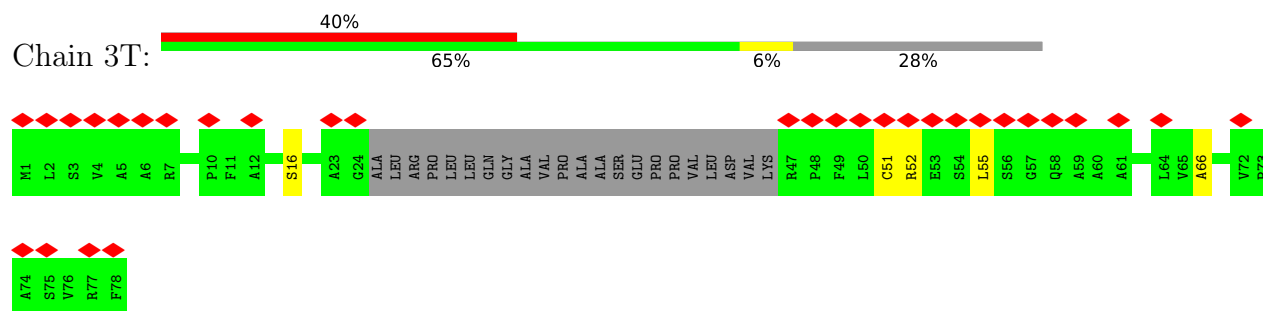
- Molecule 49: Cytochrome b-c1 complex subunit 10



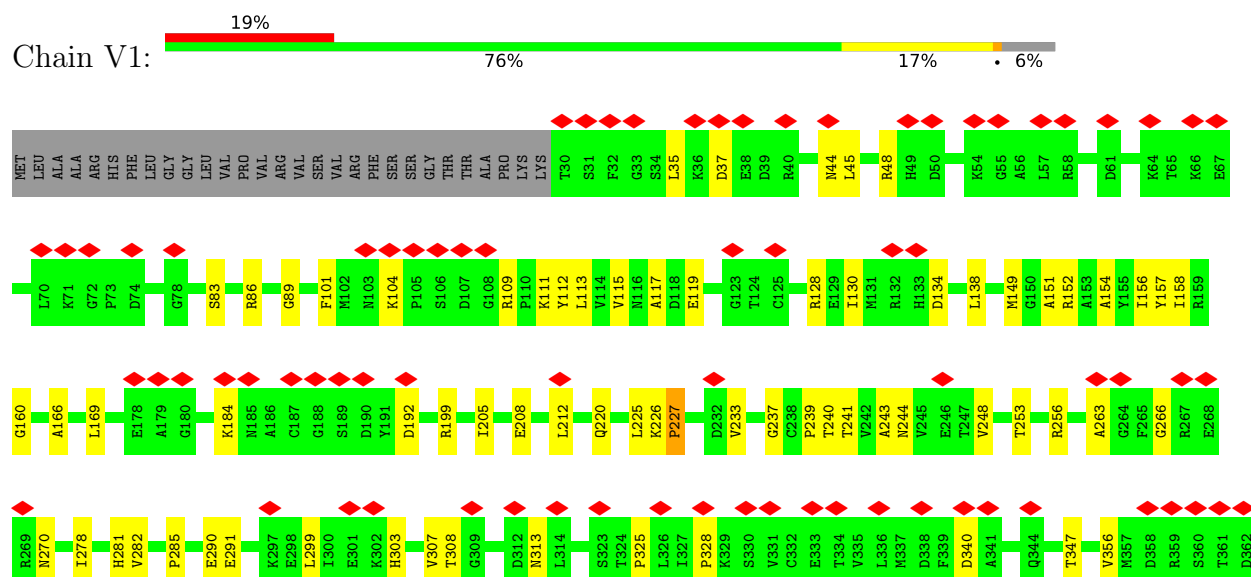
- Molecule 49: Cytochrome b-c1 complex subunit 10

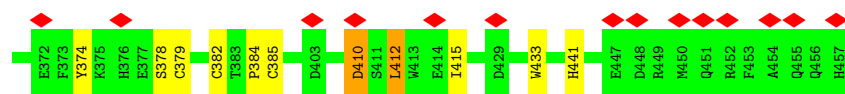


- Molecule 50: Cytochrome b-c1 complex subunit Rieske, mitochondrial



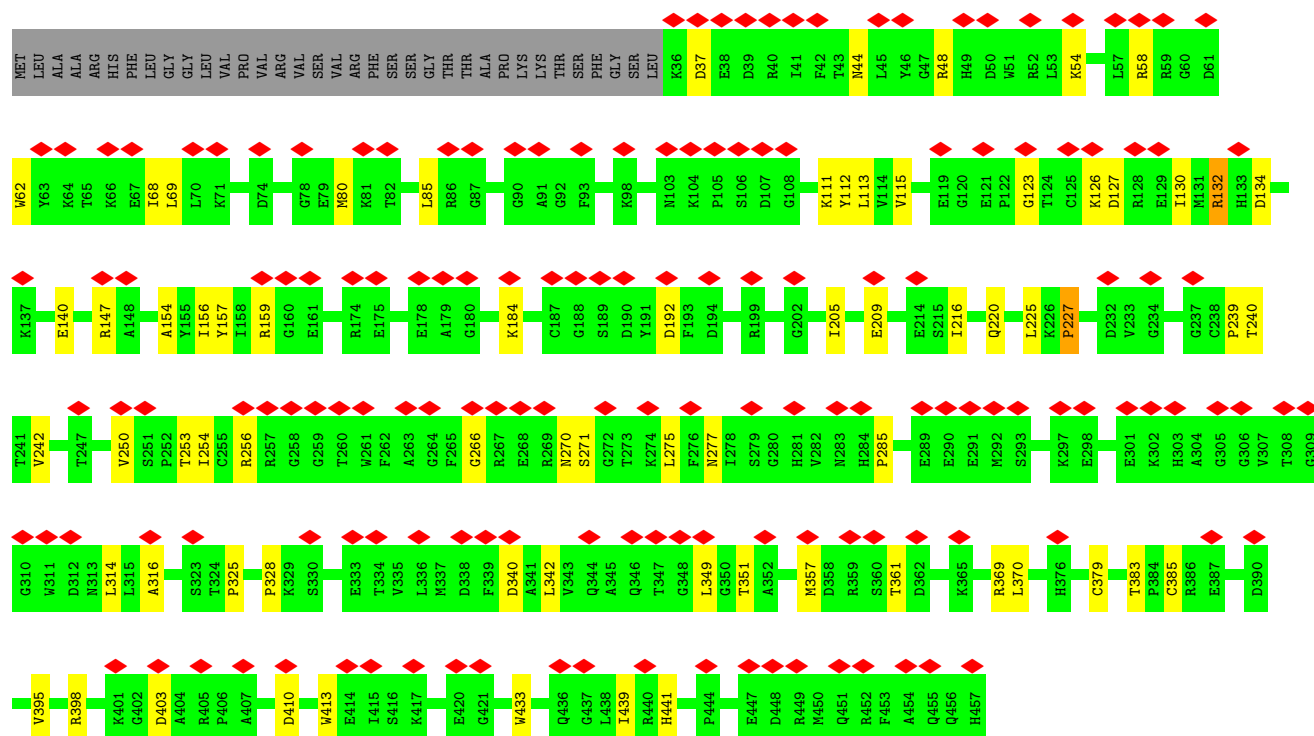
- Molecule 51: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial





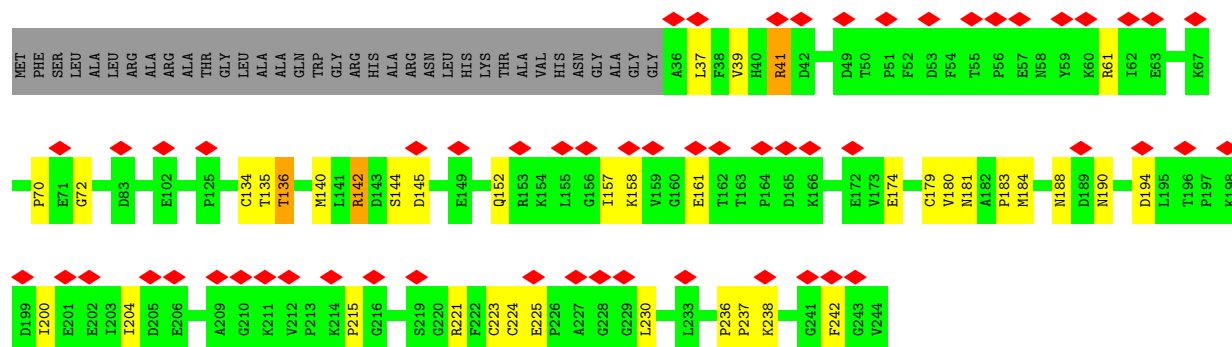
- Molecule 51: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain v1:



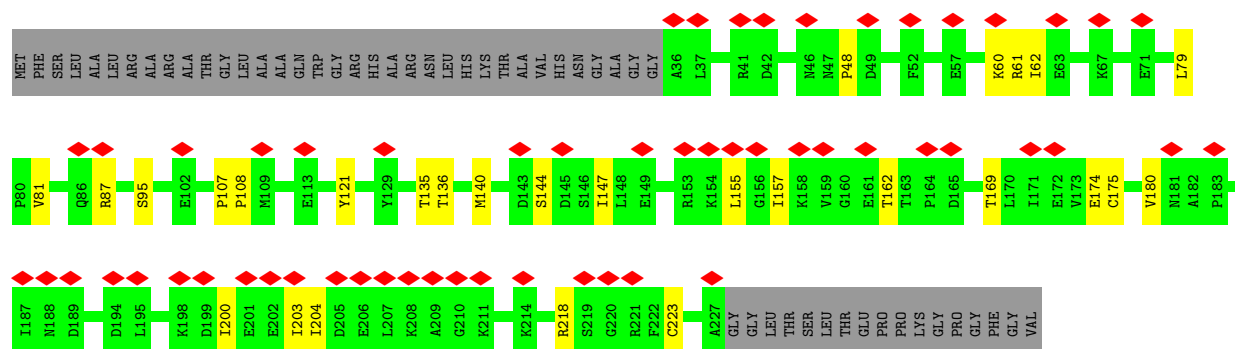
- Molecule 52: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain V2:

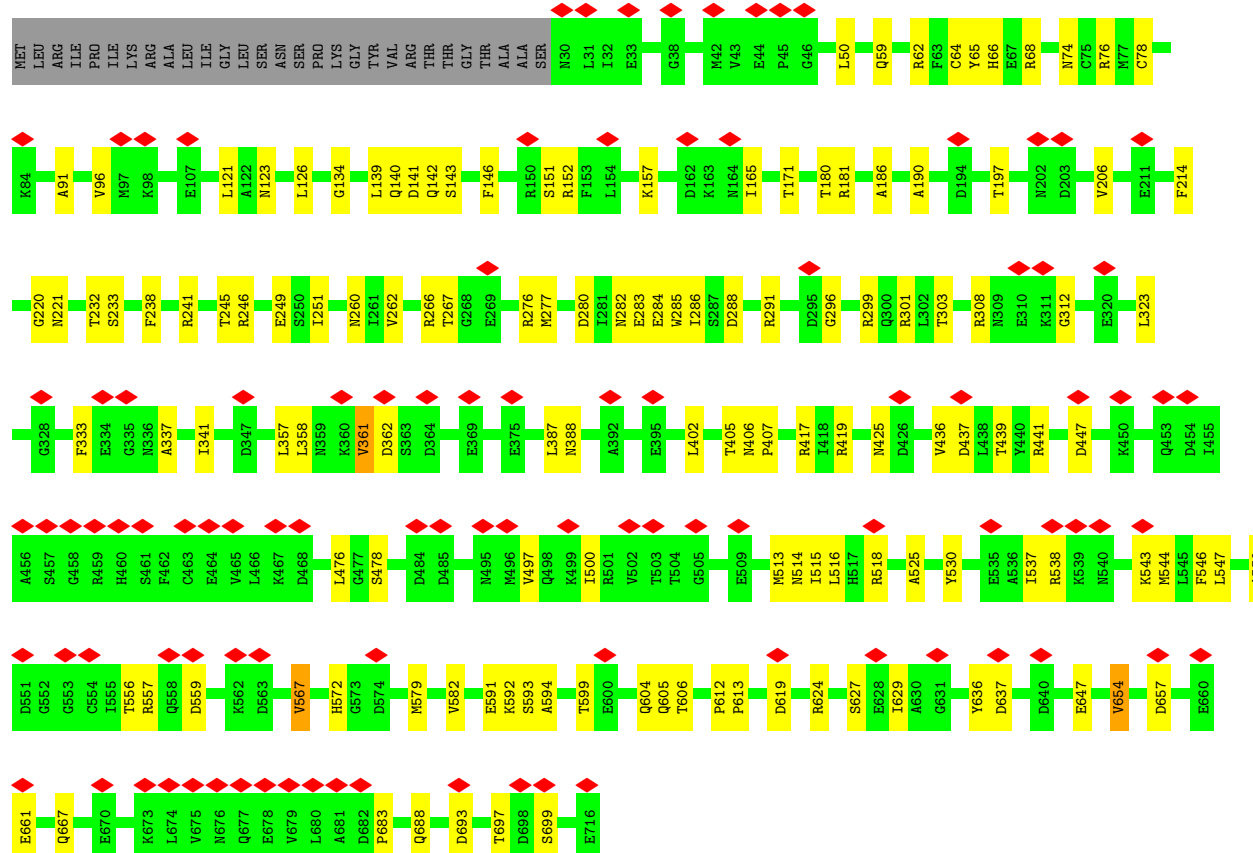


- Molecule 52: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

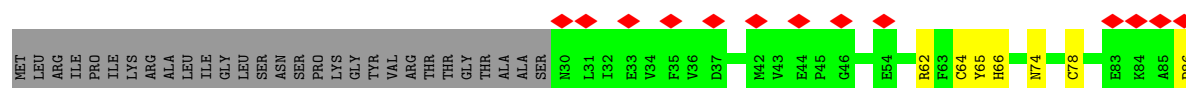
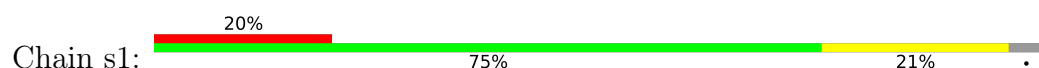
Chain v2:

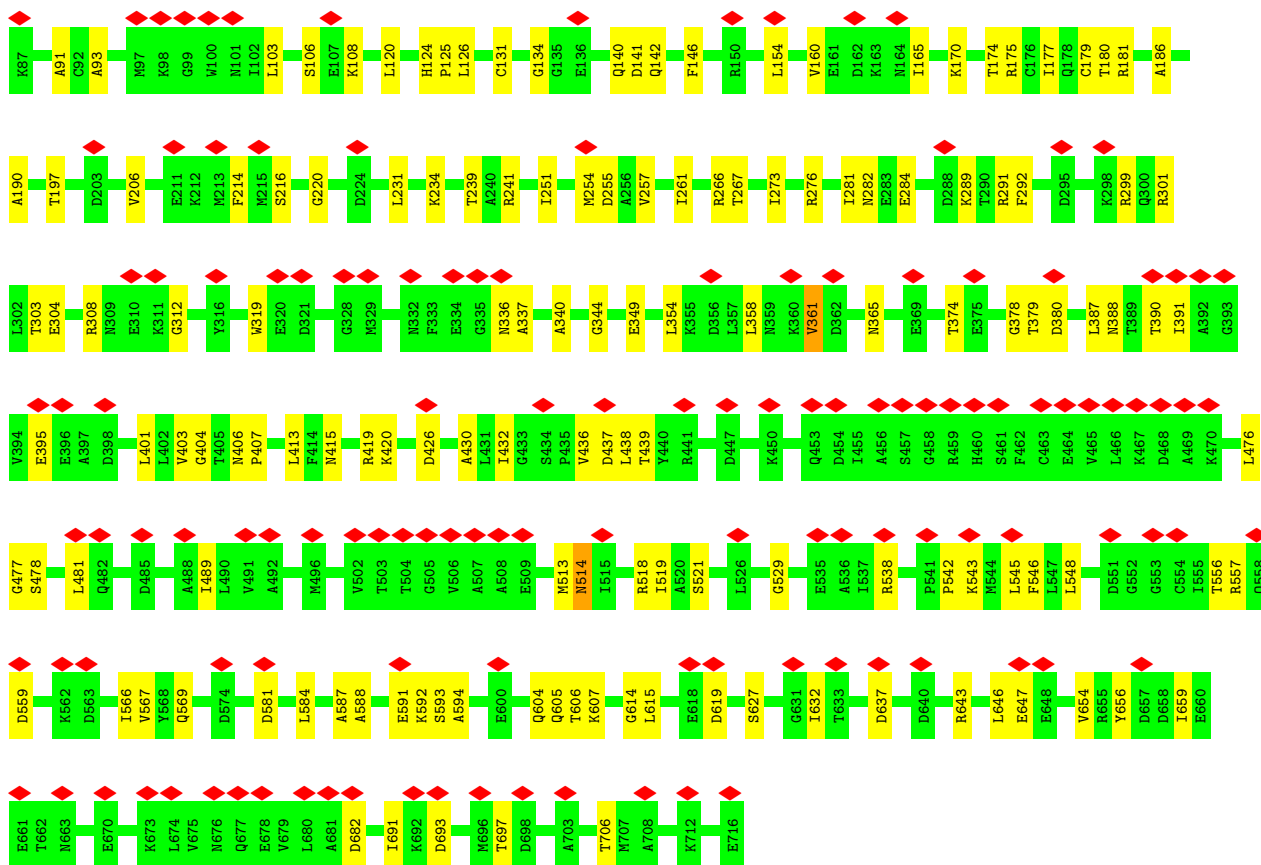


- Molecule 53: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

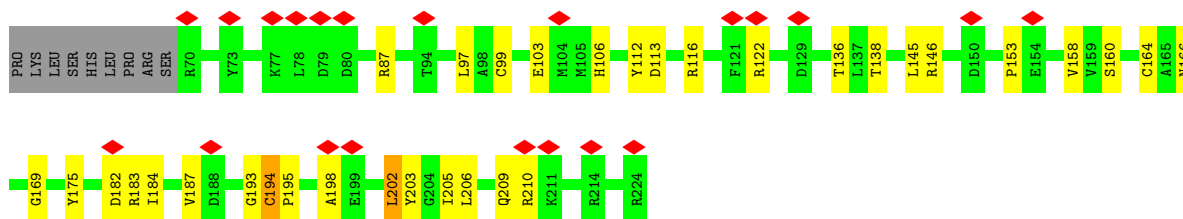
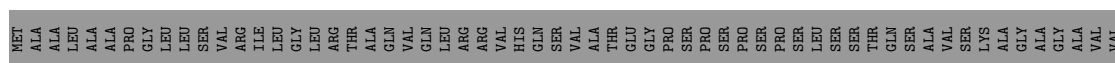


- Molecule 53: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

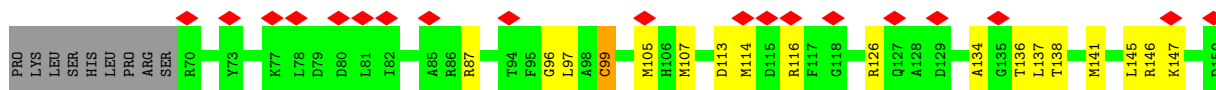
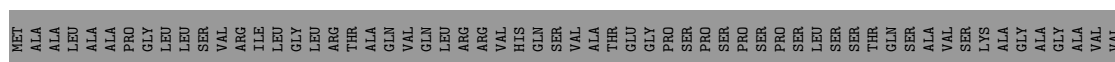


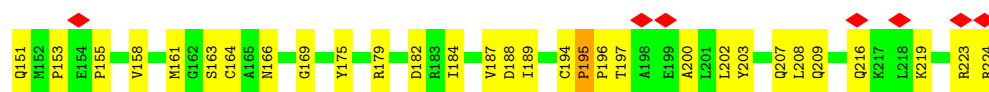


- Molecule 54: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

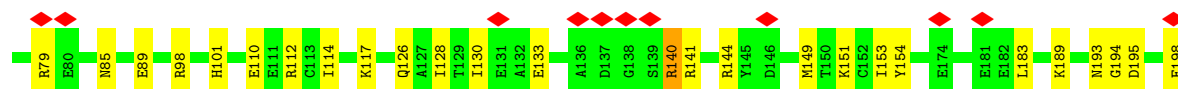
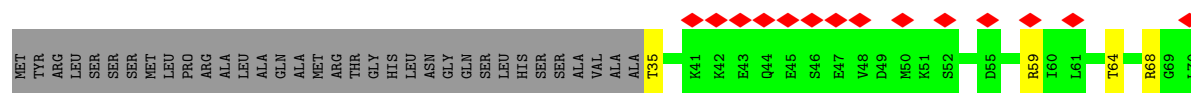


- Molecule 54: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

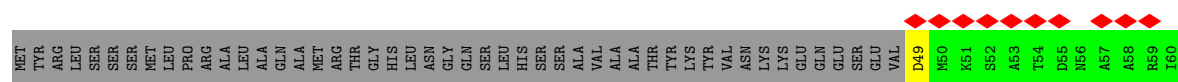




- Molecule 55: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



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



## 4 Experimental information

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

## 5 Model quality

### 5.1 Standard geometry

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

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

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

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

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

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

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

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 9   | 2a    | 255 | PRO  | CB-CG | -11.20 | 0.93        | 1.49     |
| 21  | a1    | 18  | ILE  | C-N   | 9.06   | 1.45        | 1.34     |
| 9   | 2a    | 255 | PRO  | CG-CD | -7.88  | 1.24        | 1.50     |
| 48  | 3J    | 57  | LYS  | CA-C  | 6.53   | 1.61        | 1.52     |
| 9   | 2a    | 255 | PRO  | N-CA  | 5.90   | 1.58        | 1.46     |
| 4   | 1     | 74  | ALA  | C-N   | 5.20   | 1.40        | 1.34     |

All (104) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 9   | 2a    | 255 | PRO  | CB-CG-CD | 18.22  | 164.40      | 106.10   |
| 9   | 2a    | 255 | PRO  | N-CD-CG  | -17.40 | 77.11       | 103.20   |
| 9   | 2a    | 255 | PRO  | CA-CB-CG | -16.77 | 72.64       | 104.50   |
| 10  | AL    | 210 | PRO  | CA-C-N   | 10.80  | 127.05      | 120.24   |
| 10  | AL    | 210 | PRO  | C-N-CA   | 10.80  | 127.05      | 120.24   |
| 9   | 2a    | 255 | PRO  | CA-N-CD  | -8.28  | 100.41      | 112.00   |
| 9   | 2a    | 255 | PRO  | N-CA-C   | 7.61   | 119.98      | 110.70   |
| 7   | 5     | 432 | MET  | CA-C-N   | 7.44   | 135.75      | 121.54   |
| 7   | 5     | 432 | MET  | C-N-CA   | 7.44   | 135.75      | 121.54   |
| 34  | B9    | 27  | LEU  | CA-C-N   | 7.37   | 135.62      | 121.54   |
| 34  | B9    | 27  | LEU  | C-N-CA   | 7.37   | 135.62      | 121.54   |
| 7   | 5     | 526 | LEU  | CA-CB-CG | 6.91   | 140.48      | 116.30   |
| 34  | B9    | 56  | ASP  | CA-C-N   | 6.53   | 134.02      | 121.54   |
| 34  | B9    | 56  | ASP  | C-N-CA   | 6.53   | 134.02      | 121.54   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 53  | s1    | 361 | VAL  | CA-C-N     | 6.46  | 131.57      | 122.46   |
| 53  | s1    | 361 | VAL  | C-N-CA     | 6.46  | 131.57      | 122.46   |
| 52  | V2    | 180 | VAL  | N-CA-C     | -6.46 | 107.58      | 113.71   |
| 40  | 3A    | 444 | ILE  | CG1-CB-CG2 | -6.44 | 91.39       | 110.70   |
| 53  | S1    | 283 | GLU  | CA-CB-CG   | 6.43  | 126.97      | 114.10   |
| 40  | 3L    | 250 | LEU  | CA-CB-CG   | 6.43  | 138.79      | 116.30   |
| 7   | 5a    | 230 | HIS  | N-CA-C     | 6.42  | 124.00      | 109.81   |
| 19  | AM    | 17  | GLN  | CB-CG-CD   | 6.39  | 123.47      | 112.60   |
| 27  | bm    | 112 | MET  | CA-CB-CG   | 6.39  | 126.88      | 114.10   |
| 40  | 3A    | 80  | ARG  | CA-C-N     | 6.38  | 131.93      | 122.74   |
| 40  | 3A    | 80  | ARG  | C-N-CA     | 6.38  | 131.93      | 122.74   |
| 53  | S1    | 283 | GLU  | CB-CA-C    | 6.38  | 121.98      | 112.03   |
| 19  | AM    | 17  | GLN  | CA-CB-CG   | 6.35  | 126.81      | 114.10   |
| 53  | S1    | 361 | VAL  | CA-C-N     | 6.33  | 133.64      | 121.54   |
| 53  | S1    | 361 | VAL  | C-N-CA     | 6.33  | 133.64      | 121.54   |
| 51  | v1    | 314 | LEU  | CA-CB-CG   | 6.21  | 138.02      | 116.30   |
| 42  | 3N    | 373 | GLU  | CA-CB-CG   | 6.14  | 126.38      | 114.10   |
| 43  | 3D    | 210 | TYR  | CA-CB-CG   | 6.13  | 124.94      | 113.90   |
| 40  | 3A    | 349 | SER  | CA-C-N     | 6.13  | 133.25      | 121.54   |
| 40  | 3A    | 349 | SER  | C-N-CA     | 6.13  | 133.25      | 121.54   |
| 52  | V2    | 41  | ARG  | CA-C-N     | 6.02  | 130.95      | 122.46   |
| 52  | V2    | 41  | ARG  | C-N-CA     | 6.02  | 130.95      | 122.46   |
| 53  | S1    | 654 | VAL  | N-CA-C     | -5.94 | 106.47      | 113.42   |
| 20  | ao    | 102 | PRO  | CA-C-N     | 5.92  | 132.84      | 121.54   |
| 20  | ao    | 102 | PRO  | C-N-CA     | 5.92  | 132.84      | 121.54   |
| 51  | v1    | 227 | PRO  | CA-C-N     | -5.89 | 112.48      | 119.84   |
| 51  | v1    | 227 | PRO  | C-N-CA     | -5.89 | 112.48      | 119.84   |
| 8   | 4     | 406 | TYR  | CA-CB-CG   | 5.87  | 124.47      | 113.90   |
| 3   | S2    | 375 | MET  | CB-CG-SD   | 5.85  | 130.24      | 112.70   |
| 8   | 4a    | 406 | TYR  | CA-CB-CG   | 5.83  | 124.40      | 113.90   |
| 34  | b9    | 56  | ASP  | CA-C-N     | 5.81  | 132.63      | 121.54   |
| 34  | b9    | 56  | ASP  | C-N-CA     | 5.81  | 132.63      | 121.54   |
| 13  | s6    | 49  | VAL  | CA-C-N     | 5.80  | 131.65      | 122.61   |
| 13  | s6    | 49  | VAL  | C-N-CA     | 5.80  | 131.65      | 122.61   |
| 40  | 3L    | 254 | SER  | CA-C-N     | 5.78  | 132.59      | 121.54   |
| 40  | 3L    | 254 | SER  | C-N-CA     | 5.78  | 132.59      | 121.54   |
| 7   | 5a    | 422 | TYR  | CA-CB-CG   | 5.78  | 124.30      | 113.90   |
| 51  | v1    | 370 | LEU  | CA-CB-CG   | 5.75  | 136.43      | 116.30   |
| 42  | 3N    | 133 | LEU  | N-CA-C     | 5.62  | 122.24      | 109.81   |
| 55  | S8    | 153 | ILE  | CA-CB-CG2  | 5.60  | 120.01      | 110.50   |
| 53  | S1    | 697 | THR  | CA-C-N     | 5.59  | 132.22      | 121.54   |
| 53  | S1    | 697 | THR  | C-N-CA     | 5.59  | 132.22      | 121.54   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | 1     | 200 | LEU  | CA-C-N     | 5.56  | 132.16      | 121.54   |
| 4   | 1     | 200 | LEU  | C-N-CA     | 5.56  | 132.16      | 121.54   |
| 53  | s1    | 697 | THR  | CA-C-N     | 5.56  | 132.15      | 121.54   |
| 53  | s1    | 697 | THR  | C-N-CA     | 5.56  | 132.15      | 121.54   |
| 9   | 2a    | 190 | MET  | CA-CB-CG   | 5.52  | 125.14      | 114.10   |
| 40  | 3L    | 445 | CYS  | CA-CB-SG   | 5.46  | 126.95      | 114.40   |
| 34  | B9    | 48  | PHE  | N-CA-CB    | 5.42  | 119.23      | 110.40   |
| 8   | 4     | 364 | LEU  | CA-CB-CG   | 5.39  | 135.18      | 116.30   |
| 7   | 5     | 422 | TYR  | CA-CB-CG   | 5.37  | 123.57      | 113.90   |
| 53  | S1    | 126 | LEU  | CA-CB-CG   | 5.34  | 135.01      | 116.30   |
| 42  | 3N    | 162 | GLU  | CB-CG-CD   | 5.34  | 121.67      | 112.60   |
| 7   | 5     | 230 | HIS  | N-CA-C     | 5.33  | 120.92      | 113.57   |
| 4   | 1     | 142 | TYR  | CA-CB-CG   | 5.33  | 123.49      | 113.90   |
| 16  | A5    | 115 | PRO  | CA-C-N     | 5.29  | 131.22      | 121.70   |
| 16  | A5    | 115 | PRO  | C-N-CA     | 5.29  | 131.22      | 121.70   |
| 51  | V1    | 226 | LYS  | N-CA-C     | 5.28  | 121.48      | 109.81   |
| 51  | v1    | 132 | ARG  | CA-C-N     | 5.27  | 131.60      | 121.54   |
| 51  | v1    | 132 | ARG  | C-N-CA     | 5.27  | 131.60      | 121.54   |
| 33  | B4    | 96  | GLY  | N-CA-C     | 5.27  | 123.08      | 112.34   |
| 7   | 5     | 319 | MET  | CA-CB-CG   | 5.26  | 124.62      | 114.10   |
| 40  | 3A    | 85  | LYS  | CA-C-N     | 5.25  | 129.86      | 122.46   |
| 40  | 3A    | 85  | LYS  | C-N-CA     | 5.25  | 129.86      | 122.46   |
| 34  | B9    | 28  | GLU  | CA-CB-CG   | 5.24  | 124.59      | 114.10   |
| 8   | 4     | 236 | LEU  | CA-CB-CG   | 5.23  | 134.61      | 116.30   |
| 8   | 4a    | 4   | ILE  | N-CA-C     | -5.21 | 107.75      | 112.96   |
| 55  | s8    | 151 | LYS  | CA-C-N     | 5.20  | 131.47      | 121.54   |
| 55  | s8    | 151 | LYS  | C-N-CA     | 5.20  | 131.47      | 121.54   |
| 48  | 3J    | 56  | ILE  | CG1-CB-CG2 | -5.20 | 95.10       | 110.70   |
| 2   | s3    | 80  | LEU  | CA-C-N     | 5.18  | 129.77      | 122.46   |
| 2   | s3    | 80  | LEU  | C-N-CA     | 5.18  | 129.77      | 122.46   |
| 17  | A6    | 23  | ILE  | CA-C-N     | 5.16  | 131.40      | 121.54   |
| 17  | A6    | 23  | ILE  | C-N-CA     | 5.16  | 131.40      | 121.54   |
| 9   | 2a    | 37  | LEU  | CA-CB-CG   | 5.16  | 134.37      | 116.30   |
| 8   | 4a    | 329 | LEU  | CA-CB-CG   | 5.16  | 134.35      | 116.30   |
| 53  | s1    | 126 | LEU  | CA-CB-CG   | 5.15  | 134.32      | 116.30   |
| 17  | a6    | 46  | VAL  | N-CA-C     | 5.13  | 119.96      | 108.88   |
| 2   | s3    | 160 | ILE  | CG1-CB-CG2 | -5.11 | 95.38       | 110.70   |
| 3   | s2    | 273 | VAL  | CA-C-N     | 5.10  | 129.37      | 122.07   |
| 3   | s2    | 273 | VAL  | C-N-CA     | 5.10  | 129.37      | 122.07   |
| 51  | V1    | 130 | ILE  | CA-CB-CG1  | 5.08  | 119.03      | 110.40   |
| 53  | s1    | 254 | MET  | CA-CB-CG   | 5.05  | 124.20      | 114.10   |
| 47  | 3H    | 87  | ASN  | CA-C-N     | 5.05  | 131.18      | 121.54   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 47  | 3H    | 87  | ASN  | C-N-CA     | 5.05  | 131.18      | 121.54   |
| 9   | 2     | 339 | LEU  | CA-C-N     | 5.04  | 126.06      | 120.06   |
| 9   | 2     | 339 | LEU  | C-N-CA     | 5.04  | 126.06      | 120.06   |
| 46  | 3G    | 50  | ALA  | N-CA-C     | 5.03  | 120.93      | 109.81   |
| 53  | S1    | 582 | VAL  | CG1-CB-CG2 | -5.02 | 99.75       | 110.80   |
| 3   | S2    | 139 | LEU  | CB-CG-CD1  | -5.00 | 95.68       | 110.70   |

There are no chirality outliers.

All (25) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 4   | 1     | 154 | LEU  | Peptide   |
| 4   | 1     | 199 | ASP  | Peptide   |
| 41  | 3B    | 258 | ILE  | Peptide   |
| 42  | 3C    | 26  | ASN  | Peptide   |
| 8   | 4     | 249 | ILE  | Peptide   |
| 8   | 4     | 366 | ASN  | Peptide   |
| 7   | 5a    | 437 | PHE  | Peptide   |
| 18  | A8    | 166 | ARG  | Sidechain |
| 37  | AN    | 120 | ASN  | Peptide   |
| 2   | S3    | 70  | LYS  | Peptide   |
| 54  | S7    | 153 | PRO  | Peptide   |
| 54  | S7    | 193 | GLY  | Peptide   |
| 54  | S7    | 194 | CYS  | Peptide   |
| 54  | S7    | 195 | PRO  | Peptide   |
| 51  | V1    | 227 | PRO  | Peptide   |
| 52  | V2    | 136 | THR  | Peptide   |
| 52  | V2    | 142 | ARG  | Peptide   |
| 52  | V2    | 179 | CYS  | Peptide   |
| 52  | V2    | 181 | ASN  | Peptide   |
| 54  | s7    | 134 | ALA  | Peptide   |
| 54  | s7    | 194 | CYS  | Peptide   |
| 54  | s7    | 195 | PRO  | Peptide   |
| 51  | v1    | 227 | PRO  | Peptide   |
| 51  | v1    | 253 | THR  | Peptide   |
| 52  | v2    | 87  | ARG  | Sidechain |

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 3     | 914   | 0        | 952      | 25      | 0            |
| 1   | 3a    | 893   | 0        | 935      | 17      | 0            |
| 2   | S3    | 1712  | 0        | 1667     | 37      | 0            |
| 2   | s3    | 1701  | 0        | 1655     | 31      | 0            |
| 3   | S2    | 3410  | 0        | 3348     | 71      | 0            |
| 3   | s2    | 3386  | 0        | 3319     | 69      | 0            |
| 4   | 1     | 2530  | 0        | 2615     | 49      | 0            |
| 4   | 1a    | 2522  | 0        | 2606     | 62      | 0            |
| 5   | 6     | 1290  | 0        | 1304     | 21      | 0            |
| 5   | 6a    | 1298  | 0        | 1316     | 20      | 0            |
| 6   | 4L    | 729   | 0        | 764      | 12      | 0            |
| 6   | 4l    | 727   | 0        | 758      | 16      | 0            |
| 7   | 5     | 4790  | 0        | 4975     | 100     | 0            |
| 7   | 5a    | 4790  | 0        | 4973     | 73      | 0            |
| 8   | 4     | 3630  | 0        | 3854     | 70      | 0            |
| 8   | 4a    | 3630  | 0        | 3854     | 64      | 0            |
| 9   | 2     | 2694  | 0        | 2896     | 48      | 0            |
| 9   | 2a    | 2694  | 0        | 2896     | 48      | 0            |
| 10  | AL    | 2607  | 0        | 2562     | 22      | 0            |
| 10  | al    | 2607  | 0        | 2563     | 23      | 0            |
| 11  | A9    | 2748  | 0        | 2765     | 44      | 0            |
| 11  | a9    | 2748  | 0        | 2765     | 38      | 0            |
| 12  | S4    | 1021  | 0        | 1022     | 19      | 0            |
| 12  | s4    | 1021  | 0        | 1022     | 15      | 0            |
| 13  | S6    | 748   | 0        | 721      | 16      | 0            |
| 13  | s6    | 748   | 0        | 721      | 14      | 0            |
| 14  | A2    | 671   | 0        | 688      | 14      | 0            |
| 14  | a2    | 671   | 0        | 688      | 12      | 0            |
| 15  | AB    | 628   | 0        | 627      | 4       | 0            |
| 15  | AC    | 706   | 0        | 696      | 13      | 0            |
| 15  | ab    | 628   | 0        | 627      | 12      | 0            |
| 15  | ac    | 706   | 0        | 696      | 7       | 0            |
| 16  | A5    | 927   | 0        | 968      | 11      | 0            |
| 16  | a5    | 923   | 0        | 965      | 12      | 0            |
| 17  | A6    | 957   | 0        | 979      | 12      | 0            |
| 17  | a6    | 950   | 0        | 972      | 16      | 0            |
| 18  | A8    | 1385  | 0        | 1370     | 14      | 0            |
| 18  | a8    | 1389  | 0        | 1374     | 17      | 0            |
| 19  | AM    | 1045  | 0        | 1034     | 9       | 0            |
| 19  | am    | 1045  | 0        | 1034     | 11      | 0            |
| 20  | AO    | 1161  | 0        | 1161     | 14      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 20  | ao    | 1161  | 0        | 1161     | 31      | 0            |
| 21  | A1    | 564   | 0        | 579      | 2       | 0            |
| 21  | a1    | 564   | 0        | 579      | 11      | 0            |
| 22  | A3    | 648   | 0        | 649      | 6       | 0            |
| 22  | a3    | 648   | 0        | 652      | 5       | 0            |
| 23  | C1    | 407   | 0        | 404      | 0       | 0            |
| 23  | c1    | 377   | 0        | 371      | 2       | 0            |
| 24  | C2    | 996   | 0        | 1001     | 10      | 0            |
| 24  | c2    | 996   | 0        | 1001     | 11      | 0            |
| 25  | S5    | 877   | 0        | 871      | 14      | 0            |
| 25  | s5    | 877   | 0        | 869      | 17      | 0            |
| 26  | B1    | 482   | 0        | 479      | 2       | 0            |
| 26  | b1    | 482   | 0        | 479      | 6       | 0            |
| 27  | BM    | 826   | 0        | 766      | 7       | 0            |
| 27  | bm    | 835   | 0        | 772      | 9       | 0            |
| 28  | B5    | 1166  | 0        | 1166     | 12      | 0            |
| 28  | b5    | 1158  | 0        | 1160     | 20      | 0            |
| 29  | B6    | 783   | 0        | 792      | 12      | 0            |
| 29  | b6    | 761   | 0        | 769      | 11      | 0            |
| 30  | B2    | 555   | 0        | 506      | 5       | 0            |
| 30  | b2    | 545   | 0        | 499      | 10      | 0            |
| 31  | B3    | 569   | 0        | 573      | 12      | 0            |
| 31  | b3    | 573   | 0        | 576      | 3       | 0            |
| 32  | B8    | 1302  | 0        | 1197     | 19      | 0            |
| 32  | b8    | 1302  | 0        | 1197     | 15      | 0            |
| 33  | B4    | 1044  | 0        | 1056     | 21      | 0            |
| 33  | b4    | 1044  | 0        | 1056     | 15      | 0            |
| 34  | B9    | 1541  | 0        | 1470     | 18      | 0            |
| 34  | b9    | 1534  | 0        | 1463     | 19      | 0            |
| 35  | B7    | 984   | 0        | 970      | 11      | 0            |
| 35  | b7    | 1005  | 0        | 995      | 12      | 0            |
| 36  | BL    | 1410  | 0        | 1379     | 21      | 0            |
| 36  | bl    | 1430  | 0        | 1400     | 16      | 0            |
| 37  | AN    | 1201  | 0        | 1158     | 17      | 0            |
| 37  | an    | 1201  | 0        | 1158     | 14      | 0            |
| 38  | A7    | 741   | 0        | 770      | 11      | 0            |
| 38  | a7    | 560   | 0        | 579      | 8       | 0            |
| 39  | V3    | 339   | 0        | 320      | 7       | 0            |
| 39  | v3    | 303   | 0        | 290      | 6       | 0            |
| 40  | 3A    | 3459  | 0        | 3365     | 52      | 0            |
| 40  | 3L    | 3460  | 0        | 3365     | 46      | 0            |
| 41  | 3B    | 3154  | 0        | 3158     | 30      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 41  | 3M    | 3154  | 0        | 3158     | 41      | 0            |
| 42  | 3C    | 3046  | 0        | 3110     | 36      | 0            |
| 42  | 3N    | 3046  | 0        | 3111     | 36      | 0            |
| 43  | 3D    | 1919  | 0        | 1864     | 24      | 0            |
| 43  | 3O    | 1909  | 0        | 1849     | 28      | 0            |
| 44  | 3E    | 602   | 0        | 601      | 6       | 0            |
| 44  | 3P    | 610   | 0        | 612      | 10      | 0            |
| 45  | 3F    | 900   | 0        | 887      | 12      | 0            |
| 45  | 3Q    | 879   | 0        | 864      | 8       | 0            |
| 46  | 3G    | 670   | 0        | 666      | 9       | 0            |
| 46  | 3R    | 600   | 0        | 604      | 7       | 0            |
| 47  | 3H    | 545   | 0        | 529      | 8       | 0            |
| 47  | 3S    | 545   | 0        | 531      | 5       | 0            |
| 48  | 3J    | 460   | 0        | 464      | 8       | 0            |
| 48  | 3U    | 489   | 0        | 485      | 4       | 0            |
| 49  | 3K    | 421   | 0        | 418      | 2       | 0            |
| 49  | 3V    | 438   | 0        | 443      | 3       | 0            |
| 50  | 3T    | 397   | 0        | 418      | 5       | 0            |
| 51  | V1    | 3301  | 0        | 3248     | 50      | 0            |
| 51  | v1    | 3259  | 0        | 3212     | 44      | 0            |
| 52  | V2    | 1630  | 0        | 1623     | 24      | 0            |
| 52  | v2    | 1517  | 0        | 1509     | 19      | 0            |
| 53  | S1    | 5290  | 0        | 5317     | 90      | 0            |
| 53  | s1    | 5290  | 0        | 5317     | 93      | 0            |
| 54  | S7    | 1241  | 0        | 1250     | 25      | 0            |
| 54  | s7    | 1241  | 0        | 1248     | 37      | 0            |
| 55  | S8    | 1408  | 0        | 1341     | 29      | 0            |
| 55  | s8    | 1309  | 0        | 1261     | 36      | 0            |
| 56  | AL    | 1     | 0        | 0        | 0       | 0            |
| 56  | al    | 1     | 0        | 0        | 0       | 0            |
| 57  | AL    | 31    | 0        | 12       | 1       | 0            |
| 57  | al    | 31    | 0        | 12       | 0       | 0            |
| 58  | A9    | 48    | 0        | 26       | 3       | 0            |
| 58  | a9    | 48    | 0        | 25       | 1       | 0            |
| 59  | S6    | 1     | 0        | 0        | 0       | 0            |
| 59  | s6    | 1     | 0        | 0        | 0       | 0            |
| 60  | 5a    | 37    | 0        | 0        | 0       | 0            |
| 60  | A6    | 37    | 0        | 0        | 0       | 0            |
| 60  | B9    | 37    | 0        | 0        | 1       | 0            |
| 60  | a6    | 37    | 0        | 0        | 0       | 0            |
| 61  | 3C    | 86    | 0        | 60       | 1       | 0            |
| 61  | 3N    | 86    | 0        | 60       | 2       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 62  | 3D    | 43     | 0        | 30       | 3       | 0            |
| 62  | 3O    | 43     | 0        | 30       | 2       | 0            |
| 63  | V1    | 31     | 0        | 18       | 2       | 0            |
| 63  | v1    | 31     | 0        | 19       | 0       | 0            |
| 64  | S1    | 16     | 0        | 0        | 1       | 0            |
| 64  | S7    | 8      | 0        | 0        | 3       | 0            |
| 64  | S8    | 16     | 0        | 0        | 1       | 0            |
| 64  | V1    | 8      | 0        | 0        | 1       | 0            |
| 64  | s1    | 16     | 0        | 0        | 1       | 0            |
| 64  | s7    | 8      | 0        | 0        | 2       | 0            |
| 64  | s8    | 16     | 0        | 0        | 2       | 0            |
| 64  | v1    | 8      | 0        | 0        | 1       | 0            |
| 65  | S1    | 4      | 0        | 0        | 1       | 0            |
| 65  | V2    | 4      | 0        | 0        | 1       | 0            |
| 65  | s1    | 4      | 0        | 0        | 1       | 0            |
| 65  | v2    | 4      | 0        | 0        | 1       | 0            |
| All | All   | 162102 | 0        | 161959   | 2056    | 0            |

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

All (2056) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:3D:121:CYS:SG  | 62:3D:401:HEC:CAB | 2.02                     | 1.45              |
| 43:3D:121:CYS:SG  | 62:3D:401:HEC:C3B | 2.32                     | 1.18              |
| 35:B7:7:ARG:O     | 35:B7:11:TRP:HB2  | 1.71                     | 0.91              |
| 8:4a:13:PRO:O     | 8:4a:17:LEU:HB2   | 1.75                     | 0.87              |
| 3:S2:223:HIS:CD2  | 64:S7:301:SF4:S1  | 2.69                     | 0.86              |
| 4:1:281:ARG:O     | 4:1:285:LEU:HB2   | 1.76                     | 0.85              |
| 55:S8:101:HIS:HE1 | 64:S8:301:SF4:S4  | 1.99                     | 0.84              |
| 7:5a:273:ILE:O    | 7:5a:277:MET:HB2  | 1.78                     | 0.84              |
| 36:BL:121:TYR:O   | 36:BL:125:CYS:HB2 | 1.76                     | 0.83              |
| 7:5:243:VAL:O     | 7:5:247:LEU:HB2   | 1.78                     | 0.82              |
| 3:S2:380:HIS:O    | 3:S2:384:LEU:HB2  | 1.78                     | 0.82              |
| 42:3N:296:LEU:O   | 42:3N:300:ILE:HB  | 1.82                     | 0.79              |
| 7:5:530:PRO:O     | 7:5:534:HIS:HB2   | 1.81                     | 0.79              |
| 4:1:119:SER:O     | 4:1:123:SER:HB2   | 1.85                     | 0.77              |
| 31:B3:56:ALA:O    | 31:B3:60:MET:HB3  | 1.85                     | 0.77              |
| 55:s8:128:ILE:HA  | 55:s8:146:ASP:O   | 1.85                     | 0.77              |
| 3:S2:223:HIS:NE2  | 64:S7:301:SF4:S1  | 2.57                     | 0.77              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:6a:59:TYR:O     | 5:6a:63:MET:HB2   | 1.85                     | 0.76              |
| 5:6:55:VAL:O      | 5:6:59:TYR:HB2    | 1.86                     | 0.75              |
| 20:ao:120:LEU:O   | 20:ao:124:MET:HB2 | 1.87                     | 0.74              |
| 38:a7:3:SER:N     | 38:a7:28:TYR:HH   | 1.84                     | 0.74              |
| 3:S2:223:HIS:CE1  | 54:S7:99:CYS:SG   | 2.82                     | 0.73              |
| 11:A9:56:ALA:HA   | 11:A9:125:VAL:O   | 1.87                     | 0.73              |
| 42:3C:99:GLY:O    | 42:3C:103:TYR:HB2 | 1.90                     | 0.72              |
| 28:B5:72:LYS:O    | 28:B5:76:MET:HB2  | 1.89                     | 0.71              |
| 16:A5:45:ARG:O    | 16:A5:49:GLU:HB2  | 1.90                     | 0.71              |
| 55:s8:148:ASP:O   | 55:s8:152:CYS:HB2 | 1.90                     | 0.71              |
| 41:3B:173:ILE:O   | 41:3B:177:LEU:HB2 | 1.90                     | 0.70              |
| 2:S3:168:GLU:O    | 2:S3:172:MET:HB2  | 1.90                     | 0.70              |
| 20:AO:50:MET:O    | 20:AO:54:ASN:HB2  | 1.91                     | 0.70              |
| 53:S1:78:CYS:HB3  | 65:S1:803:FES:S2  | 2.32                     | 0.70              |
| 53:s1:78:CYS:HB3  | 65:s1:803:FES:S2  | 2.32                     | 0.69              |
| 8:4:68:LEU:O      | 8:4:72:LEU:HB2    | 1.92                     | 0.69              |
| 24:c2:44:MET:O    | 24:c2:48:LEU:HB2  | 1.93                     | 0.69              |
| 7:5:374:VAL:O     | 7:5:378:LEU:HB2   | 1.93                     | 0.69              |
| 4:1:287:HIS:O     | 4:1:291:LYS:HB2   | 1.92                     | 0.68              |
| 3:S2:200:PHE:O    | 3:S2:204:PHE:HB2  | 1.93                     | 0.68              |
| 51:V1:208:GLU:O   | 51:V1:212:LEU:HB2 | 1.94                     | 0.68              |
| 46:3R:42:THR:O    | 46:3R:46:ILE:HB   | 1.94                     | 0.68              |
| 42:3C:144:THR:O   | 42:3C:148:ASN:HB2 | 1.94                     | 0.68              |
| 7:5:63:ILE:O      | 7:5:79:SER:HA     | 1.94                     | 0.67              |
| 7:5:544:LEU:O     | 7:5:548:THR:HB    | 1.94                     | 0.67              |
| 7:5a:460:GLY:O    | 7:5a:464:ALA:HB2  | 1.95                     | 0.67              |
| 55:s8:130:ILE:HA  | 55:s8:144:ARG:O   | 1.94                     | 0.66              |
| 53:s1:404:GLY:HA3 | 53:s1:477:GLY:H   | 1.59                     | 0.66              |
| 8:4a:239:GLY:O    | 8:4a:243:MET:HB2  | 1.96                     | 0.66              |
| 5:6a:63:MET:O     | 5:6a:67:PHE:HB2   | 1.96                     | 0.66              |
| 40:3L:118:ALA:HA  | 40:3L:134:LYS:O   | 1.95                     | 0.66              |
| 30:b2:94:ASP:O    | 30:b2:98:GLY:HA2  | 1.96                     | 0.66              |
| 42:3N:78:LEU:O    | 42:3N:82:MET:HB2  | 1.95                     | 0.66              |
| 3:s2:195:GLY:HA3  | 4:1a:279:ARG:HB3  | 1.77                     | 0.65              |
| 10:al:240:ALA:O   | 10:al:244:THR:HB  | 1.96                     | 0.65              |
| 25:s5:95:PRO:O    | 25:s5:99:SER:HB2  | 1.96                     | 0.64              |
| 7:5:220:ALA:O     | 7:5:224:SER:HB3   | 1.97                     | 0.64              |
| 8:4a:175:ASN:O    | 8:4a:179:LEU:HB2  | 1.98                     | 0.64              |
| 51:V1:113:LEU:O   | 51:V1:154:ALA:HA  | 1.97                     | 0.64              |
| 39:V3:81:LEU:HB3  | 52:V2:61:ARG:HD3  | 1.80                     | 0.63              |
| 4:1:134:ARG:HD3   | 4:1:200:LEU:HB3   | 1.80                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:S2:223:HIS:NE2  | 54:S7:99:CYS:SG    | 2.71                     | 0.63              |
| 4:1:90:PRO:HG3    | 4:1:162:LEU:HB3    | 1.81                     | 0.63              |
| 9:2:42:PRO:O      | 9:2:46:ASN:HB3     | 1.99                     | 0.63              |
| 3:s2:220:ALA:HB1  | 54:s7:195:PRO:HG2  | 1.81                     | 0.62              |
| 5:6:102:LEU:O     | 5:6:106:LEU:HB2    | 1.99                     | 0.62              |
| 41:3M:266:LEU:HA  | 41:3M:342:SER:O    | 1.99                     | 0.62              |
| 40:3L:308:ASN:ND2 | 40:3L:343:THR:OG1  | 2.32                     | 0.62              |
| 51:v1:113:LEU:O   | 51:v1:154:ALA:HA   | 2.00                     | 0.62              |
| 34:B9:71:PHE:O    | 34:B9:75:GLN:HB3   | 2.00                     | 0.62              |
| 17:a6:48:ASN:O    | 17:a6:52:LEU:HB3   | 1.99                     | 0.62              |
| 33:b4:33:GLN:HG3  | 33:b4:36:ARG:HH21  | 1.65                     | 0.62              |
| 46:3G:42:THR:O    | 46:3G:46:ILE:HB    | 1.99                     | 0.62              |
| 3:S2:82:LEU:HD12  | 4:1:126:LYS:HB3    | 1.82                     | 0.62              |
| 43:3O:295:MET:O   | 43:3O:299:LEU:HB2  | 2.00                     | 0.62              |
| 8:4:118:PHE:O     | 8:4:122:PHE:HB2    | 2.00                     | 0.61              |
| 3:s2:370:GLU:O    | 3:s2:374:SER:HB2   | 2.00                     | 0.61              |
| 9:2:26:LEU:HB3    | 9:2:74:ILE:HG12    | 1.83                     | 0.61              |
| 9:2:328:THR:O     | 9:2:332:MET:HB2    | 2.01                     | 0.61              |
| 16:a5:49:GLU:O    | 16:a5:53:ASN:HB2   | 2.01                     | 0.61              |
| 43:3O:281:GLU:O   | 43:3O:285:ARG:HB2  | 2.01                     | 0.61              |
| 52:V2:183:PRO:HD2 | 52:V2:194:ASP:HA   | 1.83                     | 0.61              |
| 8:4:254:THR:HG21  | 8:4:304:GLN:HE21   | 1.66                     | 0.60              |
| 9:2:187:MET:HA    | 9:2:190:MET:HG2    | 1.83                     | 0.60              |
| 30:B2:53:SER:O    | 30:B2:57:GLN:HB2   | 2.00                     | 0.60              |
| 39:v3:81:LEU:HB3  | 52:v2:61:ARG:HD3   | 1.83                     | 0.60              |
| 11:a9:86:CYS:SG   | 11:a9:87:ASP:N     | 2.74                     | 0.60              |
| 48:3J:11:TYR:HA   | 48:3J:15:PHE:HB2   | 1.83                     | 0.60              |
| 3:S2:100:GLU:HB3  | 3:S2:108:LYS:HB3   | 1.84                     | 0.60              |
| 48:3U:29:GLY:O    | 48:3U:33:PHE:HB2   | 2.01                     | 0.60              |
| 54:s7:99:CYS:HB2  | 64:s7:301:SF4:S1   | 2.42                     | 0.60              |
| 2:S3:234:LEU:HD12 | 3:S2:418:ARG:HE    | 1.67                     | 0.60              |
| 7:5a:243:VAL:O    | 7:5a:247:LEU:HB2   | 2.02                     | 0.60              |
| 15:AC:117:GLU:HG2 | 31:B3:51:TRP:HE1   | 1.66                     | 0.60              |
| 53:s1:170:LYS:HB2 | 53:s1:234:LYS:HG3  | 1.82                     | 0.60              |
| 2:S3:199:LYS:HB3  | 12:S4:126:LEU:HD11 | 1.84                     | 0.60              |
| 4:1a:138:GLN:HE21 | 4:1a:200:LEU:HB2   | 1.66                     | 0.60              |
| 53:s1:593:SER:HA  | 53:s1:606:THR:O    | 2.02                     | 0.60              |
| 6:4l:22:PHE:HB2   | 7:5a:585:LYS:HB3   | 1.84                     | 0.59              |
| 20:ao:97:ILE:HG22 | 20:ao:98:MET:HG3   | 1.85                     | 0.59              |
| 4:1:197:PRO:HG3   | 4:1:277:TYR:HB2    | 1.83                     | 0.59              |
| 8:4a:325:LEU:HD21 | 8:4a:441:MET:HE2   | 1.84                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:3D:186:ARG:HG2  | 43:3D:193:LEU:HB2  | 1.85                     | 0.59              |
| 53:s1:251:ILE:HD12 | 53:s1:604:GLN:HB2  | 1.85                     | 0.59              |
| 9:2a:216:PHE:O     | 9:2a:220:MET:HB2   | 2.02                     | 0.59              |
| 7:5:556:ILE:O      | 7:5:560:LYS:HB2    | 2.02                     | 0.59              |
| 53:s1:337:ALA:HB1  | 53:s1:543:LYS:H    | 1.65                     | 0.59              |
| 11:A9:251:ASN:O    | 11:A9:255:ASP:HB2  | 2.03                     | 0.59              |
| 8:4a:336:ARG:HH21  | 8:4a:429:SER:HA    | 1.68                     | 0.59              |
| 41:3B:234:ALA:O    | 41:3B:238:LEU:HB2  | 2.02                     | 0.59              |
| 13:S6:104:CYS:HB3  | 13:S6:107:CYS:SG   | 2.42                     | 0.59              |
| 2:s3:128:VAL:HG12  | 2:s3:143:LYS:HG2   | 1.85                     | 0.59              |
| 20:ao:128:ARG:HE   | 20:ao:132:GLU:HG2  | 1.67                     | 0.59              |
| 3:S2:98:VAL:HG11   | 17:A6:100:TRP:HE1  | 1.67                     | 0.58              |
| 1:3a:68:GLU:HG2    | 5:6a:159:LEU:HD23  | 1.83                     | 0.58              |
| 31:b3:56:ALA:O     | 31:b3:60:MET:HB3   | 2.03                     | 0.58              |
| 42:3C:45:ILE:HA    | 61:3C:401:HEM:HAB  | 1.84                     | 0.58              |
| 12:s4:99:MET:HB3   | 12:s4:126:LEU:HB2  | 1.84                     | 0.58              |
| 1:3a:6:VAL:O       | 1:3a:10:ASN:HB2    | 2.02                     | 0.58              |
| 3:s2:197:MET:SD    | 4:1a:32:GLN:NE2    | 2.76                     | 0.58              |
| 8:4a:108:MET:HB3   | 8:4a:121:LEU:HD13  | 1.84                     | 0.58              |
| 40:3A:301:ASN:O    | 40:3A:305:GLN:HB2  | 2.02                     | 0.58              |
| 41:3M:320:PRO:HA   | 50:3T:52:ARG:HE    | 1.68                     | 0.58              |
| 6:4L:16:LEU:O      | 6:4L:20:LEU:HB2    | 2.03                     | 0.58              |
| 42:3C:78:LEU:O     | 42:3C:82:MET:HB3   | 2.04                     | 0.58              |
| 10:al:146:ALA:HB1  | 10:al:157:VAL:HG21 | 1.85                     | 0.58              |
| 51:V1:225:LEU:HD21 | 53:S1:76:ARG:HH22  | 1.69                     | 0.58              |
| 11:A9:301:ILE:O    | 11:A9:305:PHE:HB2  | 2.04                     | 0.58              |
| 2:S3:111:ALA:HB3   | 2:S3:130:ASN:HB3   | 1.85                     | 0.58              |
| 2:s3:86:CYS:HA     | 2:s3:143:LYS:O     | 2.05                     | 0.57              |
| 51:V1:385:CYS:HB3  | 64:V1:502:SF4:S3   | 2.44                     | 0.57              |
| 4:1:20:LEU:HD22    | 4:1:232:ILE:HB     | 1.86                     | 0.57              |
| 22:A3:28:LEU:O     | 22:A3:32:MET:HB2   | 2.03                     | 0.57              |
| 2:s3:195:HIS:HB2   | 2:s3:198:ARG:HD2   | 1.85                     | 0.57              |
| 11:A9:221:ARG:HD2  | 11:A9:286:ARG:HG3  | 1.87                     | 0.57              |
| 10:al:223:ASP:HB3  | 10:al:226:GLU:HB2  | 1.86                     | 0.57              |
| 55:s8:181:GLU:HA   | 55:s8:184:LEU:HD12 | 1.87                     | 0.57              |
| 8:4a:150:LEU:O     | 8:4a:154:LEU:HB2   | 2.05                     | 0.57              |
| 4:1:149:ILE:HG21   | 4:1:185:TRP:HB2    | 1.86                     | 0.57              |
| 15:ac:93:ILE:HD11  | 15:ac:108:LEU:HD13 | 1.87                     | 0.57              |
| 51:v1:68:ILE:HD11  | 51:v1:256:ARG:HB3  | 1.86                     | 0.57              |
| 4:1a:90:PRO:HG3    | 4:1a:162:LEU:HB3   | 1.86                     | 0.57              |
| 34:b9:136:GLU:HG2  | 34:b9:165:PRO:HA   | 1.85                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:c1:34:PRO:HG2   | 23:c1:37:ALA:HB2   | 1.87                     | 0.57              |
| 53:S1:337:ALA:HB1  | 53:S1:543:LYS:H    | 1.69                     | 0.57              |
| 7:5a:231:PRO:HB3   | 7:5a:530:PRO:HG3   | 1.85                     | 0.57              |
| 7:5a:418:MET:HA    | 7:5a:421:MET:HB3   | 1.86                     | 0.57              |
| 4:1:26:LYS:HG2     | 4:1:37:PRO:HD2     | 1.87                     | 0.56              |
| 43:3D:222:PRO:HG3  | 47:3H:69:LEU:HD13  | 1.87                     | 0.56              |
| 51:V1:112:TYR:HB2  | 51:V1:240:THR:HG22 | 1.85                     | 0.56              |
| 52:V2:223:CYS:SG   | 52:V2:224:CYS:N    | 2.78                     | 0.56              |
| 14:A2:65:LEU:HB2   | 14:A2:79:LEU:HD11  | 1.87                     | 0.56              |
| 44:3P:98:ASP:HB3   | 44:3P:101:LYS:HG2  | 1.86                     | 0.56              |
| 2:S3:47:ARG:HH12   | 3:S2:156:GLU:HG3   | 1.68                     | 0.56              |
| 3:S2:254:ARG:HE    | 38:A7:25:GLN:HB3   | 1.70                     | 0.56              |
| 5:6:166:ILE:HD11   | 6:4L:73:VAL:HA     | 1.87                     | 0.56              |
| 29:B6:104:ILE:HB   | 35:B7:48:ASP:HB3   | 1.87                     | 0.56              |
| 3:s2:144:MET:N     | 3:s2:144:MET:SD    | 2.78                     | 0.56              |
| 4:1a:284:GLN:HA    | 4:1a:287:HIS:HB2   | 1.87                     | 0.56              |
| 7:5a:221:THR:HG23  | 7:5a:226:GLN:HB2   | 1.87                     | 0.56              |
| 42:3C:226:ILE:HD11 | 43:3D:306:MET:HE3  | 1.87                     | 0.56              |
| 51:V1:35:LEU:HB2   | 51:V1:291:GLU:HB2  | 1.88                     | 0.56              |
| 54:S7:198:ALA:O    | 54:S7:202:LEU:HB2  | 2.06                     | 0.56              |
| 3:s2:426:ALA:HB3   | 3:s2:429:PHE:HB2   | 1.88                     | 0.56              |
| 43:3D:92:PRO:HG3   | 47:3H:77:ASP:HB3   | 1.86                     | 0.56              |
| 55:S8:110:GLU:OE2  | 55:S8:141:ARG:NH1  | 2.38                     | 0.56              |
| 8:4:173:THR:HG22   | 8:4:175:ASN:H      | 1.70                     | 0.56              |
| 53:s1:478:SER:HA   | 53:s1:481:LEU:HB2  | 1.87                     | 0.56              |
| 4:1:23:VAL:O       | 4:1:27:ILE:HB      | 2.06                     | 0.56              |
| 2:s3:224:GLU:HB2   | 12:s4:118:ALA:HA   | 1.87                     | 0.56              |
| 7:5:433:THR:OG1    | 7:5:434:LYS:N      | 2.39                     | 0.56              |
| 40:3A:360:CYS:SG   | 40:3A:361:ASP:N    | 2.79                     | 0.56              |
| 40:3L:408:PRO:HA   | 40:3L:411:GLU:HB3  | 1.87                     | 0.56              |
| 53:S1:476:LEU:HB3  | 53:S1:515:ILE:HG12 | 1.88                     | 0.56              |
| 51:v1:112:TYR:HB2  | 51:v1:240:THR:HG22 | 1.87                     | 0.56              |
| 1:3:90:MET:HE3     | 5:6:149:THR:HB     | 1.88                     | 0.56              |
| 9:2:132:THR:HB     | 9:2:209:ILE:HG12   | 1.88                     | 0.56              |
| 32:B8:40:SER:OG    | 32:B8:41:TYR:N     | 2.39                     | 0.56              |
| 8:4:325:LEU:HD22   | 8:4:362:ALA:HB2    | 1.87                     | 0.55              |
| 53:S1:262:VAL:HG23 | 53:S1:276:ARG:HB2  | 1.87                     | 0.55              |
| 9:2:21:MET:HE2     | 25:S5:4:LEU:HG     | 1.89                     | 0.55              |
| 37:AN:64:ARG:HH22  | 37:AN:99:ASP:HA    | 1.70                     | 0.55              |
| 37:an:139:HIS:HB2  | 53:s1:299:ARG:HA   | 1.87                     | 0.55              |
| 42:3N:45:ILE:HA    | 61:3N:401:HEM:HAB  | 1.87                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:v2:155:LEU:HB3  | 52:v2:157:ILE:HG12 | 1.88                     | 0.55              |
| 53:s1:216:SER:HA   | 53:s1:691:ILE:HD11 | 1.87                     | 0.55              |
| 3:s2:408:GLY:H     | 3:s2:425:LYS:HB3   | 1.71                     | 0.55              |
| 9:2a:102:LEU:HD21  | 9:2a:141:ILE:HD12  | 1.88                     | 0.55              |
| 25:s5:48:GLY:O     | 25:s5:52:ALA:HB2   | 2.06                     | 0.55              |
| 3:S2:96:ARG:HB3    | 3:S2:112:HIS:HB2   | 1.87                     | 0.55              |
| 7:5:292:ALA:HA     | 7:5:295:GLN:HB2    | 1.88                     | 0.55              |
| 7:5a:296:ASN:HD22  | 7:5a:357:ARG:HE    | 1.55                     | 0.55              |
| 12:S4:82:PRO:HG3   | 12:S4:98:LYS:HD2   | 1.88                     | 0.55              |
| 39:V3:65:THR:OG1   | 39:V3:66:THR:N     | 2.39                     | 0.55              |
| 41:3M:108:GLY:HA3  | 41:3M:124:GLU:O    | 2.06                     | 0.55              |
| 42:3N:119:LEU:HD12 | 42:3N:192:LEU:HB3  | 1.89                     | 0.55              |
| 3:S2:118:2MR:HD3   | 54:S7:136:THR:HG21 | 1.86                     | 0.55              |
| 22:A3:52:ASN:ND2   | 25:S5:27:TYR:O     | 2.38                     | 0.55              |
| 42:3C:282:ARG:NH2  | 42:3C:341:GLN:O    | 2.40                     | 0.55              |
| 53:S1:591:GLU:HB3  | 53:S1:612:PRO:HD3  | 1.87                     | 0.55              |
| 7:5:61:TYR:O       | 7:5:81:LYS:HA      | 2.06                     | 0.55              |
| 20:AO:133:MET:SD   | 20:AO:137:ASN:ND2  | 2.80                     | 0.55              |
| 51:V1:253:THR:HA   | 51:V1:256:ARG:HG2  | 1.89                     | 0.55              |
| 40:3L:48:THR:OG1   | 40:3L:423:ARG:NH1  | 2.39                     | 0.55              |
| 3:S2:140:ASP:OD1   | 3:S2:404:LYS:NZ    | 2.39                     | 0.55              |
| 7:5:100:ILE:HG13   | 7:5:246:LEU:HB2    | 1.89                     | 0.55              |
| 8:4:208:PRO:HG3    | 8:4:216:LEU:HD22   | 1.89                     | 0.55              |
| 32:B8:125:SER:O    | 32:B8:129:MET:HB2  | 2.07                     | 0.55              |
| 3:s2:254:ARG:HD2   | 38:a7:25:GLN:HB3   | 1.88                     | 0.55              |
| 40:3L:295:GLY:O    | 40:3L:301:ASN:ND2  | 2.40                     | 0.55              |
| 7:5:328:HIS:O      | 7:5:332:HIS:HB3    | 2.07                     | 0.55              |
| 11:A9:83:PRO:HA    | 11:A9:106:LEU:O    | 2.07                     | 0.55              |
| 8:4a:216:LEU:O     | 8:4a:220:HIS:HB2   | 2.07                     | 0.55              |
| 10:al:275:TYR:HB3  | 16:a5:23:ARG:HH21  | 1.72                     | 0.55              |
| 25:s5:97:HIS:HA    | 25:s5:102:GLU:HB3  | 1.88                     | 0.55              |
| 40:3L:55:ASN:HD22  | 40:3L:253:VAL:H    | 1.52                     | 0.55              |
| 27:BM:135:MET:SD   | 36:BL:142:ARG:NH1  | 2.80                     | 0.54              |
| 40:3L:289:ILE:HG13 | 40:3L:456:VAL:HG22 | 1.89                     | 0.54              |
| 7:5:365:ILE:HG22   | 7:5:366:MET:HG3    | 1.90                     | 0.54              |
| 11:A9:227:PRO:HB3  | 11:A9:293:LEU:HD12 | 1.90                     | 0.54              |
| 2:s3:62:GLU:HG3    | 38:a7:69:ILE:HD12  | 1.89                     | 0.54              |
| 4:1:105:ILE:O      | 4:1:109:SER:HB3    | 2.07                     | 0.54              |
| 9:2:30:TRP:NE1     | 9:2:67:SER:OG      | 2.41                     | 0.54              |
| 40:3A:445:CYS:O    | 40:3A:449:PHE:HB2  | 2.06                     | 0.54              |
| 40:3L:403:LEU:HD12 | 40:3L:426:LEU:HD22 | 1.88                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:5:140:LEU:O      | 7:5:144:TRP:HB2   | 2.07                     | 0.54              |
| 24:C2:42:GLY:HA3   | 24:C2:61:GLN:HG2  | 1.90                     | 0.54              |
| 4:1a:207:LEU:HD12  | 4:1a:210:GLY:HA2  | 1.90                     | 0.54              |
| 7:5a:22:SER:HA     | 7:5a:27:ILE:HD12  | 1.90                     | 0.54              |
| 40:3A:222:ARG:HH21 | 40:3A:263:PRO:HB3 | 1.72                     | 0.54              |
| 48:3J:34:ARG:HD3   | 49:3K:48:ILE:HG23 | 1.90                     | 0.54              |
| 43:3O:307:LYS:O    | 43:3O:311:TRP:HB2 | 2.08                     | 0.54              |
| 55:S8:189:LYS:O    | 55:S8:193:ASN:HB2 | 2.07                     | 0.54              |
| 55:s8:204:ASN:O    | 55:s8:208:ASP:HB2 | 2.07                     | 0.54              |
| 21:A1:18:ILE:O     | 21:A1:22:SER:HB3  | 2.08                     | 0.54              |
| 4:1a:221:ALA:O     | 4:1a:225:MET:HB2  | 2.08                     | 0.54              |
| 8:4a:176:LEU:HD21  | 8:4a:245:ARG:HB3  | 1.89                     | 0.54              |
| 9:2:122:ILE:O      | 9:2:176:ARG:NH1   | 2.40                     | 0.54              |
| 14:A2:44:LEU:HD21  | 14:A2:91:MET:HE2  | 1.89                     | 0.54              |
| 2:S3:171:ASP:HB2   | 2:S3:185:ARG:HA   | 1.90                     | 0.54              |
| 8:4:36:LEU:HB2     | 27:BM:96:VAL:HG22 | 1.89                     | 0.54              |
| 2:s3:153:ASP:OD1   | 2:s3:153:ASP:N    | 2.41                     | 0.54              |
| 42:3C:32:ASN:ND2   | 42:3C:228:ASP:OD1 | 2.41                     | 0.54              |
| 40:3L:140:LEU:HA   | 40:3L:143:VAL:HB  | 1.90                     | 0.54              |
| 53:s1:186:ALA:HA   | 53:s1:190:ALA:HB3 | 1.89                     | 0.54              |
| 54:s7:87:ARG:HB2   | 54:s7:209:GLN:HG3 | 1.90                     | 0.54              |
| 8:4:254:THR:O      | 8:4:258:ALA:HB2   | 2.08                     | 0.54              |
| 2:s3:112:ASP:HB2   | 2:s3:130:ASN:HB2  | 1.89                     | 0.54              |
| 52:V2:136:THR:OG1  | 65:V2:301:FES:S2  | 2.64                     | 0.54              |
| 9:2:127:GLY:O      | 9:2:131:LEU:HB2   | 2.07                     | 0.54              |
| 8:4a:350:MET:HE2   | 34:b9:96:CYS:HA   | 1.90                     | 0.54              |
| 40:3L:469:ASN:ND2  | 43:3O:310:LYS:O   | 2.41                     | 0.54              |
| 53:S1:186:ALA:HA   | 53:S1:190:ALA:HB3 | 1.89                     | 0.54              |
| 1:3:60:ILE:HG13    | 6:4L:76:ALA:HB2   | 1.90                     | 0.53              |
| 9:2:20:THR:HG23    | 9:2:29:MET:HB2    | 1.89                     | 0.53              |
| 19:AM:141:VAL:HG22 | 28:B5:158:ARG:HB2 | 1.89                     | 0.53              |
| 28:B5:160:MET:HG2  | 28:B5:168:TRP:HB2 | 1.91                     | 0.53              |
| 7:5a:316:THR:HG21  | 7:5a:395:ILE:HG12 | 1.88                     | 0.53              |
| 8:4a:315:LEU:O     | 8:4a:319:HIS:HB3  | 2.07                     | 0.53              |
| 5:6:55:VAL:HA      | 5:6:58:ILE:HG22   | 1.91                     | 0.53              |
| 7:5:316:THR:HG21   | 7:5:395:ILE:HD12  | 1.91                     | 0.53              |
| 11:A9:238:GLN:NE2  | 11:A9:268:PRO:O   | 2.42                     | 0.53              |
| 40:3L:292:GLU:HA   | 40:3L:352:GLY:O   | 2.07                     | 0.53              |
| 49:3V:30:VAL:HA    | 49:3V:33:VAL:HG12 | 1.90                     | 0.53              |
| 52:V2:157:ILE:HG23 | 52:V2:161:GLU:HG3 | 1.90                     | 0.53              |
| 9:2:248:LEU:HD11   | 9:2:296:LEU:HD22  | 1.90                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:3L:278:ARG:NH1  | 40:3L:463:GLU:OE2  | 2.41                     | 0.53              |
| 3:S2:376:GLU:O     | 3:S2:380:HIS:ND1   | 2.39                     | 0.53              |
| 3:s2:143:SER:O     | 3:s2:147:ASN:ND2   | 2.42                     | 0.53              |
| 3:s2:412:VAL:HG23  | 3:s2:420:TYR:HB3   | 1.91                     | 0.53              |
| 11:a9:48:ARG:NH2   | 11:a9:96:LEU:O     | 2.42                     | 0.53              |
| 41:3B:63:LEU:HD13  | 41:3B:220:LEU:HB2  | 1.91                     | 0.53              |
| 51:V1:44:ASN:ND2   | 51:V1:48:ARG:O     | 2.42                     | 0.53              |
| 4:1:203:GLY:O      | 4:1:279:ARG:NH1    | 2.42                     | 0.53              |
| 3:s2:314:VAL:HB    | 3:s2:343:ILE:HD12  | 1.91                     | 0.53              |
| 53:S1:68:ARG:NH2   | 53:S1:277:MET:SD   | 2.82                     | 0.53              |
| 52:v2:140:MET:HA   | 52:v2:144:SER:H    | 1.74                     | 0.53              |
| 12:S4:151:LYS:NZ   | 53:S1:657:ASP:OD2  | 2.41                     | 0.53              |
| 2:s3:108:LYS:HB2   | 3:s2:284:LEU:HD22  | 1.91                     | 0.53              |
| 4:1a:138:GLN:NE2   | 4:1a:198:PHE:O     | 2.41                     | 0.53              |
| 7:5a:530:PRO:O     | 7:5a:534:HIS:HB3   | 2.09                     | 0.53              |
| 15:ab:79:ILE:HD12  | 15:ab:145:VAL:HB   | 1.91                     | 0.53              |
| 15:ac:123:GLU:HG2  | 15:ac:129:GLU:HA   | 1.90                     | 0.53              |
| 53:s1:276:ARG:O    | 53:s1:282:ASN:ND2  | 2.42                     | 0.53              |
| 3:S2:224:ALA:O     | 55:S8:98:ARG:NH2   | 2.42                     | 0.53              |
| 7:5:261:VAL:HG11   | 7:5:326:PHE:HB2    | 1.91                     | 0.53              |
| 8:4a:68:LEU:O      | 8:4a:72:LEU:HB2    | 2.08                     | 0.53              |
| 15:ab:116:VAL:O    | 15:ab:120:MET:HB3  | 2.09                     | 0.53              |
| 35:b7:69:CYS:O     | 35:b7:73:SER:HB3   | 2.09                     | 0.53              |
| 44:3E:156:LEU:HD12 | 44:3E:158:ASP:H    | 1.74                     | 0.53              |
| 53:S1:165:ILE:HG23 | 53:S1:214:PHE:HB3  | 1.91                     | 0.53              |
| 54:s7:200:ALA:HB2  | 55:s8:173:PHE:HB2  | 1.90                     | 0.53              |
| 3:S2:67:ASN:HB2    | 10:AL:193:LEU:HD22 | 1.91                     | 0.53              |
| 13:S6:104:CYS:CB   | 13:S6:107:CYS:SG   | 2.96                     | 0.53              |
| 10:a1:271:GLU:HG2  | 16:a5:26:ILE:HD13  | 1.91                     | 0.53              |
| 40:3L:403:LEU:HD13 | 40:3L:423:ARG:HH21 | 1.73                     | 0.53              |
| 3:s2:173:LEU:HD12  | 3:s2:347:CYS:HB3   | 1.90                     | 0.53              |
| 3:s2:266:ARG:H     | 55:s8:66:LEU:HD21  | 1.73                     | 0.53              |
| 6:4l:50:ASN:O      | 25:s5:32:ARG:NH1   | 2.42                     | 0.53              |
| 9:2a:149:LEU:HD22  | 9:2a:154:ILE:HD11  | 1.90                     | 0.53              |
| 11:a9:110:ALA:HB1  | 11:a9:148:ILE:HG12 | 1.91                     | 0.53              |
| 53:S1:419:ARG:NH1  | 53:S1:439:THR:O    | 2.42                     | 0.53              |
| 52:v2:200:ILE:HG23 | 52:v2:204:ILE:HD12 | 1.90                     | 0.53              |
| 7:5:51:LEU:HD11    | 7:5:88:LEU:HD12    | 1.90                     | 0.53              |
| 11:A9:113:LYS:HA   | 11:A9:116:ILE:HD12 | 1.89                     | 0.53              |
| 14:A2:25:GLN:NE2   | 53:S1:661:GLU:O    | 2.40                     | 0.53              |
| 15:AB:83:VAL:O     | 15:AB:87:LEU:HB2   | 2.08                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:V1:328:PRO:HB3  | 51:V1:441:HIS:HB3  | 1.91                     | 0.53              |
| 8:4:229:MET:O      | 8:4:233:ALA:HB3    | 2.09                     | 0.52              |
| 3:s2:93:GLY:HA3    | 54:s7:96:GLY:HA3   | 1.91                     | 0.52              |
| 4:1a:65:THR:O      | 4:1a:124:ASN:ND2   | 2.40                     | 0.52              |
| 40:3A:453:CYS:SG   | 40:3A:472:ARG:NH1  | 2.82                     | 0.52              |
| 43:3D:295:MET:O    | 43:3D:299:LEU:HB2  | 2.09                     | 0.52              |
| 45:3F:76:LEU:HB3   | 45:3F:80:GLN:HB3   | 1.90                     | 0.52              |
| 51:V1:158:ILE:HG21 | 51:V1:166:ALA:HB2  | 1.90                     | 0.52              |
| 53:S1:497:VAL:HG11 | 53:S1:513:MET:HB2  | 1.91                     | 0.52              |
| 51:v1:385:CYS:HB3  | 64:v1:502:SF4:S3   | 2.50                     | 0.52              |
| 7:5:174:TYR:HD2    | 7:5:232:TRP:HB3    | 1.73                     | 0.52              |
| 12:S4:84:ARG:HH21  | 53:S1:277:MET:HE2  | 1.74                     | 0.52              |
| 11:a9:169:HIS:HB2  | 11:a9:184:LYS:HZ2  | 1.73                     | 0.52              |
| 41:3M:113:THR:HB   | 41:3M:120:ALA:HB3  | 1.92                     | 0.52              |
| 42:3N:39:VAL:HG21  | 42:3N:232:ILE:HD11 | 1.92                     | 0.52              |
| 53:S1:66:HIS:HB2   | 53:S1:181:ARG:HD3  | 1.91                     | 0.52              |
| 53:s1:257:VAL:HG11 | 53:s1:413:LEU:HB3  | 1.91                     | 0.52              |
| 54:s7:216:GLN:HB3  | 54:s7:219:LYS:HB3  | 1.91                     | 0.52              |
| 3:S2:290:GLY:HA3   | 3:S2:405:GLY:HA2   | 1.90                     | 0.52              |
| 6:4L:63:ILE:HD12   | 9:2:71:LEU:HD21    | 1.92                     | 0.52              |
| 22:A3:52:ASN:HD22  | 25:S5:28:LYS:HE3   | 1.74                     | 0.52              |
| 36:BL:6:ASP:N      | 36:BL:6:ASP:OD1    | 2.42                     | 0.52              |
| 2:s3:153:ASP:HA    | 2:s3:178:PHE:HB2   | 1.92                     | 0.52              |
| 3:s2:216:ARG:HH21  | 3:s2:240:LEU:HA    | 1.74                     | 0.52              |
| 8:4a:264:LEU:HD13  | 33:b4:98:LEU:HD21  | 1.91                     | 0.52              |
| 18:a8:163:HIS:O    | 28:b5:146:LYS:NZ   | 2.42                     | 0.52              |
| 53:S1:165:ILE:HD12 | 53:S1:171:THR:HG21 | 1.91                     | 0.52              |
| 53:s1:165:ILE:HG23 | 53:s1:214:PHE:HB3  | 1.90                     | 0.52              |
| 2:S3:195:HIS:HB2   | 2:S3:198:ARG:HD2   | 1.92                     | 0.52              |
| 4:1:28:LEU:HD22    | 4:1:275:ALA:HB2    | 1.90                     | 0.52              |
| 40:3A:64:SER:OG    | 40:3A:65:SER:N     | 2.42                     | 0.52              |
| 3:S2:143:SER:HB3   | 3:S2:182:ASN:HB2   | 1.91                     | 0.52              |
| 20:AO:93:GLU:HA    | 20:AO:96:ILE:HD12  | 1.91                     | 0.52              |
| 2:s3:100:ARG:NH1   | 2:s3:158:VAL:O     | 2.43                     | 0.52              |
| 21:a1:1:MET:HE1    | 38:a7:4:ALA:HA     | 1.91                     | 0.52              |
| 42:3C:177:ARG:NH2  | 44:3P:140:MET:O    | 2.42                     | 0.52              |
| 47:3H:38:LEU:HD23  | 47:3H:40:LYS:H     | 1.74                     | 0.52              |
| 40:3L:62:GLU:OE1   | 40:3L:423:ARG:NH1  | 2.42                     | 0.52              |
| 41:3M:116:ARG:NH1  | 41:3M:188:ASN:O    | 2.43                     | 0.52              |
| 51:v1:44:ASN:ND2   | 51:v1:48:ARG:O     | 2.41                     | 0.52              |
| 2:S3:98:PHE:HB2    | 16:A5:94:MET:HE1   | 1.92                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:5:137:MET:HB3    | 7:5:186:MET:HE2    | 1.91                     | 0.52              |
| 7:5:432:MET:HG2    | 31:B3:67:ILE:HD11  | 1.91                     | 0.52              |
| 7:5:474:PRO:O      | 35:B7:55:GLN:NE2   | 2.42                     | 0.52              |
| 18:A8:147:ARG:NH1  | 25:S5:43:CYS:SG    | 2.82                     | 0.52              |
| 4:1a:282:TYR:HA    | 4:1a:285:LEU:HB3   | 1.92                     | 0.52              |
| 11:a9:142:GLU:O    | 11:a9:146:VAL:HB   | 2.10                     | 0.52              |
| 43:3D:243:GLY:H    | 62:3D:401:HEC:HBD2 | 1.74                     | 0.52              |
| 52:v2:147:ILE:HG13 | 52:v2:200:ILE:HD11 | 1.92                     | 0.52              |
| 55:s8:194:GLY:O    | 55:s8:198:GLU:HB2  | 2.10                     | 0.52              |
| 3:S2:144:MET:N     | 3:S2:144:MET:SD    | 2.82                     | 0.52              |
| 11:A9:82:ILE:HD13  | 11:A9:94:LEU:HD23  | 1.92                     | 0.52              |
| 39:V3:103:ARG:HH11 | 53:S1:441:ARG:HB3  | 1.75                     | 0.52              |
| 11:a9:140:ASP:OD1  | 11:a9:140:ASP:N    | 2.43                     | 0.52              |
| 12:s4:89:SER:O     | 53:s1:62:ARG:NH1   | 2.43                     | 0.52              |
| 37:an:87:PRO:HG2   | 37:an:90:TRP:HB2   | 1.91                     | 0.52              |
| 43:3O:126:SER:HB2  | 43:3O:177:LYS:HD2  | 1.91                     | 0.52              |
| 51:V1:113:LEU:HD21 | 51:V1:248:VAL:HG11 | 1.92                     | 0.52              |
| 8:4:456:GLY:O      | 27:BM:111:ARG:NH1  | 2.43                     | 0.52              |
| 32:b8:61:ASP:OD2   | 33:b4:36:ARG:NH1   | 2.43                     | 0.52              |
| 42:3C:334:ILE:HG12 | 46:3G:56:VAL:HG23  | 1.92                     | 0.52              |
| 51:v1:328:PRO:HB3  | 51:v1:441:HIS:HB3  | 1.92                     | 0.52              |
| 18:A8:7:LEU:O      | 20:AO:88:ARG:NH2   | 2.43                     | 0.52              |
| 24:C2:52:PRO:HB3   | 24:C2:55:ARG:HE    | 1.75                     | 0.52              |
| 7:5a:328:HIS:O     | 7:5a:332:HIS:HB3   | 2.10                     | 0.52              |
| 7:5a:577:THR:O     | 7:5a:580:GLN:NE2   | 2.43                     | 0.52              |
| 9:2a:51:ARG:HG2    | 9:2a:121:GLY:HA2   | 1.91                     | 0.52              |
| 40:3L:141:PRO:HA   | 40:3L:245:LEU:HD21 | 1.92                     | 0.52              |
| 40:3L:412:ASP:O    | 40:3L:416:SER:HB2  | 2.09                     | 0.52              |
| 48:3U:12:TYR:HA    | 48:3U:16:PHE:HB2   | 1.92                     | 0.52              |
| 53:s1:406:ASN:HD22 | 53:s1:436:VAL:HG11 | 1.74                     | 0.52              |
| 15:AC:138:LEU:HD13 | 15:AC:144:ILE:HG13 | 1.92                     | 0.52              |
| 1:3a:95:VAL:HG23   | 1:3a:98:LEU:HD23   | 1.91                     | 0.52              |
| 3:s2:333:ARG:NH1   | 3:s2:453:THR:O     | 2.43                     | 0.52              |
| 12:s4:88:GLN:NE2   | 53:s1:141:ASP:OD2  | 2.43                     | 0.52              |
| 41:3M:173:ILE:HD11 | 41:3M:441:SER:HB3  | 1.92                     | 0.52              |
| 51:V1:220:GLN:NE2  | 53:S1:197:THR:O    | 2.44                     | 0.52              |
| 54:s7:97:LEU:HD11  | 54:s7:141:MET:HE2  | 1.91                     | 0.52              |
| 3:S2:225:ALA:O     | 3:S2:228:ARG:NH1   | 2.43                     | 0.51              |
| 7:5:574:THR:HG21   | 9:2:170:LEU:HB2    | 1.91                     | 0.51              |
| 8:4:360:LEU:O      | 8:4:364:LEU:HB3    | 2.10                     | 0.51              |
| 3:s2:55:SER:OG     | 3:s2:56:LYS:N      | 2.44                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:5a:509:MET:SD    | 34:b9:33:HIS:ND1   | 2.83                     | 0.51              |
| 9:2a:131:LEU:O     | 9:2a:135:LYS:NZ    | 2.43                     | 0.51              |
| 43:3O:100:GLY:O    | 43:3O:286:LYS:NZ   | 2.43                     | 0.51              |
| 51:V1:138:LEU:HD23 | 51:V1:169:LEU:HD21 | 1.92                     | 0.51              |
| 53:S1:301:ARG:NH2  | 53:S1:591:GLU:OE1  | 2.43                     | 0.51              |
| 53:S1:593:SER:HA   | 53:S1:606:THR:O    | 2.10                     | 0.51              |
| 3:S2:138:ARG:NE    | 64:S7:301:SF4:S2   | 2.82                     | 0.51              |
| 5:6:61:GLY:HA2     | 5:6:64:LEU:HD12    | 1.92                     | 0.51              |
| 29:B6:29:SER:HB2   | 29:B6:32:GLU:HB2   | 1.91                     | 0.51              |
| 8:4a:181:PHE:O     | 36:bl:153:ARG:NH1  | 2.43                     | 0.51              |
| 39:V3:93:PRO:O     | 51:V1:152:ARG:NH2  | 2.43                     | 0.51              |
| 9:2a:316:HIS:O     | 10:al:337:ARG:NH2  | 2.43                     | 0.51              |
| 11:a9:81:ILE:HG22  | 11:a9:104:THR:HB   | 1.92                     | 0.51              |
| 40:3L:393:ASN:OD1  | 40:3L:396:ARG:NH1  | 2.44                     | 0.51              |
| 43:3O:227:LEU:HD12 | 43:3O:231:LEU:HB3  | 1.92                     | 0.51              |
| 7:5:594:ASN:ND2    | 9:2:110:PRO:O      | 2.43                     | 0.51              |
| 4:1a:22:LEU:HD11   | 4:1a:45:ILE:HA     | 1.91                     | 0.51              |
| 9:2:130:LEU:O      | 9:2:135:LYS:NZ     | 2.44                     | 0.51              |
| 15:AC:115:GLN:NE2  | 15:AC:135:ALA:O    | 2.43                     | 0.51              |
| 4:1a:172:MET:HE3   | 20:ao:49:ARG:HB3   | 1.91                     | 0.51              |
| 18:a8:166:ARG:NH1  | 28:b5:153:GLU:OE1  | 2.44                     | 0.51              |
| 34:b9:71:PHE:O     | 34:b9:75:GLN:HB3   | 2.11                     | 0.51              |
| 40:3A:446:SER:OG   | 48:3J:16:ARG:NH2   | 2.44                     | 0.51              |
| 51:V1:111:LYS:HG2  | 51:V1:239:PRO:HG2  | 1.93                     | 0.51              |
| 53:S1:437:ASP:OD1  | 53:S1:437:ASP:N    | 2.43                     | 0.51              |
| 51:v1:111:LYS:HG2  | 51:v1:239:PRO:HG2  | 1.93                     | 0.51              |
| 12:S4:75:ARG:NH2   | 12:S4:102:ASP:O    | 2.44                     | 0.51              |
| 3:s2:446:ASP:OD2   | 4:1a:281:ARG:NH1   | 2.44                     | 0.51              |
| 10:al:216:SER:OG   | 10:al:220:LYS:NZ   | 2.43                     | 0.51              |
| 11:a9:204:SER:OG   | 11:a9:205:ASP:N    | 2.44                     | 0.51              |
| 12:s4:64:LEU:HD21  | 17:a6:84:LEU:HD13  | 1.93                     | 0.51              |
| 19:am:81:ARG:NH1   | 19:am:86:ASP:OD2   | 2.44                     | 0.51              |
| 53:S1:280:ASP:O    | 53:S1:417:ARG:NH1  | 2.44                     | 0.51              |
| 53:s1:64:CYS:SG    | 53:s1:65:TYR:N     | 2.84                     | 0.51              |
| 2:S3:230:ARG:NH2   | 55:S8:128:ILE:O    | 2.44                     | 0.51              |
| 4:1:70:LEU:HA      | 4:1:73:ILE:HG22    | 1.93                     | 0.51              |
| 4:1:195:ARG:NH2    | 4:1:227:GLU:OE2    | 2.44                     | 0.51              |
| 40:3A:144:VAL:HG11 | 40:3A:245:LEU:HB3  | 1.93                     | 0.51              |
| 42:3C:39:VAL:HG21  | 42:3C:232:ILE:HD11 | 1.92                     | 0.51              |
| 51:v1:220:GLN:NE2  | 53:s1:197:THR:O    | 2.44                     | 0.51              |
| 8:4:236:LEU:HD23   | 8:4:237:LYS:HG3    | 1.92                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:S6:75:ARG:HH21  | 13:S6:76:ILE:HD11  | 1.75                     | 0.51              |
| 14:A2:83:SER:OG    | 14:A2:84:ALA:N     | 2.43                     | 0.51              |
| 17:A6:41:ALA:O     | 17:A6:45:GLU:HB2   | 2.10                     | 0.51              |
| 17:A6:117:ARG:HH21 | 17:A6:130:ASP:HB3  | 1.75                     | 0.51              |
| 7:5a:560:LYS:HD3   | 33:b4:80:PHE:HE2   | 1.76                     | 0.51              |
| 11:a9:192:ARG:NH2  | 11:a9:262:THR:OG1  | 2.42                     | 0.51              |
| 28:b5:77:LEU:HD23  | 28:b5:78:THR:HG23  | 1.92                     | 0.51              |
| 41:3B:50:ALA:O     | 41:3B:221:VAL:HA   | 2.11                     | 0.51              |
| 53:S1:251:ILE:HD12 | 53:S1:604:GLN:HB2  | 1.91                     | 0.51              |
| 53:S1:447:ASP:HB3  | 53:S1:683:PRO:HB3  | 1.91                     | 0.51              |
| 54:s7:164:CYS:HA   | 54:s7:169:GLY:H    | 1.76                     | 0.51              |
| 7:5:352:ASP:OD2    | 34:B9:93:ARG:NH1   | 2.44                     | 0.51              |
| 8:4:300:SER:O      | 8:4:308:SER:OG     | 2.28                     | 0.51              |
| 12:S4:78:ARG:HH21  | 12:S4:148:GLU:HG3  | 1.75                     | 0.51              |
| 33:B4:97:PRO:HA    | 33:B4:100:PHE:HB3  | 1.93                     | 0.51              |
| 3:s2:376:GLU:O     | 3:s2:380:HIS:ND1   | 2.42                     | 0.51              |
| 4:1a:234:MET:HA    | 4:1a:237:LEU:HB2   | 1.93                     | 0.51              |
| 8:4a:141:GLU:OE2   | 8:4a:144:ASN:ND2   | 2.44                     | 0.51              |
| 9:2a:30:TRP:NE1    | 9:2a:67:SER:OG     | 2.44                     | 0.51              |
| 53:S1:221:ASN:ND2  | 53:S1:286:ILE:O    | 2.43                     | 0.51              |
| 51:v1:205:ILE:HG12 | 51:v1:379:CYS:HB3  | 1.93                     | 0.51              |
| 7:5:161:ARG:NH2    | 34:B9:88:GLY:O     | 2.44                     | 0.51              |
| 35:B7:47:MET:SD    | 36:BL:120:ASN:ND2  | 2.79                     | 0.51              |
| 8:4a:380:PHE:HA    | 8:4a:383:MET:HG2   | 1.93                     | 0.51              |
| 11:a9:85:ARG:HH22  | 54:s7:224:ARG:HG3  | 1.76                     | 0.51              |
| 24:c2:46:ASN:OD1   | 24:c2:51:ARG:NH1   | 2.39                     | 0.51              |
| 37:an:82:ASP:HB2   | 54:s7:203:TYR:HE1  | 1.75                     | 0.51              |
| 42:3C:117:VAL:HG11 | 42:3C:302:ALA:HB2  | 1.93                     | 0.51              |
| 43:3O:192:ALA:HB1  | 62:3O:401:HEC:HBD1 | 1.92                     | 0.51              |
| 53:S1:50:LEU:HD21  | 53:S1:62:ARG:HE    | 1.74                     | 0.51              |
| 53:s1:301:ARG:NH2  | 53:s1:591:GLU:OE1  | 2.44                     | 0.51              |
| 9:2:109:ALA:HA     | 9:2:112:HIS:HB3    | 1.93                     | 0.50              |
| 12:S4:75:ARG:NH1   | 12:S4:119:ASP:OD1  | 2.45                     | 0.50              |
| 35:B7:59:CYS:HB2   | 35:B7:90:CYS:HB3   | 1.92                     | 0.50              |
| 1:3a:34:ALA:HB1    | 4:1a:63:PRO:HA     | 1.93                     | 0.50              |
| 10:al:71:ASN:ND2   | 10:al:160:GLU:OE1  | 2.44                     | 0.50              |
| 13:s6:69:VAL:HG12  | 13:s6:110:GLN:HB2  | 1.92                     | 0.50              |
| 18:a8:125:LEU:HB2  | 20:ao:66:GLU:HG2   | 1.93                     | 0.50              |
| 19:am:1:MET:SD     | 19:am:1:MET:N      | 2.82                     | 0.50              |
| 41:3M:43:LEU:HD12  | 41:3M:47:LEU:HD23  | 1.92                     | 0.50              |
| 54:S7:169:GLY:HA2  | 55:S8:151:LYS:HA   | 1.92                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:s1:437:ASP:N    | 53:s1:437:ASP:OD1  | 2.43                     | 0.50              |
| 1:3:54:LYS:HB3     | 1:3:113:TRP:HB3    | 1.93                     | 0.50              |
| 1:3:95:VAL:HG13    | 4:1:298:LEU:HD22   | 1.92                     | 0.50              |
| 2:S3:170:TRP:NE1   | 17:A6:91:MET:SD    | 2.77                     | 0.50              |
| 2:S3:210:ARG:NH2   | 11:A9:71:ASN:OD1   | 2.44                     | 0.50              |
| 10:AL:82:GLY:O     | 10:AL:155:GLN:NE2  | 2.44                     | 0.50              |
| 11:a9:239:PRO:HG2  | 11:a9:345:LEU:HD22 | 1.92                     | 0.50              |
| 45:3F:58:ASP:OD2   | 45:3F:62:ARG:NH1   | 2.43                     | 0.50              |
| 13:S6:58:ASN:ND2   | 55:S8:195:ASP:OD2  | 2.44                     | 0.50              |
| 20:AO:25:LEU:HG    | 55:S8:68:ARG:HH21  | 1.74                     | 0.50              |
| 37:AN:27:LEU:O     | 37:AN:31:PHE:HB2   | 2.12                     | 0.50              |
| 7:5a:145:GLU:OE2   | 7:5a:176:ARG:NH1   | 2.44                     | 0.50              |
| 7:5a:396:ILE:O     | 7:5a:400:ASN:HB2   | 2.11                     | 0.50              |
| 8:4a:437:MET:HA    | 8:4a:440:HIS:HB2   | 1.93                     | 0.50              |
| 51:V1:290:GLU:OE2  | 51:V1:303:HIS:ND1  | 2.44                     | 0.50              |
| 2:S3:107:PHE:HB3   | 2:S3:131:LEU:HB3   | 1.92                     | 0.50              |
| 7:5:136:ASN:ND2    | 7:5:197:GLU:OE1    | 2.44                     | 0.50              |
| 12:S4:78:ARG:NH1   | 53:S1:249:GLU:OE1  | 2.45                     | 0.50              |
| 14:A2:79:LEU:HD22  | 14:A2:87:VAL:HG23  | 1.93                     | 0.50              |
| 7:5a:142:ILE:HG12  | 8:4a:370:PRO:HB2   | 1.92                     | 0.50              |
| 33:b4:62:ASP:HB2   | 33:b4:65:LEU:HB2   | 1.93                     | 0.50              |
| 53:s1:594:ALA:O    | 53:s1:605:GLN:HA   | 2.11                     | 0.50              |
| 6:4L:59:ILE:HG23   | 9:2:27:MET:HE2     | 1.93                     | 0.50              |
| 10:AL:250:SER:O    | 10:AL:280:LYS:NZ   | 2.44                     | 0.50              |
| 15:AC:89:LEU:HD13  | 31:B3:54:ASN:HA    | 1.94                     | 0.50              |
| 33:B4:38:SER:OG    | 33:B4:42:ARG:NH1   | 2.45                     | 0.50              |
| 36:BL:7:LYS:NZ     | 36:BL:12:GLU:O     | 2.44                     | 0.50              |
| 1:3a:6:VAL:HG21    | 4:1a:87:VAL:HG11   | 1.92                     | 0.50              |
| 3:s2:282:ASP:O     | 3:s2:286:TYR:HB2   | 2.10                     | 0.50              |
| 43:3D:197:LEU:HB2  | 43:3D:274:LEU:HD11 | 1.94                     | 0.50              |
| 51:V1:278:ILE:HD11 | 51:V1:299:LEU:HD22 | 1.92                     | 0.50              |
| 51:V1:308:THR:O    | 51:V1:313:ASN:ND2  | 2.44                     | 0.50              |
| 53:S1:647:GLU:HG2  | 53:S1:654:VAL:HG21 | 1.94                     | 0.50              |
| 3:S2:402:ALA:HB2   | 3:S2:407:PHE:HB2   | 1.94                     | 0.50              |
| 8:4:261:PHE:O      | 8:4:265:SER:HB3    | 2.11                     | 0.50              |
| 11:A9:165:ILE:HG21 | 11:A9:249:ILE:HG23 | 1.94                     | 0.50              |
| 2:s3:151:PRO:HB3   | 2:s3:176:PHE:HB3   | 1.92                     | 0.50              |
| 7:5a:446:ASN:ND2   | 30:b2:54:GLN:OE1   | 2.45                     | 0.50              |
| 9:2a:3:PRO:HB3     | 10:a1:40:LEU:HD11  | 1.94                     | 0.50              |
| 18:a8:13:LEU:HD23  | 18:a8:57:LEU:HD11  | 1.93                     | 0.50              |
| 24:c2:30:ARG:HH21  | 24:c2:76:LEU:HD21  | 1.76                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:3A:58:ARG:O     | 40:3A:230:VAL:HA   | 2.12                     | 0.50              |
| 52:V2:136:THR:OG1  | 52:V2:174:GLU:O    | 2.30                     | 0.50              |
| 2:S3:118:VAL:HG21  | 2:S3:121:ARG:HH21  | 1.75                     | 0.50              |
| 7:5:511:LEU:HD11   | 31:B3:38:VAL:HG22  | 1.94                     | 0.50              |
| 8:4:101:SER:HA     | 8:4:104:ILE:HD12   | 1.94                     | 0.50              |
| 8:4:360:LEU:O      | 8:4:364:LEU:CB     | 2.60                     | 0.50              |
| 1:3a:10:ASN:HB3    | 4:1a:80:THR:HG23   | 1.94                     | 0.50              |
| 6:4l:45:SER:O      | 6:4l:49:LEU:HB2    | 2.11                     | 0.50              |
| 18:a8:23:ALA:HB3   | 18:a8:86:TRP:HE3   | 1.76                     | 0.50              |
| 20:ao:52:ARG:NH1   | 20:ao:55:GLN:OE1   | 2.44                     | 0.50              |
| 42:3N:377:LEU:O    | 45:3Q:34:ARG:NH1   | 2.45                     | 0.50              |
| 51:V1:89:GLY:HA3   | 63:V1:501:FMN:H1'2 | 1.94                     | 0.50              |
| 53:S1:220:GLY:HA3  | 53:S1:291:ARG:HD3  | 1.93                     | 0.50              |
| 54:s7:219:LYS:HE3  | 54:s7:223:ARG:HE   | 1.77                     | 0.50              |
| 55:s8:153:ILE:N    | 64:s8:301:SF4:S3   | 2.81                     | 0.50              |
| 3:S2:116:LEU:HD21  | 54:S7:97:LEU:HG    | 1.94                     | 0.50              |
| 11:A9:61:ALA:HB3   | 11:A9:82:ILE:HG23  | 1.94                     | 0.50              |
| 4:1a:195:ARG:NH1   | 4:1a:227:GLU:OE2   | 2.44                     | 0.50              |
| 22:a3:72:ASP:OD1   | 22:a3:72:ASP:N     | 2.39                     | 0.50              |
| 32:b8:33:THR:O     | 32:b8:37:LEU:HB2   | 2.11                     | 0.50              |
| 39:v3:86:ASP:O     | 39:v3:89:LYS:NZ    | 2.45                     | 0.50              |
| 42:3C:102:LEU:HD21 | 42:3C:304:MET:HE3  | 1.93                     | 0.50              |
| 53:S1:405:THR:HG21 | 53:S1:516:LEU:HD11 | 1.94                     | 0.50              |
| 5:6:81:THR:OG1     | 5:6:82:TRP:N       | 2.45                     | 0.50              |
| 9:2:25:ASN:HB3     | 9:2:28:LEU:HB2     | 1.92                     | 0.50              |
| 9:2:139:LEU:HD23   | 9:2:205:LEU:HD22   | 1.94                     | 0.50              |
| 9:2:269:GLU:O      | 9:2:273:ASN:ND2    | 2.45                     | 0.50              |
| 10:AL:64:GLY:O     | 10:AL:161:ARG:NH1  | 2.45                     | 0.50              |
| 4:1a:58:LYS:HA     | 54:s7:155:PRO:HG2  | 1.94                     | 0.50              |
| 8:4a:388:TRP:O     | 33:b4:112:LYS:NZ   | 2.44                     | 0.50              |
| 34:b9:62:GLN:OE1   | 34:b9:65:ARG:NH1   | 2.44                     | 0.50              |
| 40:3A:451:ASP:OD1  | 40:3A:472:ARG:NH2  | 2.45                     | 0.50              |
| 41:3M:70:ARG:NH1   | 41:3M:332:ASP:OD2  | 2.45                     | 0.50              |
| 54:s7:182:ASP:OD1  | 54:s7:182:ASP:N    | 2.44                     | 0.50              |
| 3:S2:312:ASP:N     | 3:S2:312:ASP:OD1   | 2.43                     | 0.49              |
| 33:B4:50:GLN:O     | 33:B4:56:ARG:NH1   | 2.44                     | 0.49              |
| 4:1a:26:LYS:NZ     | 4:1a:43:TYR:O      | 2.45                     | 0.49              |
| 7:5a:306:THR:HB    | 7:5a:336:LYS:HG2   | 1.94                     | 0.49              |
| 8:4a:400:ILE:HA    | 8:4a:403:THR:HG22  | 1.94                     | 0.49              |
| 11:a9:135:GLU:HB2  | 11:a9:140:ASP:HA   | 1.94                     | 0.49              |
| 14:a2:24:CYS:SG    | 14:a2:25:GLN:N     | 2.85                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:a2:86:GLU:HA    | 14:a2:89:ARG:HG3   | 1.94                     | 0.49              |
| 42:3N:43:VAL:HA    | 42:3N:46:ILE:HG22  | 1.94                     | 0.49              |
| 8:4:56:PHE:HB3     | 8:4:111:SER:HB3    | 1.92                     | 0.49              |
| 8:4:251:ASP:OD2    | 36:BL:154:LYS:NZ   | 2.44                     | 0.49              |
| 31:B3:84:PHE:HB3   | 31:B3:86:VAL:HG22  | 1.94                     | 0.49              |
| 3:s2:156:GLU:OE2   | 3:s2:171:ARG:NH2   | 2.45                     | 0.49              |
| 3:s2:228:ARG:NH1   | 55:s8:160:GLU:OE2  | 2.46                     | 0.49              |
| 7:5a:14:LEU:HD11   | 29:b6:75:VAL:HG22  | 1.94                     | 0.49              |
| 12:s4:111:LEU:HD23 | 12:s4:112:MET:HB2  | 1.93                     | 0.49              |
| 14:a2:27:SER:O     | 14:a2:34:ARG:NH2   | 2.45                     | 0.49              |
| 41:3B:183:LYS:HD2  | 41:3B:252:LYS:HE3  | 1.94                     | 0.49              |
| 40:3L:179:MET:HE1  | 40:3L:282:LEU:HD22 | 1.94                     | 0.49              |
| 43:3O:199:TYR:O    | 43:3O:203:ALA:HB2  | 2.11                     | 0.49              |
| 51:v1:126:LYS:HB2  | 51:v1:275:LEU:HD13 | 1.94                     | 0.49              |
| 2:S3:98:PHE:O      | 2:S3:102:HIS:HB2   | 2.12                     | 0.49              |
| 2:S3:229:PHE:O     | 53:S1:246:ARG:NH2  | 2.45                     | 0.49              |
| 6:4L:40:LEU:HD13   | 9:2:71:LEU:HD23    | 1.94                     | 0.49              |
| 8:4:317:ILE:HB     | 8:4:454:ILE:HD11   | 1.94                     | 0.49              |
| 10:AL:68:SER:HA    | 10:AL:217:ARG:HH21 | 1.76                     | 0.49              |
| 10:AL:200:PRO:O    | 10:AL:283:TRP:NE1  | 2.42                     | 0.49              |
| 11:A9:123:SER:OG   | 11:A9:124:ASN:N    | 2.46                     | 0.49              |
| 2:s3:214:GLU:OE1   | 11:a9:75:ARG:NH2   | 2.44                     | 0.49              |
| 3:s2:253:LEU:O     | 3:s2:257:GLU:HB2   | 2.12                     | 0.49              |
| 4:1a:20:LEU:HD22   | 4:1a:232:ILE:HB    | 1.94                     | 0.49              |
| 4:1a:154:LEU:HD21  | 4:1a:165:LEU:HD11  | 1.94                     | 0.49              |
| 8:4a:224:PRO:O     | 8:4a:228:SER:HB2   | 2.13                     | 0.49              |
| 27:bm:101:THR:HA   | 27:bm:104:VAL:HG12 | 1.93                     | 0.49              |
| 40:3A:126:ARG:NH1  | 40:3A:199:GLN:O    | 2.46                     | 0.49              |
| 41:3B:70:ARG:NH2   | 41:3B:249:ALA:O    | 2.45                     | 0.49              |
| 41:3B:162:LYS:HD2  | 41:3B:197:MET:HE1  | 1.93                     | 0.49              |
| 48:3J:5:THR:OG1    | 48:3J:6:ILE:N      | 2.45                     | 0.49              |
| 42:3N:137:GLN:NE2  | 42:3N:263:ASN:OD1  | 2.45                     | 0.49              |
| 53:s1:647:GLU:HG2  | 53:s1:654:VAL:HG21 | 1.93                     | 0.49              |
| 4:1:153:VAL:HG21   | 4:1:242:PHE:HE1    | 1.77                     | 0.49              |
| 5:6:134:MET:O      | 25:S5:29:ASN:ND2   | 2.45                     | 0.49              |
| 7:5:224:SER:OG     | 7:5:226:GLN:NE2    | 2.44                     | 0.49              |
| 18:A8:143:HIS:HB2  | 20:AO:115:ARG:HB3  | 1.94                     | 0.49              |
| 19:am:9:TYR:HB2    | 19:am:24:ILE:HG21  | 1.93                     | 0.49              |
| 32:b8:110:ASP:OD2  | 33:b4:72:ARG:NH1   | 2.45                     | 0.49              |
| 41:3M:90:THR:HG23  | 41:3M:95:SER:HA    | 1.93                     | 0.49              |
| 43:3O:89:LEU:HD11  | 47:3S:74:HIS:HB2   | 1.93                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 43:3O:195:PRO:HG3 | 62:3O:401:HEC:HBA1 | 1.93                     | 0.49              |
| 51:v1:285:PRO:HB2 | 52:v2:180:VAL:HG13 | 1.93                     | 0.49              |
| 53:s1:281:ILE:HA  | 53:s1:391:ILE:HD13 | 1.94                     | 0.49              |
| 7:5:446:ASN:HA    | 7:5:451:MET:HE3    | 1.94                     | 0.49              |
| 9:2:326:PHE:O     | 9:2:330:ALA:HB2    | 2.12                     | 0.49              |
| 11:A9:144:VAL:HA  | 11:A9:148:ILE:HD12 | 1.94                     | 0.49              |
| 2:s3:173:PHE:O    | 2:s3:198:ARG:NH1   | 2.46                     | 0.49              |
| 3:s2:66:TRP:HB2   | 10:al:193:LEU:HD11 | 1.93                     | 0.49              |
| 4:1a:184:MET:HE1  | 4:1a:296:LEU:HB3   | 1.94                     | 0.49              |
| 6:4l:54:MET:HB2   | 25:s5:26:PRO:HD2   | 1.94                     | 0.49              |
| 7:5a:121:LEU:HD22 | 7:5a:246:LEU:HD23  | 1.95                     | 0.49              |
| 9:2a:51:ARG:HD3   | 9:2a:120:GLN:HG3   | 1.94                     | 0.49              |
| 36:bl:28:ASN:HB3  | 36:bl:30:ILE:HG12  | 1.95                     | 0.49              |
| 51:V1:134:ASP:OD1 | 51:V1:134:ASP:N    | 2.46                     | 0.49              |
| 53:S1:637:ASP:OD1 | 53:S1:637:ASP:N    | 2.46                     | 0.49              |
| 53:s1:340:ALA:HA  | 53:s1:546:PHE:O    | 2.12                     | 0.49              |
| 53:s1:682:ASP:N   | 53:s1:682:ASP:OD1  | 2.45                     | 0.49              |
| 7:5:347:ILE:HG23  | 7:5:352:ASP:HA     | 1.95                     | 0.49              |
| 24:C2:106:LYS:O   | 36:BL:78:LYS:NZ    | 2.46                     | 0.49              |
| 37:AN:87:PRO:HG2  | 37:AN:90:TRP:HB2   | 1.95                     | 0.49              |
| 4:1a:178:ALA:HB1  | 4:1a:181:MET:HB2   | 1.95                     | 0.49              |
| 4:1a:286:MET:O    | 4:1a:290:TRP:HB2   | 2.12                     | 0.49              |
| 8:4a:431:THR:HG22 | 28:b5:67:PHE:HB2   | 1.95                     | 0.49              |
| 12:s4:78:ARG:HE   | 53:s1:607:LYS:HG3  | 1.77                     | 0.49              |
| 29:b6:83:HIS:NE2  | 36:bl:42:ASP:OD1   | 2.45                     | 0.49              |
| 40:3A:469:ASN:ND2 | 43:3D:310:LYS:O    | 2.45                     | 0.49              |
| 48:3J:28:GLY:O    | 48:3J:32:PHE:HB2   | 2.13                     | 0.49              |
| 41:3M:213:PHE:O   | 41:3M:241:ARG:NH1  | 2.46                     | 0.49              |
| 2:S3:182:ASP:N    | 2:S3:182:ASP:OD1   | 2.46                     | 0.49              |
| 7:5:198:LEU:HA    | 7:5:201:ILE:HG22   | 1.95                     | 0.49              |
| 7:5:535:ARG:NH2   | 32:B8:120:SER:OG   | 2.45                     | 0.49              |
| 8:4:166:LEU:HD22  | 9:2:276:LEU:HD11   | 1.94                     | 0.49              |
| 8:4:297:VAL:HA    | 8:4:300:SER:HB3    | 1.94                     | 0.49              |
| 10:AL:200:PRO:HG2 | 10:AL:282:PRO:HG2  | 1.94                     | 0.49              |
| 34:B9:136:GLU:HG2 | 34:B9:165:PRO:HA   | 1.93                     | 0.49              |
| 37:AN:80:ASP:OD1  | 54:S7:210:ARG:NH1  | 2.45                     | 0.49              |
| 40:3A:397:ASN:ND2 | 41:3B:107:GLY:O    | 2.46                     | 0.49              |
| 44:3E:141:SER:OG  | 44:3E:142:ALA:N    | 2.45                     | 0.49              |
| 51:V1:115:VAL:HB  | 51:V1:156:ILE:HA   | 1.95                     | 0.49              |
| 53:S1:238:PHE:HB3 | 55:S8:140:ARG:HE   | 1.77                     | 0.49              |
| 3:S2:379:ILE:HD12 | 53:S1:140:GLN:HG2  | 1.94                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:5:260:LEU:HB2   | 7:5:317:LEU:HD11   | 1.94                     | 0.49              |
| 7:5:574:THR:HB    | 9:2:171:ASN:HB2    | 1.93                     | 0.49              |
| 8:4:105:LEU:O     | 8:4:109:THR:OG1    | 2.26                     | 0.49              |
| 19:AM:57:GLY:O    | 19:AM:61:PHE:HB2   | 2.13                     | 0.49              |
| 9:2a:324:LEU:HD23 | 24:c2:49:ARG:HH22  | 1.76                     | 0.49              |
| 16:a5:40:LYS:O    | 16:a5:46:LYS:NZ    | 2.45                     | 0.49              |
| 47:3H:64:ASP:OD1  | 47:3H:64:ASP:N     | 2.45                     | 0.49              |
| 51:V1:37:ASP:N    | 51:V1:37:ASP:OD1   | 2.44                     | 0.49              |
| 53:S1:693:ASP:OD1 | 53:S1:693:ASP:N    | 2.45                     | 0.49              |
| 2:S3:227:GLN:OE1  | 2:S3:230:ARG:NH1   | 2.46                     | 0.49              |
| 2:S3:231:LYS:H    | 53:S1:246:ARG:HH21 | 1.60                     | 0.49              |
| 3:S2:148:GLU:HB3  | 3:S2:227:ILE:HB    | 1.94                     | 0.49              |
| 7:5:144:TRP:O     | 7:5:223:LYS:NZ     | 2.44                     | 0.49              |
| 33:B4:62:ASP:HB3  | 33:B4:65:LEU:HB2   | 1.94                     | 0.49              |
| 4:1a:27:ILE:HD13  | 21:a1:5:ILE:HG12   | 1.94                     | 0.49              |
| 10:a1:172:ALA:HB2 | 10:a1:237:ILE:HD11 | 1.95                     | 0.49              |
| 34:b9:89:THR:O    | 34:b9:93:ARG:NH1   | 2.46                     | 0.49              |
| 34:b9:105:ASP:OD1 | 34:b9:122:ARG:NH2  | 2.42                     | 0.49              |
| 41:3B:76:ASN:OD1  | 41:3B:76:ASN:N     | 2.46                     | 0.49              |
| 41:3B:109:LYS:O   | 41:3B:123:VAL:HA   | 2.13                     | 0.49              |
| 42:3N:186:PRO:HA  | 42:3N:189:ILE:HB   | 1.95                     | 0.49              |
| 44:3P:141:SER:OG  | 44:3P:142:ALA:N    | 2.46                     | 0.49              |
| 54:s7:147:LYS:O   | 54:s7:151:GLN:NE2  | 2.44                     | 0.49              |
| 8:4:443:PRO:O     | 8:4:447:LEU:HB2    | 2.13                     | 0.49              |
| 10:AL:112:CYS:HB3 | 10:AL:130:ARG:HB3  | 1.95                     | 0.49              |
| 13:S6:72:VAL:HG21 | 13:S6:77:ILE:HD12  | 1.95                     | 0.49              |
| 30:B2:76:ASP:N    | 30:B2:76:ASP:OD1   | 2.46                     | 0.49              |
| 31:B3:45:ARG:NH2  | 34:B9:39:TYR:OH    | 2.46                     | 0.49              |
| 35:B7:53:LEU:HA   | 35:B7:56:ARG:HD2   | 1.95                     | 0.49              |
| 6:4l:46:VAL:O     | 6:4l:50:ASN:HB2    | 2.12                     | 0.49              |
| 12:s4:78:ARG:NH1  | 12:s4:148:GLU:OE1  | 2.45                     | 0.49              |
| 14:a2:62:GLN:OE1  | 14:a2:80:ASN:ND2   | 2.46                     | 0.49              |
| 15:ab:132:ASP:OD2 | 17:a6:40:ARG:NH1   | 2.46                     | 0.49              |
| 44:3P:79:SER:OG   | 44:3P:80:HIS:N     | 2.45                     | 0.49              |
| 52:v2:136:THR:OG1 | 65:v2:301:FES:S2   | 2.65                     | 0.49              |
| 2:S3:230:ARG:NH2  | 55:S8:126:GLN:OE1  | 2.45                     | 0.48              |
| 3:S2:115:LEU:O    | 54:S7:138:THR:OG1  | 2.31                     | 0.48              |
| 11:A9:192:ARG:NH1 | 11:A9:198:ALA:O    | 2.45                     | 0.48              |
| 15:AC:69:SER:OG   | 15:AC:70:ASP:N     | 2.46                     | 0.48              |
| 22:A3:79:ASP:OD1  | 22:A3:79:ASP:N     | 2.46                     | 0.48              |
| 33:B4:91:ALA:O    | 33:B4:95:PHE:HB2   | 2.12                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BL:4:SER:OG     | 36:BL:5:TRP:N      | 2.46                     | 0.48              |
| 8:4a:456:GLY:O     | 27:bm:111:ARG:NH1  | 2.46                     | 0.48              |
| 20:ao:82:ARG:NH1   | 20:ao:125:TYR:OH   | 2.46                     | 0.48              |
| 21:a1:37:ARG:NH2   | 21:a1:51:ASP:OD2   | 2.46                     | 0.48              |
| 29:b6:11:ARG:O     | 29:b6:15:LEU:HB2   | 2.12                     | 0.48              |
| 42:3C:45:ILE:O     | 42:3C:49:LEU:HB2   | 2.13                     | 0.48              |
| 42:3C:214:ASP:HB3  | 46:3G:8:LEU:HB3    | 1.94                     | 0.48              |
| 42:3C:216:ASP:OD1  | 43:3D:317:ARG:NH2  | 2.46                     | 0.48              |
| 53:s1:354:LEU:HD22 | 53:s1:548:LEU:HG   | 1.94                     | 0.48              |
| 8:4:187:ASP:N      | 8:4:187:ASP:OD1    | 2.45                     | 0.48              |
| 10:AL:139:ARG:NH1  | 10:AL:161:ARG:O    | 2.46                     | 0.48              |
| 3:s2:96:ARG:HH22   | 17:a6:100:TRP:HA   | 1.78                     | 0.48              |
| 4:1a:134:ARG:NH2   | 4:1a:206:GLU:OE1   | 2.47                     | 0.48              |
| 10:al:81:LEU:HD23  | 10:al:83:MET:HG3   | 1.95                     | 0.48              |
| 53:s1:131:CYS:O    | 53:s1:241:ARG:NH1  | 2.44                     | 0.48              |
| 53:s1:239:THR:O    | 53:s1:266:ARG:NH2  | 2.42                     | 0.48              |
| 2:S3:72:VAL:HA     | 2:S3:87:ILE:HG22   | 1.96                     | 0.48              |
| 16:A5:44:TYR:O     | 16:A5:48:THR:OG1   | 2.30                     | 0.48              |
| 38:A7:25:GLN:OE1   | 55:S8:79:ARG:NH1   | 2.46                     | 0.48              |
| 9:2a:269:GLU:OE1   | 28:b5:157:ARG:NH2  | 2.46                     | 0.48              |
| 31:b3:33:THR:HG22  | 31:b3:35:LEU:H     | 1.78                     | 0.48              |
| 39:v3:84:ASN:OD1   | 39:v3:91:ARG:NH2   | 2.42                     | 0.48              |
| 42:3N:158:THR:HA   | 42:3N:161:VAL:HG12 | 1.94                     | 0.48              |
| 43:3O:97:SER:O     | 48:3U:52:LYS:NZ    | 2.47                     | 0.48              |
| 51:V1:112:TYR:O    | 51:V1:240:THR:HA   | 2.12                     | 0.48              |
| 53:s1:380:ASP:OD1  | 53:s1:380:ASP:N    | 2.43                     | 0.48              |
| 53:s1:407:PRO:HD2  | 53:s1:438:LEU:HD11 | 1.95                     | 0.48              |
| 55:s8:148:ASP:HB3  | 55:s8:151:LYS:HB2  | 1.96                     | 0.48              |
| 3:S2:266:ARG:O     | 3:S2:270:ASN:HB2   | 2.13                     | 0.48              |
| 7:5:8:ILE:HA       | 7:5:11:ILE:HD12    | 1.95                     | 0.48              |
| 10:AL:327:ILE:O    | 10:AL:331:PHE:HB2  | 2.13                     | 0.48              |
| 8:4a:276:CYS:HB3   | 8:4a:285:LEU:HG    | 1.95                     | 0.48              |
| 9:2a:240:MET:O     | 9:2a:244:ILE:HB    | 2.13                     | 0.48              |
| 13:s6:67:GLN:NE2   | 55:s8:108:SER:O    | 2.47                     | 0.48              |
| 36:bl:162:ARG:NH1  | 36:bl:166:GLU:OE1  | 2.46                     | 0.48              |
| 44:3P:93:ARG:HD2   | 44:3P:110:ARG:HG2  | 1.94                     | 0.48              |
| 2:S3:196:PRO:O     | 3:S2:122:LYS:NZ    | 2.47                     | 0.48              |
| 9:2:42:PRO:HA      | 9:2:45:ILE:HG22    | 1.96                     | 0.48              |
| 1:3a:69:ILE:HA     | 1:3a:72:LEU:HB2    | 1.96                     | 0.48              |
| 3:s2:221:ARG:HD2   | 54:s7:197:THR:HG23 | 1.96                     | 0.48              |
| 17:a6:27:ASP:OD1   | 17:a6:27:ASP:N     | 2.44                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:bm:70:ASP:OD1   | 34:b9:108:HIS:NE2  | 2.47                     | 0.48              |
| 40:3A:368:MET:O    | 40:3A:372:LEU:HB2  | 2.14                     | 0.48              |
| 45:3F:54:ASP:OD1   | 45:3F:54:ASP:N     | 2.47                     | 0.48              |
| 42:3N:47:THR:O     | 42:3N:51:LEU:HB2   | 2.12                     | 0.48              |
| 52:V2:37:LEU:HB3   | 52:V2:41:ARG:HH21  | 1.79                     | 0.48              |
| 53:S1:140:GLN:NE2  | 64:S1:801:SF4:S3   | 2.86                     | 0.48              |
| 53:s1:66:HIS:HB2   | 53:s1:181:ARG:HD3  | 1.96                     | 0.48              |
| 4:1:28:LEU:HD11    | 4:1:274:ARG:HH11   | 1.79                     | 0.48              |
| 8:4:180:SER:O      | 36:BL:153:ARG:NH2  | 2.45                     | 0.48              |
| 10:AL:139:ARG:NH1  | 10:AL:166:ASP:OD1  | 2.47                     | 0.48              |
| 14:A2:27:SER:O     | 14:A2:34:ARG:NH2   | 2.44                     | 0.48              |
| 2:s3:185:ARG:NH1   | 2:s3:188:THR:OG1   | 2.46                     | 0.48              |
| 8:4a:53:SER:OG     | 8:4a:54:ASN:N      | 2.47                     | 0.48              |
| 9:2a:273:ASN:O     | 19:am:140:LYS:NZ   | 2.47                     | 0.48              |
| 15:ac:131:PRO:HG2  | 15:ac:134:ASP:HB2  | 1.95                     | 0.48              |
| 19:am:87:PRO:HG3   | 19:am:127:ILE:HD13 | 1.95                     | 0.48              |
| 25:s5:15:ASP:N     | 25:s5:15:ASP:OD1   | 2.47                     | 0.48              |
| 51:V1:243:ALA:HA   | 63:V1:501:FMN:H5'2 | 1.94                     | 0.48              |
| 53:s1:592:LYS:NZ   | 53:s1:619:ASP:OD2  | 2.46                     | 0.48              |
| 7:5:564:LYS:HA     | 7:5:567:SER:HB3    | 1.95                     | 0.48              |
| 8:4:36:LEU:HD13    | 27:BM:96:VAL:HA    | 1.95                     | 0.48              |
| 14:A2:71:PHE:H     | 53:S1:362:ASP:HB3  | 1.79                     | 0.48              |
| 34:B9:105:ASP:OD1  | 34:B9:122:ARG:NH2  | 2.46                     | 0.48              |
| 5:6a:22:LYS:NZ     | 6:4l:21:MET:O      | 2.40                     | 0.48              |
| 9:2a:154:ILE:HG21  | 9:2a:195:PRO:HD3   | 1.94                     | 0.48              |
| 14:a2:19:ILE:HG23  | 14:a2:53:ILE:HA    | 1.96                     | 0.48              |
| 19:am:114:GLY:O    | 19:am:118:MET:HB2  | 2.13                     | 0.48              |
| 42:3C:6:LYS:O      | 42:3C:12:LYS:NZ    | 2.47                     | 0.48              |
| 42:3C:210:GLY:HA3  | 42:3C:314:SER:HB3  | 1.95                     | 0.48              |
| 41:3M:129:ASP:N    | 41:3M:129:ASP:OD1  | 2.45                     | 0.48              |
| 44:3P:103:SER:OG   | 44:3P:104:LYS:N    | 2.45                     | 0.48              |
| 53:S1:478:SER:O    | 53:S1:518:ARG:NH1  | 2.47                     | 0.48              |
| 15:AC:141:PRO:HA   | 15:AC:144:ILE:HG22 | 1.96                     | 0.48              |
| 3:s2:411:LEU:HD13  | 3:s2:422:CYS:HB3   | 1.94                     | 0.48              |
| 4:1a:127:TYR:HD1   | 4:1a:207:LEU:HB3   | 1.79                     | 0.48              |
| 11:a9:211:ASP:OD1  | 11:a9:211:ASP:N    | 2.46                     | 0.48              |
| 40:3A:300:ASP:OD1  | 40:3A:300:ASP:N    | 2.37                     | 0.48              |
| 42:3C:130:GLY:HA2  | 42:3C:133:LEU:HD12 | 1.96                     | 0.48              |
| 40:3L:341:PHE:HB3  | 40:3L:358:PHE:HB3  | 1.96                     | 0.48              |
| 53:S1:197:THR:HG22 | 53:S1:206:VAL:HG22 | 1.96                     | 0.48              |
| 3:S2:281:GLU:OE2   | 16:A5:86:LYS:NZ    | 2.46                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:S2:303:ARG:NH2  | 3:S2:336:GLU:OE2   | 2.47                     | 0.48              |
| 8:4:26:ASN:OD1    | 26:B1:13:HIS:NE2   | 2.45                     | 0.48              |
| 8:4:137:GLY:O     | 8:4:142:ARG:NH1    | 2.47                     | 0.48              |
| 5:6a:129:ASP:HB3  | 5:6a:135:LEU:HD21  | 1.95                     | 0.48              |
| 7:5a:153:LEU:HD21 | 8:4a:360:LEU:HD21  | 1.95                     | 0.48              |
| 7:5a:512:SER:H    | 34:b9:36:LYS:HE3   | 1.78                     | 0.48              |
| 8:4a:66:ILE:HG23  | 8:4a:107:ILE:HD11  | 1.96                     | 0.48              |
| 14:a2:56:ARG:NH2  | 53:s1:379:THR:O    | 2.47                     | 0.48              |
| 15:ac:97:LYS:NZ   | 15:ac:107:ASP:O    | 2.47                     | 0.48              |
| 20:ao:56:GLU:HA   | 20:ao:59:ARG:HE    | 1.79                     | 0.48              |
| 53:s1:518:ARG:HG3 | 53:s1:519:ILE:HG13 | 1.96                     | 0.48              |
| 4:1:54:LYS:HD3    | 4:1:55:LEU:HG      | 1.96                     | 0.48              |
| 8:4:171:VAL:HG21  | 8:4:179:LEU:HD21   | 1.95                     | 0.48              |
| 9:2:43:MET:O      | 9:2:46:ASN:ND2     | 2.45                     | 0.48              |
| 10:AL:105:ASP:HB2 | 10:AL:108:PHE:HD2  | 1.79                     | 0.48              |
| 11:A9:132:ARG:NH1 | 58:A9:501:NDP:O2X  | 2.47                     | 0.48              |
| 14:A2:19:ILE:HD13 | 14:A2:91:MET:HE1   | 1.95                     | 0.48              |
| 21:a1:14:VAL:HA   | 21:a1:17:VAL:HG12  | 1.96                     | 0.48              |
| 53:S1:296:GLY:O   | 53:S1:572:HIS:NE2  | 2.42                     | 0.48              |
| 54:S7:146:ARG:NH1 | 54:S7:184:ILE:O    | 2.46                     | 0.48              |
| 53:s1:419:ARG:NH1 | 53:s1:439:THR:O    | 2.47                     | 0.48              |
| 55:s8:90:LYS:NZ   | 55:s8:174:GLU:OE2  | 2.47                     | 0.48              |
| 3:S2:137:ASP:OD1  | 3:S2:137:ASP:N     | 2.46                     | 0.47              |
| 5:6:129:ASP:HB3   | 5:6:135:LEU:HD21   | 1.96                     | 0.47              |
| 36:BL:140:GLN:HG2 | 36:BL:144:LEU:HD22 | 1.96                     | 0.47              |
| 4:1a:281:ARG:NE   | 4:1a:284:GLN:OE1   | 2.43                     | 0.47              |
| 7:5a:460:GLY:O    | 7:5a:464:ALA:CB    | 2.62                     | 0.47              |
| 18:a8:149:GLU:OE2 | 25:s5:51:ARG:NH1   | 2.47                     | 0.47              |
| 41:3B:155:ARG:NH1 | 41:3B:200:ILE:O    | 2.47                     | 0.47              |
| 3:S2:216:ARG:HE   | 3:S2:240:LEU:HD13  | 1.78                     | 0.47              |
| 5:6:25:PRO:HG3    | 6:4L:28:SER:HB2    | 1.95                     | 0.47              |
| 8:4:375:LEU:O     | 8:4:379:LEU:HB2    | 2.14                     | 0.47              |
| 9:2:120:GLN:O     | 9:2:176:ARG:NH1    | 2.46                     | 0.47              |
| 9:2:307:THR:OG1   | 9:2:308:ASN:N      | 2.47                     | 0.47              |
| 11:A9:117:ARG:O   | 11:A9:121:GLN:HB3  | 2.14                     | 0.47              |
| 13:S6:75:ARG:NH1  | 13:S6:96:ASP:OD2   | 2.48                     | 0.47              |
| 14:A2:20:ARG:HB3  | 14:A2:66:TRP:O     | 2.15                     | 0.47              |
| 8:4a:310:MET:HE3  | 8:4a:310:MET:HB3   | 1.79                     | 0.47              |
| 9:2a:155:LEU:HD23 | 9:2a:278:MET:HG2   | 1.96                     | 0.47              |
| 26:b1:42:MET:O    | 36:bl:69:ARG:NH1   | 2.46                     | 0.47              |
| 35:b7:56:ARG:NH2  | 36:bl:120:ASN:OD1  | 2.48                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:3A:74:TRP:HB2   | 40:3A:230:VAL:HG22 | 1.97                     | 0.47              |
| 41:3M:60:ARG:NH2   | 41:3M:122:THR:OG1  | 2.47                     | 0.47              |
| 53:S1:497:VAL:HA   | 53:S1:500:ILE:HB   | 1.96                     | 0.47              |
| 54:S7:164:CYS:HA   | 54:S7:169:GLY:H    | 1.78                     | 0.47              |
| 55:s8:140:ARG:O    | 55:s8:141:ARG:NH1  | 2.44                     | 0.47              |
| 5:6:123:TRP:HH2    | 20:AO:123:GLU:HG3  | 1.79                     | 0.47              |
| 8:4:221:VAL:O      | 8:4:340:ARG:NH1    | 2.48                     | 0.47              |
| 11:A9:280:ILE:HG23 | 11:A9:353:LEU:HD11 | 1.95                     | 0.47              |
| 14:A2:19:ILE:HD12  | 14:A2:53:ILE:HB    | 1.95                     | 0.47              |
| 39:V3:94:GLN:HB3   | 52:V2:70:PRO:HA    | 1.96                     | 0.47              |
| 8:4a:159:PRO:HG3   | 9:2a:284:MET:HE1   | 1.97                     | 0.47              |
| 27:bm:138:ASN:HB3  | 36:bl:159:GLN:HE21 | 1.79                     | 0.47              |
| 45:3Q:68:ASP:OD2   | 45:3Q:72:ARG:NH1   | 2.47                     | 0.47              |
| 51:V1:160:GLY:O    | 51:V1:199:ARG:NH2  | 2.48                     | 0.47              |
| 51:V1:410:ASP:OD1  | 51:V1:410:ASP:N    | 2.39                     | 0.47              |
| 53:s1:197:THR:HG22 | 53:s1:206:VAL:HG22 | 1.96                     | 0.47              |
| 53:s1:336:ASN:O    | 53:s1:365:ASN:ND2  | 2.47                     | 0.47              |
| 2:S3:133:SER:HG    | 2:S3:138:SER:H     | 1.60                     | 0.47              |
| 3:S2:443:MET:H     | 3:S2:446:ASP:HB2   | 1.79                     | 0.47              |
| 5:6:78:TYR:HB3     | 11:A9:360:ARG:HD2  | 1.97                     | 0.47              |
| 7:5:304:PHE:HZ     | 7:5:526:LEU:HD13   | 1.80                     | 0.47              |
| 10:AL:342:GLY:O    | 10:AL:355:LYS:NZ   | 2.45                     | 0.47              |
| 15:AB:136:GLU:OE1  | 15:AB:137:LYS:NZ   | 2.46                     | 0.47              |
| 36:BL:164:LEU:HD23 | 36:BL:167:ARG:HE   | 1.79                     | 0.47              |
| 2:s3:149:LEU:HG    | 17:a6:80:ARG:HH21  | 1.80                     | 0.47              |
| 4:1a:317:TYR:O     | 21:a1:40:ARG:NH1   | 2.44                     | 0.47              |
| 7:5a:136:ASN:HA    | 7:5a:197:GLU:HA    | 1.96                     | 0.47              |
| 9:2a:108:LEU:HD23  | 9:2a:187:MET:HB3   | 1.96                     | 0.47              |
| 11:a9:270:ARG:NH2  | 11:a9:328:MET:SD   | 2.82                     | 0.47              |
| 40:3A:165:ARG:NH2  | 40:3A:211:LEU:O    | 2.48                     | 0.47              |
| 43:3O:291:LYS:O    | 43:3O:295:MET:HB2  | 2.15                     | 0.47              |
| 52:V2:134:CYS:SG   | 52:V2:135:THR:N    | 2.87                     | 0.47              |
| 2:S3:208:GLU:OE1   | 54:S7:183:ARG:NH2  | 2.47                     | 0.47              |
| 28:B5:175:GLU:HG3  | 28:B5:177:GLU:H    | 1.78                     | 0.47              |
| 32:B8:38:PRO:HD3   | 33:B4:67:ARG:HG2   | 1.96                     | 0.47              |
| 33:B4:30:ARG:HG3   | 40:3A:261:ALA:HB2  | 1.97                     | 0.47              |
| 38:A7:9:GLN:OE1    | 38:A7:12:ARG:NH2   | 2.47                     | 0.47              |
| 1:3a:28:ASN:O      | 1:3a:33:LYS:NZ     | 2.43                     | 0.47              |
| 3:s2:117:HIS:ND1   | 3:s2:462:ASP:O     | 2.47                     | 0.47              |
| 29:b6:19:ARG:HH21  | 34:b9:173:ARG:HE   | 1.63                     | 0.47              |
| 29:b6:122:ASP:OD1  | 29:b6:122:ASP:N    | 2.45                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:3C:40:CYS:HA    | 42:3C:43:VAL:HG12  | 1.97                     | 0.47              |
| 47:3H:31:VAL:HA    | 47:3H:34:HIS:HB3   | 1.96                     | 0.47              |
| 40:3L:316:CYS:O    | 41:3M:157:GLN:NE2  | 2.47                     | 0.47              |
| 41:3M:50:ALA:HB3   | 41:3M:221:VAL:HG12 | 1.97                     | 0.47              |
| 51:V1:266:GLY:N    | 51:V1:291:GLU:OE2  | 2.48                     | 0.47              |
| 53:S1:64:CYS:SG    | 53:S1:65:TYR:N     | 2.88                     | 0.47              |
| 53:S1:388:ASN:ND2  | 53:S1:513:MET:O    | 2.43                     | 0.47              |
| 51:v1:54:LYS:O     | 51:v1:58:ARG:NH1   | 2.47                     | 0.47              |
| 51:v1:126:LYS:NZ   | 51:v1:351:THR:O    | 2.44                     | 0.47              |
| 1:3:58:VAL:HA      | 1:3:61:THR:HG22    | 1.97                     | 0.47              |
| 4:1:294:LEU:HA     | 4:1:297:THR:HG22   | 1.96                     | 0.47              |
| 9:2:119:THR:HG22   | 9:2:176:ARG:HB3    | 1.95                     | 0.47              |
| 18:A8:144:SER:OG   | 18:A8:145:ARG:N    | 2.47                     | 0.47              |
| 19:AM:85:ASP:OD1   | 19:AM:85:ASP:N     | 2.45                     | 0.47              |
| 37:AN:82:ASP:N     | 37:AN:82:ASP:OD1   | 2.47                     | 0.47              |
| 7:5a:482:MET:HB3   | 7:5a:486:LEU:HB3   | 1.96                     | 0.47              |
| 8:4a:102:LEU:HD13  | 8:4a:128:PRO:HB2   | 1.96                     | 0.47              |
| 10:a1:272:ASP:OD2  | 16:a5:30:LYS:NZ    | 2.47                     | 0.47              |
| 30:b2:97:LEU:HD11  | 35:b7:100:LYS:HG3  | 1.97                     | 0.47              |
| 36:bl:159:GLN:HG2  | 36:bl:162:ARG:HH21 | 1.80                     | 0.47              |
| 40:3A:122:ALA:H    | 41:3B:300:LYS:HD2  | 1.78                     | 0.47              |
| 43:3O:104:SER:OG   | 43:3O:105:LEU:N    | 2.46                     | 0.47              |
| 51:V1:225:LEU:HB3  | 51:V1:227:PRO:HD2  | 1.96                     | 0.47              |
| 54:S7:87:ARG:HB2   | 54:S7:209:GLN:HG3  | 1.97                     | 0.47              |
| 1:3:52:SER:OG      | 1:3:54:LYS:NZ      | 2.47                     | 0.47              |
| 1:3:60:ILE:HG23    | 6:4L:72:ALA:HB1    | 1.95                     | 0.47              |
| 3:S2:220:ALA:HB2   | 55:S8:98:ARG:HE    | 1.79                     | 0.47              |
| 4:1:67:SER:O       | 4:1:71:PHE:HB2     | 2.14                     | 0.47              |
| 4:1:80:THR:O       | 4:1:84:SER:HB3     | 2.15                     | 0.47              |
| 11:A9:104:THR:HG21 | 13:S6:46:VAL:HG13  | 1.96                     | 0.47              |
| 12:S4:60:ASP:HB2   | 12:S4:62:THR:HG23  | 1.95                     | 0.47              |
| 29:B6:108:ASP:OD2  | 35:B7:71:ARG:NH2   | 2.47                     | 0.47              |
| 35:B7:69:CYS:O     | 35:B7:73:SER:HB2   | 2.14                     | 0.47              |
| 37:AN:82:ASP:HB2   | 54:S7:203:TYR:HE1  | 1.80                     | 0.47              |
| 39:V3:72:HIS:NE2   | 52:V2:215:PRO:O    | 2.48                     | 0.47              |
| 4:1a:191:ALA:HB2   | 4:1a:198:PHE:HD2   | 1.80                     | 0.47              |
| 12:s4:81:VAL:HG21  | 12:s4:150:LYS:HD3  | 1.95                     | 0.47              |
| 25:s5:7:GLN:HE21   | 25:s5:14:LEU:HD12  | 1.80                     | 0.47              |
| 28:b5:89:VAL:HG22  | 28:b5:116:PRO:HG2  | 1.97                     | 0.47              |
| 32:b8:110:ASP:OD1  | 32:b8:110:ASP:N    | 2.45                     | 0.47              |
| 40:3A:392:LYS:HG2  | 40:3A:433:ILE:HG23 | 1.97                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:3B:216:ALA:HB3  | 41:3B:244:LEU:HA   | 1.96                     | 0.47              |
| 41:3M:109:LYS:HG2  | 41:3M:124:GLU:HG2  | 1.97                     | 0.47              |
| 46:3R:25:ARG:HH11  | 46:3R:26:ALA:H     | 1.61                     | 0.47              |
| 53:S1:123:ASN:HD22 | 53:S1:157:LYS:HA   | 1.79                     | 0.47              |
| 53:s1:426:ASP:OD1  | 53:s1:426:ASP:N    | 2.46                     | 0.47              |
| 32:B8:67:ASP:O     | 33:B4:81:ARG:NH2   | 2.48                     | 0.47              |
| 7:5a:538:PRO:O     | 7:5a:542:LEU:HB2   | 2.15                     | 0.47              |
| 8:4a:326:LEU:HA    | 8:4a:329:LEU:HD22  | 1.97                     | 0.47              |
| 13:s6:32:THR:HG22  | 13:s6:55:VAL:HG22  | 1.96                     | 0.47              |
| 32:b8:38:PRO:HD3   | 33:b4:67:ARG:HG2   | 1.95                     | 0.47              |
| 42:3C:39:VAL:HG11  | 42:3C:232:ILE:HG12 | 1.96                     | 0.47              |
| 40:3L:367:ASP:OD1  | 40:3L:367:ASP:N    | 2.48                     | 0.47              |
| 45:3Q:30:LEU:HD21  | 45:3Q:70:THR:HG23  | 1.97                     | 0.47              |
| 53:S1:546:PHE:HB2  | 53:S1:567:VAL:HG22 | 1.96                     | 0.47              |
| 53:s1:693:ASP:OD1  | 53:s1:693:ASP:N    | 2.45                     | 0.47              |
| 11:A9:357:ARG:NH2  | 11:A9:364:SER:O    | 2.48                     | 0.47              |
| 24:C2:97:HIS:HB3   | 24:C2:100:ASP:HB2  | 1.96                     | 0.47              |
| 3:s2:236:LEU:HD13  | 3:s2:240:LEU:HD23  | 1.97                     | 0.47              |
| 7:5a:60:GLU:OE2    | 7:5a:81:LYS:NZ     | 2.48                     | 0.47              |
| 7:5a:204:SER:HB3   | 7:5a:266:LEU:HD11  | 1.97                     | 0.47              |
| 9:2a:210:ILE:HD12  | 9:2a:329:LEU:HD22  | 1.95                     | 0.47              |
| 12:s4:50:THR:OG1   | 12:s4:51:GLN:N     | 2.46                     | 0.47              |
| 40:3A:446:SER:O    | 48:3J:16:ARG:NH2   | 2.45                     | 0.47              |
| 42:3C:296:LEU:O    | 42:3C:300:ILE:HB   | 2.15                     | 0.47              |
| 42:3N:240:MET:HA   | 42:3N:243:VAL:HG12 | 1.96                     | 0.47              |
| 4:1:199:ASP:OD1    | 4:1:279:ARG:NH1    | 2.48                     | 0.47              |
| 11:A9:226:VAL:HG11 | 11:A9:277:VAL:HG11 | 1.97                     | 0.47              |
| 13:S6:21:GLY:N     | 13:S6:62:ASP:OD2   | 2.48                     | 0.47              |
| 13:S6:106:TYR:O    | 55:S8:141:ARG:NH2  | 2.48                     | 0.47              |
| 17:A6:120:ASP:OD1  | 17:A6:120:ASP:N    | 2.45                     | 0.47              |
| 32:B8:86:ARG:NH1   | 32:B8:99:MET:SD    | 2.81                     | 0.47              |
| 3:s2:120:THR:HG21  | 3:s2:139:LEU:HD21  | 1.97                     | 0.47              |
| 4:1a:75:PRO:HG2    | 4:1a:219:PRO:HB3   | 1.97                     | 0.47              |
| 6:4l:78:LEU:HA     | 6:4l:81:VAL:HG12   | 1.97                     | 0.47              |
| 7:5a:386:LEU:HD21  | 30:b2:65:MET:HE2   | 1.96                     | 0.47              |
| 7:5a:553:LEU:HA    | 7:5a:557:TRP:HB2   | 1.96                     | 0.47              |
| 25:s5:47:ILE:HG13  | 25:s5:51:ARG:HB3   | 1.97                     | 0.47              |
| 42:3C:304:MET:HE1  | 42:3C:362:ILE:HD12 | 1.95                     | 0.47              |
| 51:V1:374:TYR:O    | 51:V1:378:SER:HB3  | 2.15                     | 0.47              |
| 53:S1:308:ARG:NH1  | 53:S1:312:GLY:O    | 2.48                     | 0.47              |
| 51:v1:209:GLU:HA   | 51:v1:242:VAL:HG11 | 1.96                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:3:75:LEU:HA      | 1:3:78:ALA:HB3     | 1.96                     | 0.46              |
| 4:1:85:LEU:HB2     | 4:1:233:LEU:HD21   | 1.95                     | 0.46              |
| 7:5:398:ALA:HA     | 7:5:401:THR:HG22   | 1.97                     | 0.46              |
| 15:AC:115:GLN:NE2  | 15:AC:138:LEU:O    | 2.47                     | 0.46              |
| 24:C2:120:ARG:O    | 33:B4:109:ARG:NH1  | 2.46                     | 0.46              |
| 27:BM:127:ARG:HD3  | 27:BM:132:LEU:HB3  | 1.96                     | 0.46              |
| 28:B5:145:GLU:HA   | 28:B5:148:GLU:HG2  | 1.95                     | 0.46              |
| 28:B5:180:ASP:OD1  | 28:B5:180:ASP:N    | 2.42                     | 0.46              |
| 2:s3:234:LEU:HD12  | 3:s2:418:ARG:HH11  | 1.80                     | 0.46              |
| 3:s2:224:ALA:O     | 55:s8:98:ARG:NH2   | 2.46                     | 0.46              |
| 4:1a:59:GLU:HB3    | 54:s7:153:PRO:HB2  | 1.97                     | 0.46              |
| 7:5a:62:MET:HB3    | 36:bl:115:GLN:HG2  | 1.96                     | 0.46              |
| 8:4a:119:TYR:HE1   | 8:4a:157:SER:HB2   | 1.80                     | 0.46              |
| 8:4a:345:ALA:HB1   | 8:4a:348:LEU:HD11  | 1.97                     | 0.46              |
| 18:a8:47:ARG:HH21  | 28:b5:187:PRO:HB2  | 1.81                     | 0.46              |
| 24:c2:44:MET:HA    | 24:c2:47:MET:HG2   | 1.97                     | 0.46              |
| 40:3L:37:THR:OG1   | 40:3L:38:PHE:N     | 2.47                     | 0.46              |
| 43:3O:215:LEU:HB3  | 43:3O:248:ILE:HD11 | 1.97                     | 0.46              |
| 54:S7:112:TYR:HD2  | 54:S7:198:ALA:HB3  | 1.80                     | 0.46              |
| 55:s8:189:LYS:O    | 55:s8:193:ASN:HB2  | 2.15                     | 0.46              |
| 3:S2:185:MET:SD    | 3:S2:189:THR:OG1   | 2.73                     | 0.46              |
| 7:5:82:THR:HA      | 7:5:86:SER:HB3     | 1.96                     | 0.46              |
| 7:5:161:ARG:NH1    | 34:B9:89:THR:O     | 2.48                     | 0.46              |
| 8:4:118:PHE:O      | 8:4:122:PHE:CB     | 2.63                     | 0.46              |
| 9:2:106:LEU:HG     | 9:2:138:PRO:HB2    | 1.97                     | 0.46              |
| 1:3a:97:ILE:HA     | 1:3a:100:LEU:HB2   | 1.97                     | 0.46              |
| 2:s3:72:VAL:HA     | 2:s3:87:ILE:HG22   | 1.96                     | 0.46              |
| 4:1a:27:ILE:HD11   | 55:s8:77:LEU:HD13  | 1.96                     | 0.46              |
| 14:a2:18:GLU:OE2   | 14:a2:20:ARG:NH1   | 2.48                     | 0.46              |
| 15:ab:115:GLN:NE2  | 15:ab:138:LEU:O    | 2.47                     | 0.46              |
| 42:3C:33:PHE:HA    | 42:3C:36:LEU:HB2   | 1.97                     | 0.46              |
| 40:3L:411:GLU:O    | 40:3L:415:ARG:HB2  | 2.15                     | 0.46              |
| 53:S1:266:ARG:HH12 | 55:S8:117:LYS:HE2  | 1.80                     | 0.46              |
| 54:S7:182:ASP:OD1  | 54:S7:182:ASP:N    | 2.45                     | 0.46              |
| 53:s1:319:TRP:HE1  | 53:s1:615:LEU:HB3  | 1.80                     | 0.46              |
| 7:5:222:GLY:HA2    | 7:5:229:LEU:HD22   | 1.97                     | 0.46              |
| 24:C2:42:GLY:O     | 24:C2:46:ASN:ND2   | 2.47                     | 0.46              |
| 35:B7:15:VAL:HG12  | 35:B7:113:LYS:HG3  | 1.97                     | 0.46              |
| 2:s3:57:LEU:HB3    | 2:s3:83:LEU:HD21   | 1.96                     | 0.46              |
| 4:1a:315:PRO:HG3   | 20:ao:54:ASN:HD21  | 1.79                     | 0.46              |
| 8:4a:231:LEU:HA    | 8:4a:235:LEU:HB2   | 1.97                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:2a:42:PRO:HA     | 9:2a:45:ILE:HG22   | 1.96                     | 0.46              |
| 32:b8:169:GLU:OE1  | 35:b7:56:ARG:NH1   | 2.48                     | 0.46              |
| 40:3L:226:ALA:HA   | 40:3L:229:MET:HB2  | 1.97                     | 0.46              |
| 42:3N:14:ILE:O     | 42:3N:18:PHE:HB2   | 2.15                     | 0.46              |
| 49:3V:45:VAL:HG12  | 49:3V:47:TYR:H     | 1.81                     | 0.46              |
| 51:V1:48:ARG:NH1   | 52:V2:225:GLU:OE2  | 2.49                     | 0.46              |
| 53:s1:261:ILE:HG23 | 53:s1:273:ILE:HG23 | 1.97                     | 0.46              |
| 53:s1:588:ALA:H    | 53:s1:591:GLU:HB2  | 1.80                     | 0.46              |
| 3:S2:174:PHE:O     | 3:S2:178:THR:OG1   | 2.31                     | 0.46              |
| 11:A9:69:VAL:O     | 11:A9:73:LEU:HB2   | 2.16                     | 0.46              |
| 18:A8:7:LEU:HD23   | 20:AO:91:LEU:HD13  | 1.97                     | 0.46              |
| 3:s2:290:GLY:HA3   | 3:s2:405:GLY:HA2   | 1.97                     | 0.46              |
| 17:a6:55:LEU:HD13  | 17:a6:57:ILE:HD11  | 1.98                     | 0.46              |
| 18:a8:53:PRO:HB3   | 20:ao:80:ASP:HB2   | 1.96                     | 0.46              |
| 51:V1:101:PHE:O    | 51:V1:104:LYS:NZ   | 2.48                     | 0.46              |
| 53:S1:59:GLN:OE1   | 53:S1:62:ARG:NH1   | 2.43                     | 0.46              |
| 53:s1:86:PRO:O     | 53:s1:108:LYS:NZ   | 2.48                     | 0.46              |
| 55:s8:74:LEU:HD12  | 55:s8:77:LEU:HD21  | 1.96                     | 0.46              |
| 3:S2:317:ASP:OD2   | 3:S2:342:ARG:NH2   | 2.48                     | 0.46              |
| 4:1:164:THR:HA     | 4:1:167:THR:HG22   | 1.96                     | 0.46              |
| 18:A8:144:SER:OG   | 18:A8:147:ARG:NH2  | 2.49                     | 0.46              |
| 2:s3:154:SER:HB3   | 2:s3:177:PHE:HB3   | 1.98                     | 0.46              |
| 3:s2:184:ILE:HG23  | 3:s2:203:MET:HB3   | 1.98                     | 0.46              |
| 5:6a:81:THR:H      | 5:6a:84:SER:HB2    | 1.80                     | 0.46              |
| 7:5a:97:THR:HG21   | 7:5a:125:LEU:HD22  | 1.96                     | 0.46              |
| 7:5a:357:ARG:HG2   | 34:b9:32:ILE:HG23  | 1.98                     | 0.46              |
| 9:2a:115:LEU:HA    | 9:2a:118:VAL:HG12  | 1.96                     | 0.46              |
| 13:s6:31:ILE:HG12  | 13:s6:37:VAL:HB    | 1.98                     | 0.46              |
| 25:s5:33:CYS:HB3   | 25:s5:36:PHE:HB2   | 1.98                     | 0.46              |
| 45:3F:46:GLU:OE2   | 45:3F:49:ARG:NH1   | 2.49                     | 0.46              |
| 53:s1:134:GLY:HA3  | 53:s1:241:ARG:HD2  | 1.96                     | 0.46              |
| 54:s7:158:VAL:HB   | 54:s7:187:VAL:HA   | 1.98                     | 0.46              |
| 2:S3:218:VAL:O     | 17:A6:104:THR:OG1  | 2.33                     | 0.46              |
| 3:S2:458:PHE:HA    | 3:S2:461:ILE:HG12  | 1.97                     | 0.46              |
| 36:BL:79:GLU:HA    | 36:BL:85:ILE:HD11  | 1.98                     | 0.46              |
| 3:s2:254:ARG:NE    | 55:s8:76:TYR:OH    | 2.48                     | 0.46              |
| 5:6a:155:ALA:HB1   | 6:4l:65:VAL:HG11   | 1.96                     | 0.46              |
| 8:4a:109:THR:OG1   | 8:4a:121:LEU:O     | 2.34                     | 0.46              |
| 10:al:200:PRO:HG2  | 10:al:282:PRO:HG2  | 1.98                     | 0.46              |
| 11:a9:70:VAL:HG12  | 11:a9:97:MET:HG3   | 1.98                     | 0.46              |
| 28:b5:155:GLU:HB2  | 28:b5:158:ARG:HH21 | 1.79                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:3A:303:THR:HA   | 40:3A:306:VAL:HG12 | 1.98                     | 0.46              |
| 43:3D:210:TYR:O    | 43:3D:214:LEU:HB2  | 2.15                     | 0.46              |
| 42:3N:125:ALA:O    | 42:3N:129:MET:HB2  | 2.16                     | 0.46              |
| 51:v1:369:ARG:HE   | 52:v2:136:THR:HA   | 1.81                     | 0.46              |
| 53:s1:401:LEU:HA   | 53:s1:430:ALA:O    | 2.16                     | 0.46              |
| 4:1:284:GLN:HA     | 4:1:287:HIS:HB2    | 1.98                     | 0.46              |
| 5:6:161:ALA:O      | 5:6:165:ILE:HB     | 2.16                     | 0.46              |
| 6:4L:27:MET:HE2    | 6:4L:78:LEU:HD13   | 1.97                     | 0.46              |
| 7:5:75:GLU:HG3     | 7:5:77:LYS:HD3     | 1.98                     | 0.46              |
| 7:5:172:ILE:O      | 7:5:176:ARG:HB2    | 2.15                     | 0.46              |
| 8:4:315:LEU:O      | 8:4:319:HIS:HB3    | 2.15                     | 0.46              |
| 10:AL:87:PRO:O     | 10:AL:142:GLN:NE2  | 2.42                     | 0.46              |
| 4:1a:149:ILE:HG21  | 4:1a:185:TRP:HB2   | 1.98                     | 0.46              |
| 4:1a:189:THR:OG1   | 4:1a:234:MET:SD    | 2.70                     | 0.46              |
| 4:1a:260:MET:HE3   | 4:1a:264:LEU:HB3   | 1.97                     | 0.46              |
| 7:5a:237:MET:HE1   | 7:5a:248:HIS:HB2   | 1.98                     | 0.46              |
| 15:ac:81:ASP:O     | 15:ac:85:TYR:HB2   | 2.15                     | 0.46              |
| 20:ao:82:ARG:NH2   | 21:a1:46:TYR:OH    | 2.48                     | 0.46              |
| 27:bm:93:PHE:HD2   | 28:b5:75:LEU:HD13  | 1.81                     | 0.46              |
| 45:3F:41:THR:OG1   | 45:3F:42:GLU:N     | 2.47                     | 0.46              |
| 42:3N:163:TRP:O    | 42:3N:177:ARG:NH1  | 2.48                     | 0.46              |
| 43:3O:308:ARG:O    | 43:3O:312:SER:HB2  | 2.15                     | 0.46              |
| 53:s1:546:PHE:HB2  | 53:s1:567:VAL:HG22 | 1.98                     | 0.46              |
| 2:S3:212:ASP:OD2   | 11:A9:75:ARG:NH1   | 2.49                     | 0.46              |
| 7:5:319:MET:HB2    | 7:5:319:MET:HE3    | 1.75                     | 0.46              |
| 12:S4:158:LYS:HA   | 12:S4:158:LYS:HD3  | 1.76                     | 0.46              |
| 13:S6:51:ARG:HD3   | 37:AN:129:VAL:HG11 | 1.98                     | 0.46              |
| 32:B8:110:ASP:OD1  | 32:B8:110:ASP:N    | 2.47                     | 0.46              |
| 37:AN:135:ARG:NH2  | 55:S8:133:GLU:OE1  | 2.48                     | 0.46              |
| 1:3a:33:LYS:HG2    | 4:1a:61:MET:HE1    | 1.97                     | 0.46              |
| 13:s6:39:ASP:O     | 13:s6:45:ARG:NH1   | 2.49                     | 0.46              |
| 16:a5:5:LEU:O      | 16:a5:7:LYS:NZ     | 2.48                     | 0.46              |
| 24:c2:120:ARG:NH1  | 33:b4:113:GLU:OE1  | 2.49                     | 0.46              |
| 28:b5:145:GLU:O    | 28:b5:149:LEU:HB2  | 2.16                     | 0.46              |
| 32:b8:105:ILE:HG23 | 32:b8:109:LEU:HD22 | 1.96                     | 0.46              |
| 37:an:20:GLY:HA3   | 37:an:39:ILE:HG13  | 1.96                     | 0.46              |
| 40:3A:88:GLY:O     | 40:3A:92:PHE:HB2   | 2.15                     | 0.46              |
| 40:3A:292:GLU:HA   | 40:3A:352:GLY:O    | 2.16                     | 0.46              |
| 41:3B:90:THR:HG23  | 41:3B:145:GLU:HB2  | 1.97                     | 0.46              |
| 40:3L:193:GLN:O    | 40:3L:269:ARG:NH2  | 2.44                     | 0.46              |
| 40:3L:400:VAL:HG21 | 41:3M:57:PRO:HB2   | 1.98                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:3N:71:ARG:HG3   | 43:3O:280:PRO:HG2  | 1.98                     | 0.46              |
| 52:V2:152:GLN:NE2  | 52:V2:158:LYS:O    | 2.49                     | 0.46              |
| 55:S8:204:ASN:O    | 55:S8:208:ASP:HB2  | 2.15                     | 0.46              |
| 3:S2:80:MET:HE2    | 3:S2:80:MET:HB3    | 1.78                     | 0.46              |
| 4:1:312:ALA:O      | 20:AO:55:GLN:NE2   | 2.49                     | 0.46              |
| 8:4:277:LEU:HD21   | 8:4:405:MET:HB3    | 1.98                     | 0.46              |
| 15:AC:85:TYR:OH    | 31:B3:28:TRP:NE1   | 2.43                     | 0.46              |
| 15:AC:153:ASP:OD2  | 29:B6:19:ARG:NH2   | 2.48                     | 0.46              |
| 16:A5:38:PHE:O     | 16:A5:45:ARG:NH2   | 2.49                     | 0.46              |
| 25:S5:66:CYS:HA    | 25:S5:69:ARG:HE    | 1.80                     | 0.46              |
| 2:s3:125:PHE:HB2   | 2:s3:146:ALA:HB3   | 1.98                     | 0.46              |
| 3:s2:315:GLU:O     | 3:s2:342:ARG:NH2   | 2.48                     | 0.46              |
| 4:1a:289:LEU:O     | 4:1a:294:LEU:N     | 2.49                     | 0.46              |
| 30:b2:78:ASP:HB3   | 30:b2:83:HIS:HA    | 1.98                     | 0.46              |
| 46:3G:51:PRO:HA    | 46:3G:54:VAL:HB    | 1.97                     | 0.46              |
| 51:V1:325:PRO:HG2  | 51:V1:347:THR:HA   | 1.98                     | 0.46              |
| 53:S1:142:GLN:O    | 53:S1:146:PHE:HB2  | 2.16                     | 0.46              |
| 53:S1:333:PHE:HD2  | 53:S1:544:MET:HB2  | 1.81                     | 0.46              |
| 53:S1:572:HIS:O    | 53:S1:699:SER:OG   | 2.34                     | 0.46              |
| 51:v1:159:ARG:NH2  | 52:v2:175:CYS:O    | 2.49                     | 0.46              |
| 53:s1:292:PHE:HB3  | 53:s1:706:THR:HG21 | 1.98                     | 0.46              |
| 53:s1:390:THR:HG22 | 53:s1:659:ILE:HD13 | 1.98                     | 0.46              |
| 3:S2:358:VAL:HG12  | 3:S2:364:SER:HB3   | 1.96                     | 0.46              |
| 9:2:207:ILE:O      | 9:2:211:LEU:HB2    | 2.16                     | 0.46              |
| 11:A9:188:GLU:OE2  | 11:A9:202:ARG:NE   | 2.45                     | 0.46              |
| 2:s3:148:GLU:HG2   | 2:s3:149:LEU:HD22  | 1.97                     | 0.46              |
| 3:s2:432:LEU:HD22  | 3:s2:456:ILE:HG21  | 1.98                     | 0.46              |
| 4:1a:311:THR:OG1   | 20:ao:51:MET:SD    | 2.66                     | 0.46              |
| 5:6a:150:TRP:HE1   | 9:2a:19:ILE:HD11   | 1.81                     | 0.46              |
| 8:4a:76:MET:HE1    | 8:4a:230:ILE:HD13  | 1.98                     | 0.46              |
| 36:bl:4:SER:OG     | 36:bl:5:TRP:N      | 2.49                     | 0.46              |
| 42:3C:248:ASP:N    | 42:3C:248:ASP:OD1  | 2.47                     | 0.46              |
| 42:3N:33:PHE:HA    | 42:3N:36:LEU:HB2   | 1.98                     | 0.46              |
| 54:s7:163:SER:OG   | 64:s7:301:SF4:S3   | 2.70                     | 0.46              |
| 55:s8:168:VAL:HG21 | 55:s8:201:ILE:HG21 | 1.98                     | 0.46              |
| 3:S2:196:ALA:HB2   | 4:1:278:PRO:HB3    | 1.98                     | 0.45              |
| 3:S2:383:LYS:NZ    | 53:S1:141:ASP:OD1  | 2.43                     | 0.45              |
| 7:5:297:ASP:HB2    | 7:5:300:LYS:HB2    | 1.96                     | 0.45              |
| 11:A9:248:GLY:HA3  | 11:A9:265:PHE:HZ   | 1.81                     | 0.45              |
| 12:S4:50:THR:OG1   | 12:S4:51:GLN:N     | 2.47                     | 0.45              |
| 36:BL:56:HIS:O     | 36:BL:60:ARG:HB2   | 2.16                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:s2:80:MET:N      | 3:s2:80:MET:SD     | 2.89                     | 0.45              |
| 7:5a:393:ASP:O     | 7:5a:397:GLU:HB2   | 2.17                     | 0.45              |
| 32:b8:83:GLN:HE22  | 32:b8:86:ARG:HH21  | 1.64                     | 0.45              |
| 40:3A:113:VAL:HG11 | 40:3A:120:LEU:HD11 | 1.97                     | 0.45              |
| 40:3A:426:LEU:HA   | 40:3A:429:TRP:HB2  | 1.97                     | 0.45              |
| 41:3M:322:ASP:HB2  | 50:3T:55:LEU:HB3   | 1.98                     | 0.45              |
| 42:3N:359:PHE:HA   | 42:3N:362:ILE:HG22 | 1.98                     | 0.45              |
| 51:v1:325:PRO:HD3  | 51:v1:433:TRP:HB3  | 1.98                     | 0.45              |
| 53:s1:220:GLY:HA3  | 53:s1:291:ARG:HD3  | 1.98                     | 0.45              |
| 53:s1:266:ARG:HD2  | 53:s1:267:THR:HG23 | 1.98                     | 0.45              |
| 3:S2:185:MET:O     | 3:S2:189:THR:OG1   | 2.34                     | 0.45              |
| 36:BL:92:TRP:HH2   | 36:BL:150:TYR:HB2  | 1.81                     | 0.45              |
| 1:3a:80:GLN:OE1    | 20:ao:58:ARG:NH1   | 2.48                     | 0.45              |
| 3:s2:271:ARG:HD3   | 4:1a:284:GLN:HE22  | 1.82                     | 0.45              |
| 3:s2:404:LYS:HZ1   | 3:s2:457:VAL:HG22  | 1.80                     | 0.45              |
| 4:1a:105:ILE:HG21  | 4:1a:237:LEU:HD11  | 1.98                     | 0.45              |
| 11:a9:136:THR:OG1  | 11:a9:137:ARG:N    | 2.50                     | 0.45              |
| 13:s6:88:HIS:HD2   | 13:s6:107:CYS:SG   | 2.28                     | 0.45              |
| 20:ao:69:ILE:HD11  | 22:a3:53:TYR:HA    | 1.97                     | 0.45              |
| 36:bl:66:ARG:HH11  | 36:bl:68:TYR:HE1   | 1.64                     | 0.45              |
| 47:3S:54:ARG:NH2   | 47:3S:63:GLU:OE1   | 2.47                     | 0.45              |
| 51:V1:119:GLU:OE2  | 51:V1:128:ARG:N    | 2.49                     | 0.45              |
| 53:s1:538:ARG:NH1  | 53:s1:559:ASP:OD2  | 2.49                     | 0.45              |
| 1:3:80:GLN:NE2     | 4:1:315:PRO:O      | 2.49                     | 0.45              |
| 3:S2:246:GLU:HG3   | 38:A7:30:GLU:HB3   | 1.98                     | 0.45              |
| 7:5:231:PRO:HB3    | 7:5:530:PRO:HG3    | 1.98                     | 0.45              |
| 17:A6:34:ARG:HG2   | 17:A6:86:VAL:HG11  | 1.98                     | 0.45              |
| 34:B9:31:CYS:HB3   | 34:B9:36:LYS:HB3   | 1.97                     | 0.45              |
| 2:s3:215:VAL:O     | 11:a9:209:ARG:NH2  | 2.49                     | 0.45              |
| 5:6a:78:TYR:HB3    | 11:a9:360:ARG:HD2  | 1.97                     | 0.45              |
| 7:5a:536:ILE:HD12  | 32:b8:126:TRP:HZ2  | 1.82                     | 0.45              |
| 11:a9:61:ALA:HA    | 11:a9:66:GLY:HA3   | 1.97                     | 0.45              |
| 11:a9:72:HIS:ND1   | 11:a9:246:SER:OG   | 2.50                     | 0.45              |
| 20:ao:48:TRP:HD1   | 20:ao:51:MET:HE3   | 1.80                     | 0.45              |
| 43:3D:109:SER:OG   | 43:3D:112:ARG:NH2  | 2.50                     | 0.45              |
| 41:3M:72:GLU:O     | 41:3M:188:ASN:ND2  | 2.50                     | 0.45              |
| 42:3N:145:VAL:HG21 | 42:3N:268:ILE:HG12 | 1.98                     | 0.45              |
| 42:3N:373:GLU:OE1  | 45:3Q:21:TYR:OH    | 2.32                     | 0.45              |
| 53:S1:74:ASN:OD1   | 53:S1:180:THR:OG1  | 2.33                     | 0.45              |
| 51:v1:250:VAL:HG13 | 51:v1:254:ILE:HD11 | 1.97                     | 0.45              |
| 51:v1:410:ASP:OD1  | 51:v1:410:ASP:N    | 2.50                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:5:492:ILE:O     | 7:5:496:LEU:HB2    | 2.16                     | 0.45              |
| 8:4:7:PRO:HB2     | 8:4:34:ILE:HD11    | 1.98                     | 0.45              |
| 13:S6:52:GLN:HG3  | 37:AN:127:GLN:H    | 1.81                     | 0.45              |
| 15:AC:120:MET:HE1 | 34:B9:21:LYS:HA    | 1.97                     | 0.45              |
| 31:B3:42:LEU:HD11 | 34:B9:42:CYS:HB2   | 1.97                     | 0.45              |
| 3:s2:174:PHE:O    | 3:s2:178:THR:OG1   | 2.31                     | 0.45              |
| 7:5a:367:PRO:O    | 7:5a:371:SER:HB3   | 2.16                     | 0.45              |
| 8:4a:104:ILE:O    | 8:4a:108:MET:HB2   | 2.17                     | 0.45              |
| 9:2a:298:TYR:O    | 9:2a:303:THR:OG1   | 2.31                     | 0.45              |
| 37:an:134:THR:HB  | 55:s8:144:ARG:HB2  | 1.98                     | 0.45              |
| 42:3C:165:TRP:O   | 42:3C:174:THR:OG1  | 2.34                     | 0.45              |
| 44:3E:118:THR:O   | 44:3E:122:THR:OG1  | 2.33                     | 0.45              |
| 40:3L:164:GLU:HA  | 40:3L:167:VAL:HB   | 1.98                     | 0.45              |
| 47:3S:64:ASP:OD1  | 47:3S:64:ASP:N     | 2.49                     | 0.45              |
| 54:S7:206:LEU:HB3 | 54:S7:210:ARG:HH21 | 1.80                     | 0.45              |
| 55:s8:49:ASP:N    | 55:s8:49:ASP:OD1   | 2.50                     | 0.45              |
| 7:5:539:MET:O     | 7:5:543:ASN:HB2    | 2.16                     | 0.45              |
| 16:A5:52:THR:O    | 16:A5:56:LEU:HB2   | 2.17                     | 0.45              |
| 34:B9:50:GLU:OE2  | 34:B9:59:ARG:NH2   | 2.49                     | 0.45              |
| 2:s3:172:MET:HA   | 2:s3:196:PRO:HD2   | 1.99                     | 0.45              |
| 11:a9:92:MET:HE2  | 54:s7:188:ASP:HA   | 1.99                     | 0.45              |
| 37:an:122:SER:OG  | 54:s7:207:GLN:OE1  | 2.33                     | 0.45              |
| 40:3L:58:ARG:O    | 40:3L:230:VAL:HA   | 2.17                     | 0.45              |
| 51:V1:109:ARG:NH1 | 51:V1:237:GLY:O    | 2.50                     | 0.45              |
| 53:S1:406:ASN:ND2 | 53:S1:688:GLN:O    | 2.48                     | 0.45              |
| 51:v1:123:GLY:O   | 51:v1:277:ASN:ND2  | 2.49                     | 0.45              |
| 53:s1:406:ASN:OD1 | 53:s1:406:ASN:N    | 2.49                     | 0.45              |
| 2:S3:216:LYS:HE2  | 11:A9:209:ARG:HD3  | 1.98                     | 0.45              |
| 3:S2:279:THR:HG23 | 16:A5:13:GLY:HA3   | 1.97                     | 0.45              |
| 8:4:187:ASP:OD1   | 8:4:192:ASN:ND2    | 2.49                     | 0.45              |
| 11:A9:48:ARG:NH2  | 11:A9:98:GLY:O     | 2.49                     | 0.45              |
| 20:AO:10:MET:HE2  | 20:AO:10:MET:HB3   | 1.83                     | 0.45              |
| 36:BL:34:THR:HA   | 36:BL:37:TYR:HB3   | 1.99                     | 0.45              |
| 3:s2:204:PHE:HE2  | 54:s7:105:MET:HB3  | 1.81                     | 0.45              |
| 5:6a:63:MET:HA    | 5:6a:66:VAL:HG12   | 1.98                     | 0.45              |
| 7:5a:101:MET:HE3  | 7:5a:101:MET:HB3   | 1.77                     | 0.45              |
| 12:s4:167:ASN:O   | 39:v3:99:ARG:NH1   | 2.49                     | 0.45              |
| 43:3D:98:HIS:NE2  | 43:3D:208:GLU:OE2  | 2.45                     | 0.45              |
| 46:3R:20:SER:O    | 46:3R:24:GLN:NE2   | 2.46                     | 0.45              |
| 54:S7:103:GLU:HA  | 54:S7:106:HIS:HB2  | 1.98                     | 0.45              |
| 53:s1:74:ASN:OD1  | 53:s1:180:THR:OG1  | 2.34                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:4:361:MET:HB3    | 8:4:441:MET:HE3    | 1.98                     | 0.45              |
| 8:4:431:THR:OG1    | 28:B5:66:ARG:NH1   | 2.48                     | 0.45              |
| 10:AL:282:PRO:O    | 10:AL:286:GLN:NE2  | 2.50                     | 0.45              |
| 13:S6:87:GLY:HA2   | 55:S8:112:ARG:HH12 | 1.82                     | 0.45              |
| 29:B6:101:LYS:HE2  | 29:B6:101:LYS:HB2  | 1.79                     | 0.45              |
| 37:AN:45:GLU:OE1   | 37:AN:51:LYS:NZ    | 2.49                     | 0.45              |
| 3:s2:263:THR:O     | 3:s2:327:TYR:OH    | 2.34                     | 0.45              |
| 4:1a:85:LEU:HB3    | 4:1a:233:LEU:HD11  | 1.99                     | 0.45              |
| 9:2a:179:MET:HE1   | 9:2a:251:LEU:HD11  | 1.99                     | 0.45              |
| 11:a9:136:THR:HG23 | 11:a9:139:PHE:H    | 1.81                     | 0.45              |
| 40:3A:230:VAL:HG11 | 40:3A:417:LEU:HB3  | 1.99                     | 0.45              |
| 53:S1:303:THR:HG22 | 53:S1:613:PRO:HG2  | 1.99                     | 0.45              |
| 51:v1:134:ASP:OD1  | 51:v1:134:ASP:N    | 2.47                     | 0.45              |
| 53:s1:643:ARG:NH1  | 53:s1:656:TYR:OH   | 2.50                     | 0.45              |
| 54:s7:146:ARG:NH1  | 54:s7:184:ILE:O    | 2.49                     | 0.45              |
| 3:S2:386:THR:OG1   | 3:S2:387:GLU:N     | 2.50                     | 0.45              |
| 7:5:15:LEU:HD21    | 7:5:94:LEU:HD21    | 1.97                     | 0.45              |
| 7:5:448:PRO:HA     | 7:5:451:MET:HB2    | 1.98                     | 0.45              |
| 19:AM:118:MET:HB3  | 19:AM:118:MET:HE2  | 1.86                     | 0.45              |
| 24:C2:1:MET:HA     | 28:B5:169:TYR:H    | 1.82                     | 0.45              |
| 7:5a:328:HIS:O     | 7:5a:332:HIS:CB    | 2.64                     | 0.45              |
| 8:4a:124:ALA:HA    | 9:2a:256:PRO:HD3   | 1.98                     | 0.45              |
| 15:ab:83:VAL:HA    | 15:ab:86:VAL:HG12  | 1.98                     | 0.45              |
| 20:ao:80:ASP:HA    | 20:ao:83:THR:HG22  | 1.97                     | 0.45              |
| 32:b8:58:ARG:NH1   | 32:b8:60:GLU:OE1   | 2.49                     | 0.45              |
| 40:3A:97:ALA:HB1   | 40:3A:150:ILE:HG23 | 1.99                     | 0.45              |
| 41:3B:70:ARG:HD3   | 41:3B:117:GLU:HG3  | 1.99                     | 0.45              |
| 43:3D:322:ARG:NH2  | 44:3E:79:SER:O     | 2.50                     | 0.45              |
| 40:3L:410:CYS:HA   | 40:3L:413:ILE:HG22 | 1.98                     | 0.45              |
| 41:3M:309:LEU:HD11 | 41:3M:338:ILE:HD12 | 1.99                     | 0.45              |
| 53:s1:160:VAL:H    | 53:s1:174:THR:HG22 | 1.82                     | 0.45              |
| 53:s1:308:ARG:NH1  | 53:s1:312:GLY:O    | 2.47                     | 0.45              |
| 7:5:88:LEU:HD11    | 7:5:468:ILE:HD12   | 1.99                     | 0.45              |
| 7:5:512:SER:OG     | 7:5:513:MET:N      | 2.50                     | 0.45              |
| 8:4:36:LEU:HA      | 8:4:39:LEU:HD12    | 1.99                     | 0.45              |
| 11:A9:150:ARG:O    | 11:A9:154:GLN:HB2  | 2.17                     | 0.45              |
| 11:A9:206:ILE:H    | 58:A9:501:NDP:H42N | 1.82                     | 0.45              |
| 4:1a:239:THR:HG23  | 4:1a:262:GLU:HG2   | 1.98                     | 0.45              |
| 7:5a:326:PHE:HA    | 7:5a:329:ILE:HD12  | 1.98                     | 0.45              |
| 9:2a:17:PRO:HA     | 9:2a:20:THR:HG22   | 1.99                     | 0.45              |
| 23:c1:40:ASN:OD1   | 23:c1:40:ASN:N     | 2.50                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:b7:39:MET:HG3   | 35:b7:41:ALA:H     | 1.81                     | 0.45              |
| 37:an:29:ARG:O     | 37:an:33:ARG:HB2   | 2.17                     | 0.45              |
| 40:3A:71:VAL:HA    | 40:3A:232:ALA:O    | 2.16                     | 0.45              |
| 43:3D:290:LEU:HD21 | 48:3J:43:ILE:HG23  | 1.99                     | 0.45              |
| 52:V2:238:LYS:HE3  | 52:V2:242:PHE:HB3  | 1.98                     | 0.45              |
| 55:s8:101:HIS:H    | 55:s8:149:MET:HE1  | 1.82                     | 0.45              |
| 55:s8:125:ALA:HB1  | 55:s8:151:LYS:HB3  | 1.98                     | 0.45              |
| 3:S2:265:ASN:O     | 3:S2:269:ARG:HB2   | 2.16                     | 0.45              |
| 7:5:202:MET:HE2    | 7:5:265:PRO:HG2    | 1.98                     | 0.45              |
| 34:B9:109:PRO:HA   | 34:B9:112:LYS:HB2  | 1.99                     | 0.45              |
| 8:4a:63:THR:HA     | 8:4a:66:ILE:HB     | 1.99                     | 0.45              |
| 15:ac:85:TYR:O     | 15:ac:89:LEU:HB2   | 2.17                     | 0.45              |
| 40:3A:58:ARG:NH2   | 40:3A:417:LEU:O    | 2.50                     | 0.45              |
| 41:3B:50:ALA:HB3   | 41:3B:221:VAL:HG12 | 1.99                     | 0.45              |
| 42:3C:138:MET:HE2  | 42:3C:269:LYS:H    | 1.81                     | 0.45              |
| 52:V2:200:ILE:HG23 | 52:V2:204:ILE:HD12 | 1.98                     | 0.45              |
| 53:S1:387:LEU:N    | 53:S1:599:THR:O    | 2.46                     | 0.45              |
| 54:s7:169:GLY:HA2  | 55:s8:151:LYS:HA   | 1.99                     | 0.45              |
| 1:3:73:LEU:O       | 4:1:160:TYR:OH     | 2.30                     | 0.44              |
| 4:1:102:ILE:HG23   | 4:1:150:LEU:HD13   | 1.99                     | 0.44              |
| 5:6:56:PHE:O       | 5:6:60:LEU:HB2     | 2.17                     | 0.44              |
| 7:5:6:THR:O        | 7:5:10:LEU:HB2     | 2.16                     | 0.44              |
| 8:4:282:LEU:HB2    | 8:4:342:MET:HG3    | 1.98                     | 0.44              |
| 8:4:378:GLU:O      | 8:4:382:THR:OG1    | 2.30                     | 0.44              |
| 9:2:338:PRO:HA     | 18:A8:170:TRP:HZ2  | 1.82                     | 0.44              |
| 34:B9:55:LYS:NZ    | 40:3A:53:LEU:O     | 2.49                     | 0.44              |
| 7:5a:261:VAL:O     | 7:5a:264:HIS:ND1   | 2.49                     | 0.44              |
| 8:4a:352:PHE:HB3   | 8:4a:355:MET:HB3   | 1.99                     | 0.44              |
| 10:al:77:ILE:HG13  | 10:al:270:VAL:HG22 | 1.99                     | 0.44              |
| 41:3M:155:ARG:HD3  | 41:3M:198:GLY:HA2  | 1.97                     | 0.44              |
| 45:3Q:23:ASN:OD1   | 45:3Q:28:ASN:ND2   | 2.48                     | 0.44              |
| 51:v1:369:ARG:NH2  | 52:v2:174:GLU:OE1  | 2.50                     | 0.44              |
| 3:S2:52:MET:HE3    | 3:S2:52:MET:HB3    | 1.82                     | 0.44              |
| 8:4:41:LEU:HD23    | 8:4:58:SER:HB2     | 1.98                     | 0.44              |
| 9:2:87:GLN:HE21    | 9:2:87:GLN:HB2     | 1.60                     | 0.44              |
| 38:A7:46:SER:O     | 38:A7:46:SER:OG    | 2.35                     | 0.44              |
| 20:ao:128:ARG:NH2  | 25:s5:102:GLU:OE2  | 2.51                     | 0.44              |
| 26:b1:45:GLN:O     | 36:bl:69:ARG:NH2   | 2.51                     | 0.44              |
| 40:3A:121:ASN:HB3  | 40:3A:132:LEU:HB2  | 2.00                     | 0.44              |
| 45:3F:27:PHE:HE2   | 45:3F:34:ARG:HA    | 1.83                     | 0.44              |
| 53:S1:245:THR:HG22 | 53:S1:266:ARG:HB2  | 1.99                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:S1:594:ALA:O    | 53:S1:605:GLN:HA   | 2.18                     | 0.44              |
| 53:s1:566:ILE:O    | 53:s1:581:ASP:N    | 2.46                     | 0.44              |
| 55:s8:170:GLY:HA2  | 55:s8:171:PRO:HD3  | 1.86                     | 0.44              |
| 2:S3:58:SER:HA     | 2:S3:77:VAL:HG21   | 2.00                     | 0.44              |
| 10:AL:190:ILE:HD12 | 10:AL:308:THR:HA   | 1.99                     | 0.44              |
| 26:B1:35:THR:OG1   | 26:B1:38:ARG:NH1   | 2.50                     | 0.44              |
| 7:5a:545:SER:HA    | 7:5a:549:SER:HB3   | 1.99                     | 0.44              |
| 15:ab:84:LEU:O     | 15:ab:88:LYS:HB2   | 2.17                     | 0.44              |
| 41:3B:197:MET:HE3  | 41:3B:197:MET:HB2  | 1.84                     | 0.44              |
| 40:3L:302:VAL:HG21 | 40:3L:432:ARG:HB3  | 1.99                     | 0.44              |
| 51:V1:184:LYS:HD2  | 51:V1:192:ASP:HB3  | 1.99                     | 0.44              |
| 51:V1:285:PRO:HG3  | 52:V2:142:ARG:HH22 | 1.82                     | 0.44              |
| 53:s1:66:HIS:NE2   | 53:s1:284:GLU:OE1  | 2.48                     | 0.44              |
| 3:S2:145:MET:HA    | 3:S2:148:GLU:HB2   | 1.98                     | 0.44              |
| 7:5:217:LEU:HD11   | 7:5:280:LEU:HD13   | 2.00                     | 0.44              |
| 7:5:460:GLY:O      | 7:5:464:ALA:CB     | 2.65                     | 0.44              |
| 8:4:208:PRO:HG2    | 8:4:291:VAL:HA     | 1.98                     | 0.44              |
| 17:A6:53:MET:HB3   | 17:A6:55:LEU:HG    | 1.98                     | 0.44              |
| 2:s3:184:ARG:NH1   | 3:s2:110:ASP:OD2   | 2.50                     | 0.44              |
| 4:1a:30:TYR:HE2    | 21:a1:2:TRP:HA     | 1.82                     | 0.44              |
| 7:5a:283:LEU:HB2   | 32:b8:144:PHE:HE2  | 1.83                     | 0.44              |
| 8:4a:242:GLY:O     | 8:4a:246:ILE:HB    | 2.18                     | 0.44              |
| 18:a8:47:ARG:NH2   | 28:b5:188:ASP:OD1  | 2.44                     | 0.44              |
| 47:3H:86:LYS:HB2   | 47:3H:89:LYS:HD3   | 2.00                     | 0.44              |
| 41:3M:101:ARG:O    | 41:3M:105:ALA:HB3  | 2.17                     | 0.44              |
| 44:3P:87:ASP:OD1   | 44:3P:87:ASP:N     | 2.49                     | 0.44              |
| 53:s1:140:GLN:NE2  | 64:s1:801:SF4:S3   | 2.91                     | 0.44              |
| 1:3:69:ILE:HD12    | 4:1:147:ALA:HB3    | 2.00                     | 0.44              |
| 4:1:6:ILE:O        | 4:1:10:LEU:HB2     | 2.16                     | 0.44              |
| 11:a9:48:ARG:O     | 11:a9:102:GLN:NE2  | 2.49                     | 0.44              |
| 11:a9:152:ILE:O    | 11:a9:156:SER:HB3  | 2.18                     | 0.44              |
| 16:a5:44:TYR:O     | 16:a5:48:THR:OG1   | 2.33                     | 0.44              |
| 40:3A:310:ILE:HD11 | 40:3A:388:VAL:HA   | 1.99                     | 0.44              |
| 42:3N:144:THR:O    | 42:3N:148:ASN:HB2  | 2.18                     | 0.44              |
| 52:v2:162:THR:HB   | 52:v2:169:THR:HG22 | 1.99                     | 0.44              |
| 54:s7:137:LEU:HD11 | 54:s7:145:LEU:HD22 | 1.99                     | 0.44              |
| 2:S3:215:VAL:HG11  | 2:S3:217:ARG:HH11  | 1.82                     | 0.44              |
| 7:5:63:ILE:HB      | 7:5:80:PHE:HB2     | 2.00                     | 0.44              |
| 8:4:175:ASN:HB3    | 8:4:178:ILE:HB     | 2.00                     | 0.44              |
| 8:4:400:ILE:HA     | 8:4:403:THR:HG22   | 2.00                     | 0.44              |
| 9:2:333:SER:OG     | 9:2:334:THR:N      | 2.50                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:A5:49:GLU:O     | 16:A5:53:ASN:ND2   | 2.46                     | 0.44              |
| 29:B6:90:MET:HE3   | 29:B6:90:MET:HB2   | 1.79                     | 0.44              |
| 17:a6:76:VAL:HG22  | 17:a6:78:ASP:H     | 1.83                     | 0.44              |
| 18:a8:71:PHE:HA    | 18:a8:74:ILE:HG22  | 2.00                     | 0.44              |
| 27:bm:127:ARG:HD3  | 27:bm:134:ILE:HA   | 2.00                     | 0.44              |
| 32:b8:82:SER:HB3   | 32:b8:119:THR:H    | 1.83                     | 0.44              |
| 37:an:98:THR:OG1   | 37:an:100:ASP:OD1  | 2.35                     | 0.44              |
| 44:3E:92:ARG:HA    | 46:3G:24:GLN:HA    | 2.00                     | 0.44              |
| 40:3L:165:ARG:NH2  | 40:3L:211:LEU:O    | 2.45                     | 0.44              |
| 51:V1:205:ILE:HG12 | 51:V1:379:CYS:HB3  | 1.98                     | 0.44              |
| 51:v1:132:ARG:HH21 | 52:v2:223:CYS:HB3  | 1.82                     | 0.44              |
| 53:s1:142:GLN:O    | 53:s1:146:PHE:HB2  | 2.17                     | 0.44              |
| 53:s1:344:GLY:N    | 53:s1:521:SER:OG   | 2.49                     | 0.44              |
| 3:S2:146:CYS:H     | 3:S2:178:THR:HG21  | 1.83                     | 0.44              |
| 8:4:116:ILE:HG21   | 18:A8:168:PHE:HB3  | 1.99                     | 0.44              |
| 13:S6:54:GLU:O     | 37:AN:131:TYR:OH   | 2.35                     | 0.44              |
| 9:2a:176:ARG:NH1   | 9:2a:225:MET:SD    | 2.91                     | 0.44              |
| 16:a5:51:ILE:HG13  | 16:a5:55:LYS:HE2   | 2.00                     | 0.44              |
| 36:bl:38:ASP:HA    | 36:bl:41:VAL:HG22  | 1.99                     | 0.44              |
| 37:an:121:VAL:HG13 | 37:an:127:GLN:HA   | 2.00                     | 0.44              |
| 42:3C:257:MET:SD   | 43:3D:204:ARG:NH1  | 2.91                     | 0.44              |
| 48:3J:54:LYS:H     | 48:3J:54:LYS:HG3   | 1.64                     | 0.44              |
| 53:S1:592:LYS:NZ   | 53:S1:619:ASP:OD2  | 2.51                     | 0.44              |
| 51:v1:403:ASP:OD1  | 51:v1:403:ASP:N    | 2.41                     | 0.44              |
| 1:3:80:GLN:O       | 25:S5:27:TYR:OH    | 2.35                     | 0.44              |
| 3:S2:370:GLU:O     | 3:S2:374:SER:OG    | 2.34                     | 0.44              |
| 7:5:64:THR:O       | 29:B6:96:THR:OG1   | 2.36                     | 0.44              |
| 8:4:13:PRO:O       | 8:4:17:LEU:HB2     | 2.18                     | 0.44              |
| 14:A2:65:LEU:HB3   | 14:A2:77:VAL:HB    | 2.00                     | 0.44              |
| 29:B6:5:THR:HG23   | 29:B6:8:GLU:H      | 1.83                     | 0.44              |
| 8:4a:318:ALA:HB2   | 8:4a:373:ILE:HG13  | 1.99                     | 0.44              |
| 9:2a:26:LEU:HA     | 9:2a:29:MET:HG2    | 1.99                     | 0.44              |
| 43:3D:262:THR:HG21 | 47:3H:27:PRO:HD2   | 1.99                     | 0.44              |
| 40:3L:193:GLN:OE1  | 44:3P:92:ARG:NH2   | 2.49                     | 0.44              |
| 53:S1:78:CYS:SG    | 53:S1:91:ALA:N     | 2.90                     | 0.44              |
| 53:S1:402:LEU:HD22 | 53:S1:407:PRO:HG2  | 1.99                     | 0.44              |
| 53:S1:425:ASN:OD1  | 53:S1:425:ASN:N    | 2.51                     | 0.44              |
| 52:v2:107:PRO:HA   | 52:v2:108:PRO:HD3  | 1.86                     | 0.44              |
| 53:s1:349:GLU:HG2  | 53:s1:646:LEU:HD11 | 1.99                     | 0.44              |
| 8:4:336:ARG:HH22   | 8:4:429:SER:HA     | 1.83                     | 0.44              |
| 8:4:360:LEU:HG     | 8:4:364:LEU:HD13   | 1.98                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:2:102:LEU:HD22   | 9:2:138:PRO:HB3    | 2.00                     | 0.44              |
| 15:AB:122:MET:O    | 15:AB:126:PHE:HB2  | 2.17                     | 0.44              |
| 4:1a:79:LEU:HD22   | 4:1a:222:LEU:HD22  | 1.99                     | 0.44              |
| 14:a2:50:ASN:OD1   | 14:a2:50:ASN:N     | 2.46                     | 0.44              |
| 20:ao:75:PHE:HZ    | 21:a1:47:LEU:HD13  | 1.83                     | 0.44              |
| 39:v3:85:LEU:HD21  | 52:v2:60:LYS:HG2   | 2.00                     | 0.44              |
| 41:3B:51:SER:OG    | 41:3B:225:VAL:O    | 2.35                     | 0.44              |
| 42:3C:15:ASN:HA    | 42:3C:19:ILE:HB    | 2.00                     | 0.44              |
| 43:3O:209:ASP:OD1  | 43:3O:209:ASP:N    | 2.49                     | 0.44              |
| 53:S1:579:MET:HE2  | 53:S1:579:MET:HB3  | 1.95                     | 0.44              |
| 51:v1:112:TYR:O    | 51:v1:240:THR:HA   | 2.18                     | 0.44              |
| 7:5:186:MET:HE3    | 7:5:186:MET:HB2    | 1.73                     | 0.43              |
| 15:AC:76:LEU:HD11  | 29:B6:20:ARG:HH21  | 1.83                     | 0.43              |
| 25:S5:48:GLY:O     | 25:S5:52:ALA:CB    | 2.66                     | 0.43              |
| 27:BM:85:MET:HE3   | 27:BM:85:MET:HB3   | 1.83                     | 0.43              |
| 7:5a:89:PHE:HZ     | 7:5a:251:THR:HA    | 1.82                     | 0.43              |
| 7:5a:128:MET:HG2   | 7:5a:251:THR:HB    | 1.99                     | 0.43              |
| 7:5a:171:ALA:O     | 7:5a:175:ASN:HB2   | 2.18                     | 0.43              |
| 10:al:74:ALA:HA    | 10:al:77:ILE:HG22  | 2.00                     | 0.43              |
| 14:a2:43:GLU:HA    | 14:a2:46:LYS:HG2   | 1.99                     | 0.43              |
| 20:ao:81:ARG:O     | 25:s5:105:ARG:NH2  | 2.50                     | 0.43              |
| 26:b1:56:TRP:HH2   | 28:b5:134:GLU:HB2  | 1.82                     | 0.43              |
| 28:b5:160:MET:HE1  | 28:b5:166:GLY:HA3  | 2.00                     | 0.43              |
| 37:an:80:ASP:OD1   | 37:an:80:ASP:N     | 2.41                     | 0.43              |
| 42:3C:118:LEU:HD22 | 42:3C:192:LEU:HD21 | 2.00                     | 0.43              |
| 45:3F:44:VAL:O     | 45:3F:48:ILE:HB    | 2.18                     | 0.43              |
| 51:V1:149:MET:SD   | 51:V1:241:THR:OG1  | 2.69                     | 0.43              |
| 7:5:542:LEU:HA     | 7:5:545:SER:HB2    | 2.00                     | 0.43              |
| 10:AL:139:ARG:NH2  | 57:AL:502:DGT:N7   | 2.66                     | 0.43              |
| 13:S6:90:LYS:HE2   | 13:S6:90:LYS:HB3   | 1.87                     | 0.43              |
| 19:AM:14:ASP:OD1   | 19:AM:14:ASP:N     | 2.50                     | 0.43              |
| 32:B8:82:SER:OG    | 32:B8:83:GLN:N     | 2.51                     | 0.43              |
| 1:3a:71:LEU:HB3    | 5:6a:152:MET:HE1   | 2.00                     | 0.43              |
| 14:a2:23:LEU:HD11  | 14:a2:34:ARG:HG3   | 2.01                     | 0.43              |
| 16:a5:45:ARG:O     | 16:a5:49:GLU:HB2   | 2.18                     | 0.43              |
| 22:a3:18:VAL:HG13  | 55:s8:61:LEU:HD21  | 2.00                     | 0.43              |
| 33:b4:128:SER:OG   | 33:b4:129:TYR:N    | 2.51                     | 0.43              |
| 53:S1:538:ARG:NH1  | 53:S1:559:ASP:OD2  | 2.51                     | 0.43              |
| 51:v1:225:LEU:HD22 | 53:s1:93:ALA:HB3   | 2.00                     | 0.43              |
| 7:5:211:ILE:HG23   | 7:5:212:PRO:HD3    | 2.00                     | 0.43              |
| 20:AO:109:SER:OG   | 20:AO:111:PHE:O    | 2.35                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:5a:176:ARG:NH2   | 8:4a:367:LEU:O     | 2.51                     | 0.43              |
| 8:4a:337:ILE:HD13  | 8:4a:345:ALA:HB2   | 2.00                     | 0.43              |
| 8:4a:452:LYS:H     | 8:4a:452:LYS:HG2   | 1.62                     | 0.43              |
| 35:b7:33:GLU:O     | 35:b7:35:LYS:NZ    | 2.48                     | 0.43              |
| 51:V1:325:PRO:HD3  | 51:V1:433:TRP:HB3  | 1.98                     | 0.43              |
| 52:V2:184:MET:HE2  | 52:V2:184:MET:HB2  | 1.88                     | 0.43              |
| 53:s1:78:CYS:SG    | 53:s1:91:ALA:N     | 2.91                     | 0.43              |
| 54:s7:161:MET:HG2  | 54:s7:196:PRO:HG2  | 2.00                     | 0.43              |
| 55:s8:101:HIS:CD2  | 64:s8:301:SF4:S1   | 3.11                     | 0.43              |
| 3:S2:417:SER:O     | 3:S2:417:SER:OG    | 2.36                     | 0.43              |
| 5:6:19:LEU:HD22    | 5:6:32:LEU:HD13    | 2.00                     | 0.43              |
| 6:4L:51:SER:HA     | 25:S5:32:ARG:HH21  | 1.82                     | 0.43              |
| 7:5:556:ILE:HD12   | 33:B4:76:ILE:HG22  | 2.00                     | 0.43              |
| 8:4:179:LEU:HD22   | 8:4:249:ILE:HD12   | 1.99                     | 0.43              |
| 11:A9:61:ALA:HA    | 11:A9:66:GLY:HA3   | 2.00                     | 0.43              |
| 12:S4:91:VAL:HG12  | 12:S4:95:LYS:HG3   | 2.01                     | 0.43              |
| 28:B5:102:PRO:HG2  | 28:B5:105:TYR:HB3  | 1.99                     | 0.43              |
| 4:1a:158:GLY:HA3   | 4:1a:315:PRO:HB2   | 2.01                     | 0.43              |
| 20:ao:69:ILE:HD12  | 20:ao:69:ILE:HA    | 1.86                     | 0.43              |
| 30:b2:72:ARG:HD3   | 30:b2:72:ARG:HA    | 1.85                     | 0.43              |
| 32:b8:34:LYS:NZ    | 33:b4:70:TYR:OH    | 2.50                     | 0.43              |
| 34:b9:101:GLU:OE2  | 34:b9:122:ARG:NE   | 2.52                     | 0.43              |
| 34:b9:168:TRP:O    | 34:b9:172:THR:HB   | 2.19                     | 0.43              |
| 40:3A:86:ASN:HA    | 40:3A:211:LEU:HD21 | 1.99                     | 0.43              |
| 41:3B:77:LEU:HD11  | 41:3B:189:PRO:HD2  | 1.99                     | 0.43              |
| 41:3B:254:ARG:HH12 | 41:3M:259:ARG:HD3  | 1.84                     | 0.43              |
| 42:3C:207:ASN:OD1  | 42:3C:210:GLY:N    | 2.47                     | 0.43              |
| 41:3M:257:GLU:HG3  | 41:3M:438:MET:HB3  | 2.01                     | 0.43              |
| 42:3N:314:SER:OG   | 42:3N:315:LEU:N    | 2.51                     | 0.43              |
| 7:5:83:ASP:N       | 7:5:83:ASP:OD1     | 2.51                     | 0.43              |
| 33:B4:123:ARG:HD2  | 36:BL:144:LEU:HD21 | 1.99                     | 0.43              |
| 2:s3:203:LEU:HD12  | 3:s2:122:LYS:HG3   | 2.00                     | 0.43              |
| 4:1a:289:LEU:HD23  | 4:1a:289:LEU:HA    | 1.88                     | 0.43              |
| 7:5a:426:ILE:O     | 7:5a:430:VAL:HB    | 2.18                     | 0.43              |
| 11:a9:359:TYR:HA   | 11:a9:362:LEU:HB2  | 1.98                     | 0.43              |
| 13:s6:45:ARG:O     | 13:s6:48:PHE:HB2   | 2.19                     | 0.43              |
| 18:a8:151:ASN:OD1  | 18:a8:151:ASN:N    | 2.51                     | 0.43              |
| 34:b9:66:GLU:HA    | 34:b9:69:GLU:HG2   | 2.00                     | 0.43              |
| 40:3A:70:THR:HA    | 40:3A:133:ILE:O    | 2.19                     | 0.43              |
| 42:3N:50:PHE:HA    | 42:3N:53:MET:HE2   | 2.00                     | 0.43              |
| 50:3T:16:SER:O     | 50:3T:16:SER:OG    | 2.36                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:s1:395:GLU:OE2  | 53:s1:420:LYS:NZ   | 2.43                     | 0.43              |
| 53:s1:403:VAL:HA   | 53:s1:432:ILE:HB   | 1.99                     | 0.43              |
| 2:S3:147:ASP:OD1   | 2:S3:147:ASP:N     | 2.51                     | 0.43              |
| 7:5:79:SER:N       | 7:5:139:GLN:OE1    | 2.48                     | 0.43              |
| 7:5:286:LEU:HD22   | 7:5:411:ILE:HD11   | 1.99                     | 0.43              |
| 7:5:328:HIS:O      | 7:5:332:HIS:CB     | 2.66                     | 0.43              |
| 7:5:466:PHE:O      | 7:5:470:TYR:HB2    | 2.18                     | 0.43              |
| 7:5:594:ASN:HA     | 7:5:597:LEU:HB2    | 1.99                     | 0.43              |
| 12:S4:115:ALA:HB2  | 53:S1:267:THR:HB   | 2.00                     | 0.43              |
| 18:A8:111:VAL:O    | 18:A8:116:GLY:N    | 2.49                     | 0.43              |
| 32:B8:38:PRO:HD2   | 33:B4:70:TYR:HD2   | 1.84                     | 0.43              |
| 35:B7:12:ASP:OD1   | 35:B7:12:ASP:N     | 2.44                     | 0.43              |
| 3:s2:169:TRP:HA    | 3:s2:172:VAL:HG12  | 1.99                     | 0.43              |
| 3:s2:460:GLU:HG2   | 3:s2:461:ILE:HG13  | 2.00                     | 0.43              |
| 7:5a:108:MET:HB2   | 7:5a:114:ILE:HD13  | 2.00                     | 0.43              |
| 8:4a:72:LEU:O      | 8:4a:76:MET:N      | 2.51                     | 0.43              |
| 9:2a:108:LEU:HD11  | 9:2a:191:LEU:HD22  | 2.00                     | 0.43              |
| 10:a1:250:SER:O    | 10:a1:280:LYS:NZ   | 2.51                     | 0.43              |
| 20:ao:65:LEU:HD23  | 22:a3:50:PRO:HD2   | 2.00                     | 0.43              |
| 27:bm:112:MET:HB3  | 27:bm:112:MET:HE3  | 1.71                     | 0.43              |
| 40:3A:214:THR:HA   | 40:3A:217:THR:HG22 | 2.01                     | 0.43              |
| 40:3A:337:LEU:O    | 40:3A:364:SER:OG   | 2.37                     | 0.43              |
| 43:3D:177:LYS:HE2  | 43:3D:177:LYS:HB2  | 1.79                     | 0.43              |
| 46:3G:53:PHE:HA    | 46:3G:56:VAL:HG12  | 1.99                     | 0.43              |
| 49:3K:23:MET:HE3   | 49:3K:23:MET:HB2   | 1.83                     | 0.43              |
| 51:V1:83:SER:HA    | 51:V1:263:ALA:HB2  | 2.01                     | 0.43              |
| 51:V1:111:LYS:HB2  | 51:V1:151:ALA:HA   | 2.00                     | 0.43              |
| 51:v1:270:ASN:ND2  | 51:v1:340:ASP:OD1  | 2.51                     | 0.43              |
| 51:v1:383:THR:HG21 | 53:s1:120:LEU:HG   | 2.00                     | 0.43              |
| 53:s1:388:ASN:ND2  | 53:s1:513:MET:O    | 2.47                     | 0.43              |
| 54:s7:107:MET:HE3  | 54:s7:114:MET:HG2  | 2.00                     | 0.43              |
| 2:S3:210:ARG:HD2   | 11:A9:48:ARG:HH11  | 1.84                     | 0.43              |
| 3:S2:223:HIS:HE1   | 54:S7:99:CYS:SG    | 2.40                     | 0.43              |
| 3:S2:367:LYS:HE2   | 3:S2:367:LYS:HB2   | 1.85                     | 0.43              |
| 4:1:169:GLN:NE2    | 4:1:240:ILE:O      | 2.52                     | 0.43              |
| 8:4:307:TRP:NE1    | 8:4:383:MET:SD     | 2.92                     | 0.43              |
| 9:2:102:LEU:O      | 9:2:106:LEU:HB2    | 2.17                     | 0.43              |
| 15:AC:132:ASP:HA   | 15:AC:135:ALA:HB3  | 2.00                     | 0.43              |
| 18:A8:126:SER:O    | 18:A8:126:SER:OG   | 2.36                     | 0.43              |
| 11:a9:126:VAL:HG12 | 11:a9:161:VAL:HG21 | 2.01                     | 0.43              |
| 19:am:130:LEU:HD23 | 19:am:130:LEU:HA   | 1.92                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:b6:106:PRO:HB3  | 29:b6:119:PRO:HA   | 2.01                     | 0.43              |
| 40:3A:406:THR:OG1  | 41:3B:387:GLU:OE2  | 2.36                     | 0.43              |
| 40:3L:170:ARG:HH21 | 50:3T:51:CYS:HA    | 1.83                     | 0.43              |
| 51:V1:412:LEU:HA   | 51:V1:415:ILE:HG12 | 2.00                     | 0.43              |
| 52:V2:236:PRO:HA   | 52:V2:237:PRO:HD3  | 1.87                     | 0.43              |
| 55:S8:149:MET:SD   | 55:S8:154:TYR:OH   | 2.71                     | 0.43              |
| 51:v1:340:ASP:OD1  | 51:v1:340:ASP:N    | 2.51                     | 0.43              |
| 54:s7:146:ARG:HA   | 54:s7:146:ARG:HD2  | 1.81                     | 0.43              |
| 1:3:73:LEU:HD23    | 4:1:151:LEU:HD13   | 2.01                     | 0.43              |
| 2:S3:214:GLU:HA    | 11:A9:68:TYR:HE1   | 1.84                     | 0.43              |
| 3:S2:216:ARG:HH11  | 38:A7:34:ARG:HH21  | 1.67                     | 0.43              |
| 9:2:2:ASN:HD21     | 9:2:5:THR:HG23     | 1.84                     | 0.43              |
| 9:2:193:ILE:HB     | 9:2:266:ILE:HG12   | 2.01                     | 0.43              |
| 12:S4:112:MET:O    | 55:S8:144:ARG:NH1  | 2.51                     | 0.43              |
| 14:A2:38:VAL:O     | 53:S1:667:GLN:NE2  | 2.51                     | 0.43              |
| 19:AM:113:MET:HE2  | 19:AM:113:MET:HB2  | 1.81                     | 0.43              |
| 32:B8:170:ARG:HD3  | 32:B8:170:ARG:HA   | 1.78                     | 0.43              |
| 7:5a:147:VAL:HB    | 7:5a:252:MET:HG2   | 2.00                     | 0.43              |
| 7:5a:347:ILE:HG23  | 7:5a:352:ASP:HA    | 2.00                     | 0.43              |
| 9:2a:292:PHE:HB3   | 9:2a:295:ARG:HH21  | 1.84                     | 0.43              |
| 17:a6:21:LYS:HA    | 17:a6:21:LYS:HD2   | 1.86                     | 0.43              |
| 20:ao:79:LYS:HB3   | 20:ao:79:LYS:HE3   | 1.85                     | 0.43              |
| 24:c2:12:LYS:HB3   | 24:c2:15:PRO:HG3   | 2.00                     | 0.43              |
| 37:an:113:ILE:HG12 | 55:s8:198:GLU:HB3  | 2.01                     | 0.43              |
| 43:3D:105:LEU:HB3  | 43:3D:110:ILE:HD11 | 1.99                     | 0.43              |
| 45:3F:68:ASP:HA    | 45:3F:71:MET:HE2   | 2.01                     | 0.43              |
| 40:3L:133:ILE:HD13 | 40:3L:143:VAL:HG13 | 2.01                     | 0.43              |
| 41:3M:92:LYS:HE2   | 41:3M:143:ALA:HB1  | 2.01                     | 0.43              |
| 55:S8:59:ARG:HA    | 55:S8:64:THR:HG22  | 2.01                     | 0.43              |
| 55:S8:114:ILE:O    | 55:S8:140:ARG:NH1  | 2.52                     | 0.43              |
| 1:3:27:MET:HE1     | 4:1:62:ARG:HE      | 1.84                     | 0.43              |
| 7:5:476:SER:OG     | 7:5:477:ILE:N      | 2.51                     | 0.43              |
| 10:AL:65:ASN:HD21  | 10:AL:238:GLU:HB2  | 1.84                     | 0.43              |
| 10:AL:168:VAL:HA   | 10:AL:171:GLU:HG2  | 2.01                     | 0.43              |
| 11:A9:283:MET:HG2  | 11:A9:357:ARG:HH12 | 1.84                     | 0.43              |
| 2:s3:51:ASP:OD1    | 2:s3:51:ASP:N      | 2.51                     | 0.43              |
| 2:s3:227:GLN:HG2   | 55:s8:151:LYS:HZ1  | 1.84                     | 0.43              |
| 5:6a:123:TRP:HZ3   | 20:ao:120:LEU:HD12 | 1.84                     | 0.43              |
| 7:5a:313:MET:HG3   | 7:5a:328:HIS:HD2   | 1.82                     | 0.43              |
| 13:s6:25:SER:HG    | 13:s6:29:GLU:H     | 1.65                     | 0.43              |
| 26:b1:53:GLU:HG2   | 26:b1:54:VAL:HG23  | 1.99                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:b5:81:PRO:HA    | 28:b5:84:ILE:HG22  | 2.00                     | 0.43              |
| 41:3B:259:ARG:NH1  | 41:3B:447:THR:O    | 2.52                     | 0.43              |
| 41:3M:240:MET:H    | 41:3M:240:MET:HG2  | 1.57                     | 0.43              |
| 43:3O:170:LYS:HD3  | 43:3O:170:LYS:HA   | 1.78                     | 0.43              |
| 46:3R:51:PRO:HA    | 46:3R:54:VAL:HG22  | 1.99                     | 0.43              |
| 51:V1:270:ASN:ND2  | 51:V1:340:ASP:OD1  | 2.52                     | 0.43              |
| 53:S1:288:ASP:HA   | 53:S1:291:ARG:HG2  | 2.00                     | 0.43              |
| 54:S7:113:ASP:OD2  | 54:S7:116:ARG:N    | 2.49                     | 0.43              |
| 55:S8:200:GLU:OE2  | 55:S8:204:ASN:ND2  | 2.47                     | 0.43              |
| 3:S2:251:PHE:HD2   | 3:S2:341:LEU:HD21  | 1.84                     | 0.43              |
| 7:5:60:GLU:H       | 29:B6:100:SER:HB3  | 1.84                     | 0.43              |
| 7:5:487:LYS:HE2    | 7:5:487:LYS:HB2    | 1.83                     | 0.43              |
| 17:A6:118:PRO:O    | 17:A6:124:LYS:NZ   | 2.48                     | 0.43              |
| 31:B3:24:ASP:OD1   | 31:B3:24:ASP:N     | 2.48                     | 0.43              |
| 7:5a:291:CYS:HB2   | 7:5a:304:PHE:HE2   | 1.83                     | 0.43              |
| 10:a1:231:SER:O    | 10:a1:235:GLN:HB2  | 2.19                     | 0.43              |
| 17:a6:55:LEU:HD23  | 17:a6:55:LEU:HA    | 1.90                     | 0.43              |
| 18:a8:127:LYS:HD2  | 22:a3:76:PRO:HD2   | 2.00                     | 0.43              |
| 40:3A:58:ARG:HB2   | 40:3A:230:VAL:HG12 | 2.00                     | 0.43              |
| 40:3A:120:LEU:HD13 | 41:3B:299:ILE:HG23 | 2.01                     | 0.43              |
| 40:3L:70:THR:OG1   | 40:3L:410:CYS:SG   | 2.72                     | 0.43              |
| 41:3M:286:PHE:HB3  | 41:3M:327:ASN:HD21 | 1.84                     | 0.43              |
| 42:3N:37:LEU:HD13  | 61:3N:402:HEM:HBB2 | 2.01                     | 0.43              |
| 42:3N:216:ASP:HB2  | 45:3Q:64:LYS:HG3   | 1.99                     | 0.43              |
| 53:S1:357:LEU:HD23 | 53:S1:627:SER:HB2  | 2.01                     | 0.43              |
| 51:v1:69:LEU:O     | 51:v1:147:ARG:NH1  | 2.52                     | 0.43              |
| 51:v1:266:GLY:HA3  | 51:v1:271:SER:HA   | 2.00                     | 0.43              |
| 51:v1:342:LEU:HD12 | 51:v1:349:LEU:HB2  | 2.01                     | 0.43              |
| 52:v2:203:ILE:HD11 | 52:v2:218:ARG:HD2  | 2.01                     | 0.43              |
| 54:s7:202:LEU:HD23 | 54:s7:202:LEU:HA   | 1.91                     | 0.43              |
| 1:3:64:LEU:HD12    | 5:6:163:ILE:HD13   | 2.01                     | 0.42              |
| 7:5:64:THR:HA      | 7:5:78:MET:O       | 2.19                     | 0.42              |
| 7:5:205:ASN:ND2    | 36:BL:121:TYR:OH   | 2.51                     | 0.42              |
| 9:2:187:MET:HE2    | 9:2:187:MET:HB3    | 1.84                     | 0.42              |
| 10:AL:232:ALA:O    | 10:AL:236:ASP:HB2  | 2.19                     | 0.42              |
| 37:AN:137:LYS:HE2  | 37:AN:137:LYS:HB2  | 1.94                     | 0.42              |
| 3:s2:98:VAL:HG21   | 17:a6:100:TRP:HE1  | 1.84                     | 0.42              |
| 7:5a:363:THR:HG21  | 31:b3:67:ILE:HG21  | 2.01                     | 0.42              |
| 9:2a:271:MET:HE1   | 9:2a:276:LEU:HA    | 2.01                     | 0.42              |
| 12:s4:104:ARG:NH2  | 17:a6:130:ASP:OD1  | 2.49                     | 0.42              |
| 42:3C:328:LEU:HB2  | 42:3C:361:ILE:HG21 | 2.00                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:3L:70:THR:HG21 | 40:3L:407:THR:HG22 | 2.00                     | 0.42              |
| 46:3R:46:ILE:O    | 46:3R:50:ALA:HB3   | 2.18                     | 0.42              |
| 53:s1:304:GLU:HG2 | 53:s1:615:LEU:HD12 | 2.01                     | 0.42              |
| 53:s1:478:SER:O   | 53:s1:518:ARG:NH1  | 2.52                     | 0.42              |
| 55:s8:131:GLU:O   | 55:s8:144:ARG:HB3  | 2.18                     | 0.42              |
| 5:6:80:GLU:OE1    | 11:A9:360:ARG:NH1  | 2.52                     | 0.42              |
| 7:5:535:ARG:HB3   | 33:B4:11:LEU:HD22  | 2.02                     | 0.42              |
| 12:S4:146:ASP:OD2 | 53:S1:605:GLN:NE2  | 2.52                     | 0.42              |
| 37:AN:139:HIS:HB2 | 53:S1:299:ARG:HA   | 2.01                     | 0.42              |
| 38:A7:19:ASP:OD1  | 38:A7:19:ASP:N     | 2.51                     | 0.42              |
| 2:s3:110:LEU:HA   | 2:s3:131:LEU:HG    | 2.01                     | 0.42              |
| 4:1a:316:PRO:HG3  | 20:ao:57:ARG:HB3   | 2.00                     | 0.42              |
| 7:5a:421:MET:HA   | 7:5a:501:ALA:HB2   | 2.01                     | 0.42              |
| 8:4a:54:ASN:N     | 8:4a:54:ASN:OD1    | 2.51                     | 0.42              |
| 9:2a:95:LEU:HD13  | 9:2a:148:LEU:HB3   | 2.01                     | 0.42              |
| 18:a8:108:ASP:HA  | 18:a8:111:VAL:HG12 | 2.00                     | 0.42              |
| 28:b5:58:LYS:HB2  | 34:b9:107:TRP:HZ2  | 1.84                     | 0.42              |
| 35:b7:96:VAL:HA   | 35:b7:99:MET:HE3   | 1.99                     | 0.42              |
| 41:3B:180:VAL:HA  | 41:3B:254:ARG:HE   | 1.83                     | 0.42              |
| 46:3G:18:SER:OG   | 46:3G:19:LEU:N     | 2.52                     | 0.42              |
| 53:S1:388:ASN:H   | 53:S1:514:ASN:HB3  | 1.84                     | 0.42              |
| 55:S8:194:GLY:O   | 55:S8:198:GLU:HB2  | 2.19                     | 0.42              |
| 54:s7:97:LEU:O    | 54:s7:136:THR:OG1  | 2.31                     | 0.42              |
| 3:S2:117:HIS:NE2  | 54:S7:175:TYR:OH   | 2.43                     | 0.42              |
| 3:S2:457:VAL:HG23 | 3:S2:460:GLU:HG2   | 2.00                     | 0.42              |
| 4:1:204:GLU:OE2   | 54:S7:122:ARG:NH1  | 2.43                     | 0.42              |
| 15:AC:125:GLU:OE2 | 30:B2:44:TYR:OH    | 2.37                     | 0.42              |
| 38:A7:49:LEU:HD13 | 53:S1:152:ARG:HB2  | 2.00                     | 0.42              |
| 25:s5:48:GLY:O    | 25:s5:52:ALA:CB    | 2.67                     | 0.42              |
| 32:b8:160:GLN:OE1 | 35:b7:37:ARG:NH2   | 2.51                     | 0.42              |
| 37:an:95:HIS:HB3  | 55:s8:93:LEU:HB2   | 2.01                     | 0.42              |
| 40:3A:274:GLU:HB3 | 46:3G:18:SER:HB3   | 2.01                     | 0.42              |
| 51:V1:382:CYS:HB3 | 51:V1:384:PRO:HD2  | 2.01                     | 0.42              |
| 52:V2:145:ASP:OD1 | 52:V2:145:ASP:N    | 2.52                     | 0.42              |
| 53:S1:323:LEU:HB3 | 53:S1:629:ILE:HG21 | 2.00                     | 0.42              |
| 51:v1:157:TYR:HB2 | 51:v1:216:ILE:HD11 | 2.01                     | 0.42              |
| 5:6:13:LEU:HD23   | 5:6:99:GLU:HG3     | 2.01                     | 0.42              |
| 5:6:44:LEU:HD11   | 5:6:53:LEU:HG      | 2.00                     | 0.42              |
| 8:4:304:GLN:O     | 36:BL:148:ALA:N    | 2.52                     | 0.42              |
| 8:4:336:ARG:HA    | 8:4:336:ARG:HD3    | 1.89                     | 0.42              |
| 8:4:343:ILE:O     | 8:4:346:ARG:NH1    | 2.46                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:A9:324:ILE:HD12 | 11:A9:324:ILE:HA   | 1.97                     | 0.42              |
| 58:A9:501:NDP:O2N  | 58:A9:501:NDP:O7N  | 2.37                     | 0.42              |
| 13:S6:107:CYS:SG   | 13:S6:108:GLY:N    | 2.92                     | 0.42              |
| 32:B8:161:TYR:HA   | 32:B8:162:PRO:HD3  | 1.90                     | 0.42              |
| 3:s2:84:PHE:O      | 4:1a:127:TYR:OH    | 2.38                     | 0.42              |
| 7:5a:586:LEU:HD21  | 19:am:45:PRO:HG3   | 2.02                     | 0.42              |
| 8:4a:51:ASN:O      | 28:b5:135:LYS:NZ   | 2.52                     | 0.42              |
| 8:4a:118:PHE:O     | 8:4a:122:PHE:CB    | 2.67                     | 0.42              |
| 10:al:39:GLY:H     | 10:al:42:ALA:HB3   | 1.83                     | 0.42              |
| 11:a9:220:TYR:HB3  | 11:a9:226:VAL:HG12 | 2.01                     | 0.42              |
| 12:s4:102:ASP:N    | 12:s4:102:ASP:OD1  | 2.49                     | 0.42              |
| 13:s6:77:ILE:HD12  | 13:s6:77:ILE:HA    | 1.91                     | 0.42              |
| 15:ab:88:LYS:HB2   | 15:ab:88:LYS:HE2   | 1.90                     | 0.42              |
| 28:b5:72:LYS:O     | 28:b5:76:MET:HB2   | 2.19                     | 0.42              |
| 29:b6:118:PRO:HA   | 29:b6:119:PRO:HD3  | 1.85                     | 0.42              |
| 34:b9:114:MET:HE2  | 34:b9:114:MET:HB3  | 1.90                     | 0.42              |
| 41:3B:51:SER:HB2   | 41:3B:230:LEU:HD23 | 2.02                     | 0.42              |
| 42:3C:8:HIS:O      | 42:3C:12:LYS:N     | 2.53                     | 0.42              |
| 42:3C:8:HIS:HB3    | 42:3C:11:PHE:HB2   | 2.01                     | 0.42              |
| 40:3L:187:LEU:HA   | 40:3L:190:THR:HG22 | 2.02                     | 0.42              |
| 42:3N:117:VAL:HG21 | 42:3N:302:ALA:HB2  | 2.01                     | 0.42              |
| 45:3Q:36:ASP:OD1   | 45:3Q:90:TYR:OH    | 2.37                     | 0.42              |
| 51:V1:117:ALA:HB3  | 51:V1:157:TYR:O    | 2.19                     | 0.42              |
| 53:S1:341:ILE:HD11 | 53:S1:537:ILE:HG13 | 2.01                     | 0.42              |
| 51:v1:184:LYS:HD2  | 51:v1:192:ASP:HB3  | 2.00                     | 0.42              |
| 53:s1:387:LEU:HA   | 53:s1:514:ASN:HB2  | 2.01                     | 0.42              |
| 5:6:140:GLY:HA2    | 25:S5:26:PRO:HG3   | 2.01                     | 0.42              |
| 7:5:71:MET:HG2     | 8:4:380:PHE:HE2    | 1.84                     | 0.42              |
| 7:5:221:THR:HG22   | 7:5:226:GLN:HB2    | 2.01                     | 0.42              |
| 7:5:554:ASP:OD1    | 8:4:213:HIS:NE2    | 2.49                     | 0.42              |
| 8:4:307:TRP:HA     | 8:4:310:MET:HE2    | 2.00                     | 0.42              |
| 9:2:170:LEU:HD11   | 9:2:288:LEU:HD13   | 2.00                     | 0.42              |
| 11:A9:127:ILE:HG23 | 11:A9:165:ILE:HB   | 2.00                     | 0.42              |
| 20:AO:25:LEU:HD12  | 20:AO:25:LEU:HA    | 1.94                     | 0.42              |
| 21:A1:23:THR:HA    | 21:A1:26:ILE:HG22  | 2.02                     | 0.42              |
| 25:S5:7:GLN:NE2    | 25:S5:15:ASP:OD1   | 2.52                     | 0.42              |
| 25:S5:53:LYS:HE3   | 25:S5:53:LYS:HB2   | 1.82                     | 0.42              |
| 4:1a:170:GLU:HG2   | 4:1a:247:TYR:H     | 1.85                     | 0.42              |
| 7:5a:346:ILE:O     | 7:5a:350:LEU:HB2   | 2.18                     | 0.42              |
| 11:a9:201:ILE:HD13 | 11:a9:263:PHE:HB2  | 2.01                     | 0.42              |
| 11:a9:206:ILE:HG12 | 58:a9:501:NDP:H42N | 2.01                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 13:s6:87:GLY:HA2  | 55:s8:112:ARG:HH12 | 1.84                     | 0.42              |
| 15:ab:90:TYR:OH   | 15:ab:117:GLU:OE1  | 2.38                     | 0.42              |
| 18:a8:82:PHE:HD2  | 21:a1:66:LEU:HD11  | 1.84                     | 0.42              |
| 24:c2:43:LEU:HD22 | 24:c2:53:VAL:HG12  | 2.00                     | 0.42              |
| 40:3A:85:LYS:HG2  | 40:3A:210:ARG:HH22 | 1.84                     | 0.42              |
| 43:3O:96:TRP:HB2  | 43:3O:99:ARG:HB2   | 2.01                     | 0.42              |
| 47:3S:48:LEU:HD21 | 47:3S:69:LEU:HD12  | 2.02                     | 0.42              |
| 53:S1:134:GLY:HA3 | 53:S1:241:ARG:HD2  | 2.00                     | 0.42              |
| 53:S1:260:ASN:OD1 | 53:S1:276:ARG:NH2  | 2.53                     | 0.42              |
| 51:v1:369:ARG:NE  | 52:v2:135:THR:O    | 2.53                     | 0.42              |
| 53:s1:637:ASP:OD1 | 53:s1:637:ASP:N    | 2.52                     | 0.42              |
| 1:3:18:ILE:HD12   | 4:1:76:THR:HB      | 2.01                     | 0.42              |
| 1:3:63:LEU:HD22   | 6:4L:72:ALA:HB2    | 2.02                     | 0.42              |
| 32:B8:73:GLY:HA3  | 33:B4:79:ASN:HD22  | 1.83                     | 0.42              |
| 8:4a:152:TYR:HD2  | 8:4a:215:TRP:HB3   | 1.84                     | 0.42              |
| 17:a6:120:ASP:OD1 | 17:a6:120:ASP:N    | 2.53                     | 0.42              |
| 25:s5:65:GLU:O    | 25:s5:69:ARG:HA    | 2.20                     | 0.42              |
| 25:s5:102:GLU:H   | 25:s5:102:GLU:HG3  | 1.58                     | 0.42              |
| 43:3D:96:TRP:H    | 43:3D:99:ARG:HB2   | 1.84                     | 0.42              |
| 41:3M:54:ASN:HB2  | 41:3M:56:ALA:HB2   | 2.01                     | 0.42              |
| 51:V1:86:ARG:NH1  | 51:V1:270:ASN:OD1  | 2.46                     | 0.42              |
| 51:v1:37:ASP:OD1  | 51:v1:37:ASP:N     | 2.48                     | 0.42              |
| 53:s1:627:SER:OG  | 53:s1:632:ILE:O    | 2.35                     | 0.42              |
| 2:S3:64:VAL:HA    | 2:S3:67:ILE:HG22   | 2.01                     | 0.42              |
| 2:S3:208:GLU:HB3  | 2:S3:223:VAL:HG23  | 2.01                     | 0.42              |
| 3:S2:223:HIS:HD2  | 54:S7:194:CYS:HB3  | 1.85                     | 0.42              |
| 4:1:34:ARG:HE     | 4:1:34:ARG:HB2     | 1.73                     | 0.42              |
| 4:1:181:MET:HE3   | 4:1:181:MET:HB3    | 1.82                     | 0.42              |
| 7:5:372:CYS:HA    | 7:5:375:ILE:HG22   | 2.02                     | 0.42              |
| 8:4:424:ILE:HG13  | 33:B4:56:ARG:HH21  | 1.83                     | 0.42              |
| 9:2:140:SER:HB2   | 25:S5:3:PHE:HD2    | 1.85                     | 0.42              |
| 14:A2:30:SER:HB3  | 14:A2:63:PRO:HG3   | 2.01                     | 0.42              |
| 18:A8:20:VAL:HG12 | 18:A8:25:LEU:HG    | 2.02                     | 0.42              |
| 32:B8:121:PRO:HG3 | 33:B4:15:PRO:HB3   | 2.00                     | 0.42              |
| 33:B4:123:ARG:HB3 | 33:B4:126:ASN:HB3  | 2.01                     | 0.42              |
| 1:3a:65:PHE:HB3   | 4:1a:144:VAL:HG11  | 2.01                     | 0.42              |
| 3:s2:117:HIS:NE2  | 54:s7:175:TYR:OH   | 2.41                     | 0.42              |
| 3:s2:323:ARG:N    | 3:s2:328:ASP:OD2   | 2.53                     | 0.42              |
| 3:s2:354:GLY:O    | 20:ao:8:GLN:NE2    | 2.44                     | 0.42              |
| 5:6a:125:MET:N    | 5:6a:125:MET:SD    | 2.93                     | 0.42              |
| 13:s6:54:GLU:O    | 37:an:131:TYR:OH   | 2.35                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:b9:29:SER:HB2   | 34:b9:80:TYR:H     | 1.84                     | 0.42              |
| 40:3L:285:ALA:O    | 40:3L:359:VAL:HA   | 2.18                     | 0.42              |
| 41:3M:51:SER:HB3   | 41:3M:230:LEU:HD12 | 2.00                     | 0.42              |
| 53:S1:406:ASN:HD21 | 53:S1:436:VAL:HG21 | 1.84                     | 0.42              |
| 53:s1:569:GLN:HG2  | 53:s1:584:LEU:HB2  | 2.01                     | 0.42              |
| 1:3:64:LEU:HA      | 1:3:67:LEU:HG      | 2.01                     | 0.42              |
| 7:5:226:GLN:O      | 7:5:230:HIS:N      | 2.53                     | 0.42              |
| 9:2:313:MET:HA     | 9:2:316:HIS:HB2    | 2.02                     | 0.42              |
| 12:S4:86:ASN:HD21  | 53:S1:284:GLU:HB3  | 1.85                     | 0.42              |
| 18:A8:151:ASN:ND2  | 28:B5:170:GLN:OE1  | 2.53                     | 0.42              |
| 36:BL:117:GLU:HB3  | 36:BL:121:TYR:HA   | 2.02                     | 0.42              |
| 5:6a:66:VAL:HG23   | 6:4l:75:LEU:HD21   | 2.02                     | 0.42              |
| 7:5a:257:ILE:H     | 7:5a:257:ILE:HG12  | 1.69                     | 0.42              |
| 7:5a:475:THR:HA    | 35:b7:55:GLN:HE22  | 1.84                     | 0.42              |
| 9:2a:240:MET:HE3   | 9:2a:240:MET:HB3   | 1.89                     | 0.42              |
| 20:ao:85:GLN:OE1   | 25:s5:105:ARG:NH2  | 2.52                     | 0.42              |
| 30:b2:69:ILE:O     | 30:b2:73:PHE:HB2   | 2.20                     | 0.42              |
| 41:3M:114:ALA:HB3  | 50:3T:66:ALA:HB3   | 2.01                     | 0.42              |
| 41:3M:358:VAL:HA   | 41:3M:361:VAL:HG12 | 2.02                     | 0.42              |
| 43:3O:98:HIS:NE2   | 43:3O:208:GLU:OE2  | 2.46                     | 0.42              |
| 43:3O:115:GLN:OE1  | 43:3O:140:TYR:OH   | 2.37                     | 0.42              |
| 43:3O:295:MET:HE1  | 48:3U:33:PHE:HE2   | 1.85                     | 0.42              |
| 55:S8:117:LYS:HA   | 55:S8:130:ILE:HD11 | 2.02                     | 0.42              |
| 53:s1:358:LEU:HA   | 53:s1:361:VAL:HG12 | 2.02                     | 0.42              |
| 54:s7:189:ILE:HG21 | 54:s7:208:LEU:HB2  | 2.02                     | 0.42              |
| 3:S2:379:ILE:HG21  | 53:S1:143:SER:HB3  | 2.02                     | 0.42              |
| 4:1:215:TYR:HD2    | 4:1:219:PRO:HB2    | 1.85                     | 0.42              |
| 8:4:50:LYS:HB2     | 8:4:58:SER:HB3     | 2.02                     | 0.42              |
| 9:2:335:MET:HB2    | 24:C2:37:LEU:HD21  | 2.02                     | 0.42              |
| 31:B3:24:ASP:OD1   | 31:B3:27:GLN:NE2   | 2.46                     | 0.42              |
| 1:3a:79:ILE:HD12   | 1:3a:79:ILE:HA     | 1.94                     | 0.42              |
| 3:s2:375:MET:HE3   | 53:s1:124:HIS:HB3  | 2.02                     | 0.42              |
| 4:1a:61:MET:HG3    | 54:s7:126:ARG:HE   | 1.84                     | 0.42              |
| 6:4l:63:ILE:HG12   | 9:2a:71:LEU:HD21   | 2.02                     | 0.42              |
| 6:4l:77:LEU:HD21   | 9:2a:57:THR:HA     | 2.02                     | 0.42              |
| 7:5a:361:ASN:HB2   | 7:5a:435:PRO:HB3   | 2.01                     | 0.42              |
| 8:4a:359:TRP:CD1   | 8:4a:415:GLN:HE22  | 2.37                     | 0.42              |
| 9:2a:27:MET:HE2    | 9:2a:27:MET:HB2    | 1.90                     | 0.42              |
| 16:a5:66:LYS:HD3   | 16:a5:66:LYS:HA    | 1.83                     | 0.42              |
| 27:bm:119:GLU:OE2  | 27:bm:122:ARG:NH2  | 2.53                     | 0.42              |
| 28:b5:95:GLU:HA    | 28:b5:116:PRO:HD3  | 2.02                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:b6:120:MET:H    | 29:b6:120:MET:HG2  | 1.66                     | 0.42              |
| 40:3A:305:GLN:HB3  | 40:3A:395:LEU:HD11 | 2.01                     | 0.42              |
| 40:3L:274:GLU:HG2  | 46:3R:18:SER:HB2   | 2.00                     | 0.42              |
| 51:V1:282:VAL:HA   | 51:V1:307:VAL:HA   | 2.02                     | 0.42              |
| 51:v1:357:MET:HB3  | 51:v1:361:THR:HG21 | 2.02                     | 0.42              |
| 1:3:34:ALA:HB1     | 4:1:63:PRO:HA      | 2.02                     | 0.42              |
| 1:3:81:THR:O       | 22:A3:46:ASN:ND2   | 2.53                     | 0.42              |
| 4:1:75:PRO:HB2     | 4:1:222:LEU:HD23   | 2.02                     | 0.42              |
| 7:5:149:ILE:HD13   | 7:5:149:ILE:HA     | 1.88                     | 0.42              |
| 7:5:600:ILE:HD13   | 7:5:600:ILE:HA     | 1.96                     | 0.42              |
| 30:B2:53:SER:O     | 30:B2:57:GLN:CB    | 2.68                     | 0.42              |
| 3:s2:65:PRO:HD2    | 9:2a:51:ARG:HH12   | 1.84                     | 0.42              |
| 4:1a:196:ALA:HA    | 4:1a:199:ASP:HB3   | 2.01                     | 0.42              |
| 4:1a:302:MET:HE2   | 4:1a:302:MET:HB2   | 1.93                     | 0.42              |
| 10:al:150:LEU:HD13 | 10:al:156:GLY:HA2  | 2.01                     | 0.42              |
| 12:s4:150:LYS:HE2  | 12:s4:152:VAL:HG12 | 2.01                     | 0.42              |
| 17:a6:84:LEU:HA    | 17:a6:87:ILE:HG22  | 2.02                     | 0.42              |
| 20:ao:88:ARG:HA    | 20:ao:88:ARG:HD2   | 1.85                     | 0.42              |
| 21:a1:3:PHE:HE2    | 37:an:13:ARG:HH21  | 1.68                     | 0.42              |
| 32:b8:166:LEU:HB2  | 32:b8:170:ARG:HH21 | 1.85                     | 0.42              |
| 41:3B:272:VAL:HG12 | 41:3B:337:GLY:HA3  | 2.02                     | 0.42              |
| 53:S1:221:ASN:HD21 | 53:S1:286:ILE:H    | 1.67                     | 0.42              |
| 53:S1:525:ALA:HB1  | 53:S1:530:TYR:HB2  | 2.02                     | 0.42              |
| 54:S7:146:ARG:HA   | 54:S7:146:ARG:HD2  | 1.82                     | 0.42              |
| 55:S8:149:MET:HB2  | 55:S8:183:LEU:HB3  | 2.02                     | 0.42              |
| 53:s1:170:LYS:O    | 53:s1:231:LEU:HA   | 2.20                     | 0.42              |
| 53:s1:266:ARG:HH12 | 55:s8:117:LYS:HE2  | 1.84                     | 0.42              |
| 7:5:159:TYR:HB3    | 8:4:416:ARG:HG2    | 2.01                     | 0.41              |
| 8:4:281:ASP:OD1    | 8:4:281:ASP:N      | 2.52                     | 0.41              |
| 11:A9:157:LYS:HA   | 11:A9:157:LYS:HD2  | 1.86                     | 0.41              |
| 12:S4:126:LEU:HD12 | 12:S4:126:LEU:HA   | 1.88                     | 0.41              |
| 29:B6:26:GLN:OE1   | 34:B9:175:ARG:NH1  | 2.53                     | 0.41              |
| 3:s2:392:PRO:HA    | 3:s2:393:PRO:HD3   | 1.89                     | 0.41              |
| 3:s2:435:LEU:O     | 3:s2:439:SER:OG    | 2.37                     | 0.41              |
| 4:1a:87:VAL:HG23   | 4:1a:88:PRO:HD3    | 2.02                     | 0.41              |
| 7:5a:378:LEU:HA    | 7:5a:381:THR:HG22  | 2.01                     | 0.41              |
| 8:4a:190:TRP:HA    | 8:4a:193:ASN:HB2   | 2.02                     | 0.41              |
| 9:2a:29:MET:HE3    | 9:2a:141:ILE:HA    | 2.02                     | 0.41              |
| 14:a2:54:LEU:HD21  | 53:s1:529:GLY:HA3  | 2.01                     | 0.41              |
| 34:b9:95:GLU:HA    | 34:b9:98:LYS:HG3   | 2.01                     | 0.41              |
| 42:3C:78:LEU:O     | 42:3C:82:MET:CB    | 2.68                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:3F:10:SER:OG    | 45:3F:11:SER:N     | 2.53                     | 0.41              |
| 41:3M:49:ILE:HD12  | 41:3M:220:LEU:HB3  | 2.02                     | 0.41              |
| 42:3N:345:HIS:HA   | 42:3N:346:PRO:HA   | 1.94                     | 0.41              |
| 52:V2:194:ASP:OD2  | 52:V2:221:ARG:NH1  | 2.52                     | 0.41              |
| 51:v1:316:ALA:HB3  | 51:v1:357:MET:HB2  | 2.01                     | 0.41              |
| 4:1:20:LEU:HA      | 4:1:23:VAL:HG22    | 2.03                     | 0.41              |
| 7:5:312:LEU:HD21   | 7:5:395:ILE:HG21   | 2.01                     | 0.41              |
| 16:A5:33:ASP:HA    | 16:A5:36:LYS:HG2   | 2.01                     | 0.41              |
| 2:s3:47:ARG:HA     | 3:s2:162:GLN:HB2   | 2.01                     | 0.41              |
| 3:s2:390:GLN:O     | 38:a7:60:ARG:NH2   | 2.47                     | 0.41              |
| 9:2a:328:THR:O     | 9:2a:332:MET:HB2   | 2.20                     | 0.41              |
| 13:s6:78:ALA:HB1   | 13:s6:90:LYS:HG2   | 2.01                     | 0.41              |
| 16:a5:68:LEU:O     | 16:a5:72:LEU:HB2   | 2.20                     | 0.41              |
| 24:c2:99:GLU:H     | 24:c2:99:GLU:HG3   | 1.62                     | 0.41              |
| 28:b5:171:PHE:HA   | 28:b5:172:PRO:HD3  | 1.89                     | 0.41              |
| 36:bl:137:LYS:HE2  | 36:bl:137:LYS:HB2  | 1.92                     | 0.41              |
| 53:S1:121:LEU:HD21 | 53:S1:139:LEU:HD21 | 2.01                     | 0.41              |
| 53:S1:232:THR:OG1  | 53:S1:233:SER:N    | 2.54                     | 0.41              |
| 51:v1:395:VAL:HG22 | 51:v1:398:ARG:HH12 | 1.85                     | 0.41              |
| 52:v2:62:ILE:HD12  | 52:v2:81:VAL:HG22  | 2.02                     | 0.41              |
| 2:S3:84:GLU:HA     | 2:S3:141:ARG:O     | 2.20                     | 0.41              |
| 2:S3:93:ILE:HD13   | 2:S3:93:ILE:HA     | 1.94                     | 0.41              |
| 3:S2:267:ILE:HB    | 4:1:278:PRO:HG2    | 2.00                     | 0.41              |
| 7:5:477:ILE:HD11   | 35:B7:55:GLN:HA    | 2.01                     | 0.41              |
| 11:A9:73:LEU:HD13  | 11:A9:250:VAL:HG22 | 2.01                     | 0.41              |
| 11:A9:354:ARG:NH1  | 11:A9:362:LEU:O    | 2.53                     | 0.41              |
| 37:AN:36:ASP:OD2   | 55:S8:85:ASN:ND2   | 2.50                     | 0.41              |
| 4:1a:13:ILE:HD12   | 4:1a:13:ILE:HA     | 1.91                     | 0.41              |
| 7:5a:295:GLN:HE21  | 7:5a:300:LYS:HB3   | 1.85                     | 0.41              |
| 18:a8:83:THR:HA    | 18:a8:86:TRP:HD1   | 1.84                     | 0.41              |
| 19:am:77:SER:HA    | 19:am:80:VAL:HG12  | 2.02                     | 0.41              |
| 40:3A:53:LEU:HD11  | 40:3A:246:ALA:HB1  | 2.03                     | 0.41              |
| 40:3A:278:ARG:NH2  | 40:3A:280:ASP:OD2  | 2.47                     | 0.41              |
| 43:3D:146:LYS:HE3  | 43:3D:146:LYS:HB3  | 1.93                     | 0.41              |
| 43:3D:181:ASN:OD1  | 43:3D:184:ALA:N    | 2.47                     | 0.41              |
| 45:3F:53:GLU:OE2   | 45:3F:57:ASN:ND2   | 2.52                     | 0.41              |
| 41:3M:101:ARG:O    | 41:3M:105:ALA:CB   | 2.69                     | 0.41              |
| 43:3O:99:ARG:NH2   | 43:3O:209:ASP:OD1  | 2.49                     | 0.41              |
| 46:3R:71:LYS:HA    | 46:3R:71:LYS:HD2   | 1.81                     | 0.41              |
| 52:V2:140:MET:HA   | 52:V2:144:SER:HB2  | 2.03                     | 0.41              |
| 52:v2:48:PRO:HA    | 52:v2:95:SER:HB3   | 2.01                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:S2:197:MET:H     | 3:S2:197:MET:HG2   | 1.72                     | 0.41              |
| 7:5:538:PRO:HB2    | 32:B8:117:VAL:HB   | 2.02                     | 0.41              |
| 19:AM:44:ASN:O     | 19:AM:55:ARG:NH1   | 2.54                     | 0.41              |
| 28:B5:58:LYS:HB2   | 28:B5:58:LYS:HE3   | 1.87                     | 0.41              |
| 4:1a:85:LEU:HD23   | 4:1a:105:ILE:HD12  | 2.03                     | 0.41              |
| 5:6a:25:PRO:HG3    | 6:4l:28:SER:HB3    | 2.01                     | 0.41              |
| 8:4a:370:PRO:HB3   | 8:4a:375:LEU:HD22  | 2.03                     | 0.41              |
| 9:2a:19:ILE:O      | 9:2a:23:SER:HB3    | 2.20                     | 0.41              |
| 11:a9:57:THR:HG21  | 11:a9:120:VAL:HG12 | 2.01                     | 0.41              |
| 46:3G:80:ASN:O     | 47:3H:58:ARG:NH1   | 2.52                     | 0.41              |
| 42:3N:207:ASN:OD1  | 42:3N:210:GLY:N    | 2.53                     | 0.41              |
| 51:v1:80:MET:HE1   | 51:v1:85:LEU:HD12  | 2.02                     | 0.41              |
| 53:s1:125:PRO:HD2  | 53:s1:175:ARG:HA   | 2.02                     | 0.41              |
| 53:s1:406:ASN:HA   | 53:s1:407:PRO:HD3  | 1.95                     | 0.41              |
| 3:S2:184:ILE:HG23  | 3:S2:203:MET:HB3   | 2.01                     | 0.41              |
| 3:S2:237:PRO:HG2   | 3:S2:240:LEU:HB2   | 2.02                     | 0.41              |
| 7:5:177:ILE:HB     | 7:5:229:LEU:HD21   | 2.03                     | 0.41              |
| 7:5:508:THR:OG1    | 34:B9:36:LYS:NZ    | 2.51                     | 0.41              |
| 16:A5:66:LYS:H     | 16:A5:66:LYS:HG2   | 1.72                     | 0.41              |
| 27:BM:121:GLU:HA   | 36:BL:9:VAL:HG21   | 2.02                     | 0.41              |
| 34:B9:44:MET:HE2   | 34:B9:44:MET:HB2   | 1.93                     | 0.41              |
| 1:3a:49:LEU:HD23   | 1:3a:49:LEU:HA     | 1.96                     | 0.41              |
| 3:s2:97:LEU:HD22   | 3:s2:109:CYS:HB2   | 2.02                     | 0.41              |
| 5:6a:33:ILE:HD13   | 5:6a:33:ILE:HA     | 1.94                     | 0.41              |
| 5:6a:40:CYS:O      | 5:6a:44:LEU:HB2    | 2.21                     | 0.41              |
| 11:a9:261:LYS:HE3  | 11:a9:261:LYS:HB2  | 1.93                     | 0.41              |
| 33:b4:9:ALA:HB3    | 33:b4:12:ALA:H     | 1.85                     | 0.41              |
| 40:3L:233:ALA:HB1  | 40:3L:237:VAL:HG21 | 2.02                     | 0.41              |
| 42:3N:14:ILE:HD13  | 42:3N:14:ILE:HA    | 1.96                     | 0.41              |
| 49:3V:12:GLU:O     | 49:3V:16:ASN:HB2   | 2.20                     | 0.41              |
| 53:s1:103:LEU:HB3  | 53:s1:106:SER:HB3  | 2.01                     | 0.41              |
| 53:s1:255:ASP:OD1  | 53:s1:289:LYS:NZ   | 2.52                     | 0.41              |
| 53:s1:301:ARG:HH12 | 53:s1:588:ALA:HB2  | 1.86                     | 0.41              |
| 7:5:74:MET:HE3     | 7:5:74:MET:HB3     | 1.84                     | 0.41              |
| 12:S4:112:MET:HE2  | 12:S4:112:MET:HB3  | 1.90                     | 0.41              |
| 17:A6:49:THR:HG23  | 17:A6:53:MET:HE2   | 2.01                     | 0.41              |
| 30:B2:62:SER:OG    | 31:B3:75:LYS:O     | 2.37                     | 0.41              |
| 3:s2:294:ARG:O     | 3:s2:321:GLY:N     | 2.51                     | 0.41              |
| 6:4l:80:LYS:HE3    | 9:2a:48:LYS:HD3    | 2.02                     | 0.41              |
| 7:5a:125:LEU:HD12  | 7:5a:125:LEU:HA    | 1.92                     | 0.41              |
| 8:4a:21:LYS:HA     | 8:4a:21:LYS:HD3    | 1.91                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:a9:214:LEU:HD12 | 11:a9:352:VAL:HG11 | 2.03                     | 0.41              |
| 11:a9:360:ARG:O    | 11:a9:360:ARG:NH1  | 2.49                     | 0.41              |
| 30:b2:43:ARG:HD3   | 30:b2:48:PRO:HA    | 2.02                     | 0.41              |
| 40:3A:450:TYR:OH   | 40:3A:480:PHE:O    | 2.39                     | 0.41              |
| 42:3C:242:LEU:HD23 | 42:3C:242:LEU:HA   | 1.97                     | 0.41              |
| 43:3D:114:PHE:HE2  | 43:3D:148:LEU:HD13 | 1.86                     | 0.41              |
| 41:3M:123:VAL:HG11 | 41:3M:133:LEU:HB3  | 2.03                     | 0.41              |
| 42:3N:359:PHE:O    | 42:3N:363:LEU:HB2  | 2.20                     | 0.41              |
| 43:3O:281:GLU:O    | 43:3O:285:ARG:CB   | 2.69                     | 0.41              |
| 55:S8:85:ASN:O     | 55:S8:89:GLU:N     | 2.44                     | 0.41              |
| 51:v1:413:TRP:HB2  | 51:v1:439:ILE:HD13 | 2.01                     | 0.41              |
| 7:5:224:SER:OG     | 7:5:224:SER:O      | 2.38                     | 0.41              |
| 16:A5:93:LYS:HD3   | 16:A5:93:LYS:HA    | 1.84                     | 0.41              |
| 28:B5:171:PHE:HA   | 28:B5:172:PRO:HD3  | 1.94                     | 0.41              |
| 34:B9:76:HIS:ND1   | 34:B9:78:GLN:O     | 2.54                     | 0.41              |
| 37:AN:116:ASN:OD1  | 37:AN:116:ASN:N    | 2.54                     | 0.41              |
| 7:5a:558:LEU:HD11  | 8:4a:211:GLY:HA2   | 2.01                     | 0.41              |
| 7:5a:568:THR:HA    | 7:5a:571:THR:HG22  | 2.02                     | 0.41              |
| 14:a2:16:LEU:HD12  | 14:a2:69:TYR:HE1   | 1.86                     | 0.41              |
| 18:a8:93:ASN:OD1   | 18:a8:93:ASN:N     | 2.44                     | 0.41              |
| 18:a8:147:ARG:HD3  | 18:a8:148:PRO:HD2  | 2.02                     | 0.41              |
| 35:b7:84:GLN:O     | 35:b7:88:ASP:HB2   | 2.20                     | 0.41              |
| 38:a7:65:PRO:HA    | 38:a7:66:PRO:HD3   | 1.93                     | 0.41              |
| 42:3N:328:LEU:HB2  | 42:3N:361:ILE:HG21 | 2.03                     | 0.41              |
| 53:s1:303:THR:HB   | 53:s1:614:GLY:HA3  | 2.02                     | 0.41              |
| 1:3:29:LEU:O       | 11:A9:355:ARG:NH1  | 2.54                     | 0.41              |
| 1:3:98:LEU:HD23    | 4:1:298:LEU:HD11   | 2.03                     | 0.41              |
| 4:1:235:ASN:O      | 4:1:239:THR:OG1    | 2.34                     | 0.41              |
| 6:4L:20:LEU:HB3    | 7:5:592:LEU:HD12   | 2.03                     | 0.41              |
| 14:A2:23:LEU:HB2   | 14:A2:57:GLU:HG3   | 2.01                     | 0.41              |
| 17:A6:130:ASP:OD1  | 17:A6:130:ASP:N    | 2.54                     | 0.41              |
| 1:3a:57:LEU:O      | 1:3a:61:THR:OG1    | 2.33                     | 0.41              |
| 2:s3:93:ILE:HG13   | 2:s3:94:PRO:HD3    | 2.01                     | 0.41              |
| 3:s2:50:ALA:HB2    | 3:s2:63:PRO:HA     | 2.02                     | 0.41              |
| 3:s2:188:THR:HG23  | 3:s2:200:PHE:HA    | 2.03                     | 0.41              |
| 7:5a:149:ILE:HG13  | 8:4a:369:LEU:HD13  | 2.02                     | 0.41              |
| 8:4a:230:ILE:HD12  | 8:4a:230:ILE:HA    | 1.92                     | 0.41              |
| 8:4a:421:ASN:HD22  | 34:b9:100:PRO:HG3  | 1.86                     | 0.41              |
| 9:2a:127:GLY:HA2   | 9:2a:130:LEU:HB3   | 2.02                     | 0.41              |
| 11:a9:125:VAL:HG12 | 11:a9:163:ARG:HB3  | 2.03                     | 0.41              |
| 20:ao:61:LEU:O     | 20:ao:65:LEU:HB2   | 2.20                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:a1:52:ARG:NH1   | 21:a1:58:ASN:OD1   | 2.44                     | 0.41              |
| 38:a7:5:THR:O      | 38:a7:9:GLN:HB2    | 2.20                     | 0.41              |
| 39:v3:68:LYS:HA    | 39:v3:68:LYS:HD3   | 1.93                     | 0.41              |
| 45:3F:36:ASP:OD1   | 45:3F:90:TYR:OH    | 2.35                     | 0.41              |
| 45:3F:45:LYS:HE2   | 45:3F:45:LYS:HB2   | 1.86                     | 0.41              |
| 40:3L:93:LEU:HD11  | 40:3L:220:LEU:HB2  | 2.02                     | 0.41              |
| 40:3L:274:GLU:OE1  | 40:3L:276:ARG:NE   | 2.54                     | 0.41              |
| 45:3Q:99:ILE:HD13  | 45:3Q:99:ILE:HA    | 1.94                     | 0.41              |
| 51:v1:115:VAL:HB   | 51:v1:156:ILE:HA   | 2.01                     | 0.41              |
| 53:s1:407:PRO:HB2  | 53:s1:415:ASN:HB2  | 2.02                     | 0.41              |
| 3:S2:376:GLU:HG3   | 53:S1:151:SER:HB3  | 2.03                     | 0.41              |
| 7:5:149:ILE:HG22   | 7:5:150:MET:HE2    | 2.02                     | 0.41              |
| 7:5:316:THR:HA     | 7:5:319:MET:HB3    | 2.02                     | 0.41              |
| 7:5:464:ALA:HA     | 7:5:467:VAL:HG12   | 2.03                     | 0.41              |
| 8:4:365:ALA:O      | 8:4:374:ASN:ND2    | 2.52                     | 0.41              |
| 10:AL:180:ARG:HH21 | 10:AL:182:GLN:HE21 | 1.68                     | 0.41              |
| 12:S4:79:ILE:HD12  | 12:S4:134:ALA:HB1  | 2.03                     | 0.41              |
| 15:AB:80:LYS:HA    | 15:AB:80:LYS:HD3   | 1.90                     | 0.41              |
| 17:A6:112:GLU:H    | 17:A6:112:GLU:HG2  | 1.68                     | 0.41              |
| 37:AN:132:SER:OG   | 37:AN:134:THR:OG1  | 2.39                     | 0.41              |
| 39:V3:97:SER:HB3   | 52:V2:72:GLY:HA3   | 2.03                     | 0.41              |
| 3:s2:62:LYS:HD2    | 3:s2:62:LYS:HA     | 1.86                     | 0.41              |
| 3:s2:397:TYR:OH    | 3:s2:406:GLU:OE2   | 2.37                     | 0.41              |
| 3:s2:448:VAL:HA    | 3:s2:451:ILE:HG22  | 2.03                     | 0.41              |
| 6:4l:54:MET:HA     | 6:4l:57:MET:HG3    | 2.03                     | 0.41              |
| 7:5a:539:MET:O     | 7:5a:543:ASN:HB2   | 2.21                     | 0.41              |
| 8:4a:133:ILE:HD13  | 8:4a:219:ALA:HB1   | 2.02                     | 0.41              |
| 8:4a:348:LEU:H     | 8:4a:415:GLN:HA    | 1.86                     | 0.41              |
| 9:2a:13:ILE:HD12   | 9:2a:13:ILE:HA     | 1.95                     | 0.41              |
| 9:2a:108:LEU:HD13  | 9:2a:157:LEU:HB3   | 2.03                     | 0.41              |
| 10:al:170:LEU:HA   | 10:al:173:MET:HE3  | 2.03                     | 0.41              |
| 10:al:204:VAL:HB   | 10:al:255:VAL:HG12 | 2.03                     | 0.41              |
| 11:a9:211:ASP:O    | 11:a9:215:ASN:ND2  | 2.51                     | 0.41              |
| 13:s6:107:CYS:O    | 55:s8:141:ARG:NH2  | 2.54                     | 0.41              |
| 19:am:53:VAL:HA    | 19:am:56:VAL:HG12  | 2.02                     | 0.41              |
| 24:c2:13:PHE:HE2   | 24:c2:74:PHE:HB3   | 1.86                     | 0.41              |
| 40:3A:276:ARG:HH21 | 40:3A:465:LEU:HD23 | 1.86                     | 0.41              |
| 41:3B:76:ASN:HA    | 41:3B:196:ARG:HH12 | 1.86                     | 0.41              |
| 41:3B:293:LEU:HB3  | 41:3B:309:LEU:HG   | 2.03                     | 0.41              |
| 41:3M:138:LEU:HD11 | 41:3M:238:LEU:HB2  | 2.03                     | 0.41              |
| 41:3M:348:GLY:O    | 41:3M:352:ASN:HB2  | 2.20                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:3O:242:ILE:HG23 | 43:3O:244:MET:H    | 1.85                     | 0.41              |
| 47:3S:42:VAL:HA    | 47:3S:45:ARG:HB3   | 2.03                     | 0.41              |
| 51:V1:48:ARG:HH22  | 52:V2:230:LEU:HG   | 1.86                     | 0.41              |
| 51:V1:281:HIS:H    | 52:V2:142:ARG:HD3  | 1.86                     | 0.41              |
| 51:V1:307:VAL:HG11 | 51:V1:356:VAL:HG11 | 2.03                     | 0.41              |
| 52:V2:190:ASN:HB3  | 52:V2:215:PRO:HB3  | 2.03                     | 0.41              |
| 53:S1:358:LEU:HA   | 53:S1:361:VAL:HG12 | 2.03                     | 0.41              |
| 53:S1:556:THR:OG1  | 53:S1:557:ARG:N    | 2.54                     | 0.41              |
| 54:S7:160:SER:OG   | 54:S7:166:ASN:OD1  | 2.38                     | 0.41              |
| 51:v1:127:ASP:HA   | 51:v1:130:ILE:HG22 | 2.01                     | 0.41              |
| 53:s1:542:PRO:HG2  | 53:s1:545:LEU:HB2  | 2.02                     | 0.41              |
| 53:s1:556:THR:OG1  | 53:s1:557:ARG:N    | 2.54                     | 0.41              |
| 54:s7:163:SER:HA   | 54:s7:166:ASN:HD22 | 1.86                     | 0.41              |
| 5:6:165:ILE:HG12   | 9:2:42:PRO:HG2     | 2.03                     | 0.41              |
| 7:5:406:ALA:HB2    | 32:B8:152:SER:HB2  | 2.03                     | 0.41              |
| 8:4:79:ALA:HB2     | 8:4:436:LEU:HD21   | 2.03                     | 0.41              |
| 8:4:148:TYR:O      | 8:4:152:TYR:HB2    | 2.21                     | 0.41              |
| 8:4:303:ILE:HD12   | 8:4:303:ILE:HA     | 1.96                     | 0.41              |
| 9:2:88:GLN:HA      | 9:2:148:LEU:HD11   | 2.02                     | 0.41              |
| 10:AL:62:VAL:HG12  | 10:AL:205:ILE:HB   | 2.03                     | 0.41              |
| 11:A9:207:PHE:HD1  | 11:A9:214:LEU:HD11 | 1.86                     | 0.41              |
| 18:A8:154:ILE:HG12 | 24:C2:92:GLY:HA3   | 2.02                     | 0.41              |
| 22:A3:18:VAL:HG13  | 22:A3:19:LEU:HD12  | 2.03                     | 0.41              |
| 33:B4:115:LEU:HB3  | 33:B4:121:LEU:HB2  | 2.03                     | 0.41              |
| 38:A7:65:PRO:HA    | 38:A7:66:PRO:HD3   | 1.95                     | 0.41              |
| 2:s3:208:GLU:OE2   | 54:s7:179:ARG:NH1  | 2.52                     | 0.41              |
| 4:1a:24:GLU:O      | 4:1a:28:LEU:HB2    | 2.21                     | 0.41              |
| 7:5a:492:ILE:HD13  | 7:5a:492:ILE:HA    | 1.97                     | 0.41              |
| 8:4a:341:THR:HG22  | 8:4a:343:ILE:H     | 1.86                     | 0.41              |
| 20:ao:83:THR:HA    | 20:ao:86:ILE:HG22  | 2.03                     | 0.41              |
| 27:bm:117:ARG:NH1  | 36:bl:108:GLU:OE2  | 2.51                     | 0.41              |
| 29:b6:109:THR:HG22 | 29:b6:116:VAL:HG22 | 2.03                     | 0.41              |
| 30:b2:56:ILE:HD12  | 30:b2:56:ILE:HA    | 1.97                     | 0.41              |
| 36:bl:7:LYS:HE3    | 36:bl:12:GLU:HB3   | 2.03                     | 0.41              |
| 41:3B:130:ILE:HA   | 41:3B:133:LEU:HD12 | 2.03                     | 0.41              |
| 41:3M:250:LYS:HA   | 41:3M:250:LYS:HD2  | 1.87                     | 0.41              |
| 44:3P:120:THR:HA   | 44:3P:123:VAL:HG12 | 2.02                     | 0.41              |
| 53:S1:624:ARG:NE   | 53:S1:636:TYR:O    | 2.50                     | 0.41              |
| 53:s1:476:LEU:HD11 | 53:s1:489:ILE:HG22 | 2.02                     | 0.41              |
| 1:3:17:LEU:HA      | 1:3:20:VAL:HG12    | 2.03                     | 0.40              |
| 1:3:55:PHE:O       | 1:3:59:ALA:HB2     | 2.20                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:S3:104:ASN:HB3   | 38:A7:96:THR:HG22  | 2.03                     | 0.40              |
| 7:5:283:LEU:HB2    | 32:B8:144:PHE:HE2  | 1.85                     | 0.40              |
| 8:4:345:ALA:HA     | 8:4:423:MET:HE1    | 2.03                     | 0.40              |
| 9:2:249:LEU:HD23   | 9:2:249:LEU:HA     | 1.94                     | 0.40              |
| 32:B8:71:GLY:HA3   | 33:B4:76:ILE:HG23  | 2.02                     | 0.40              |
| 32:B8:122:THR:OG1  | 32:B8:124:VAL:O    | 2.35                     | 0.40              |
| 36:BL:85:ILE:O     | 36:BL:89:GLU:HB2   | 2.20                     | 0.40              |
| 38:A7:33:LYS:O     | 38:A7:36:GLN:NE2   | 2.49                     | 0.40              |
| 4:1a:288:LEU:O     | 4:1a:292:ASN:HB2   | 2.21                     | 0.40              |
| 17:a6:44:ARG:HD3   | 17:a6:44:ARG:HA    | 1.87                     | 0.40              |
| 24:c2:120:ARG:HD2  | 33:b4:116:ILE:HG13 | 2.02                     | 0.40              |
| 26:b1:46:ARG:HE    | 26:b1:46:ARG:HB3   | 1.60                     | 0.40              |
| 30:b2:96:GLU:HG3   | 30:b2:97:LEU:HD12  | 2.03                     | 0.40              |
| 40:3A:336:LYS:HD3  | 40:3A:336:LYS:HA   | 1.85                     | 0.40              |
| 40:3L:58:ARG:HG2   | 40:3L:417:LEU:HD12 | 2.03                     | 0.40              |
| 41:3M:197:MET:H    | 41:3M:197:MET:HG2  | 1.67                     | 0.40              |
| 43:3O:208:GLU:OE1  | 43:3O:275:ARG:NH2  | 2.54                     | 0.40              |
| 3:S2:339:GLN:OE1   | 3:S2:342:ARG:NE    | 2.53                     | 0.40              |
| 7:5:378:LEU:HD12   | 7:5:378:LEU:HA     | 1.96                     | 0.40              |
| 7:5:459:PHE:HA     | 7:5:462:ILE:HG22   | 2.03                     | 0.40              |
| 8:4:15:THR:O       | 8:4:93:LYS:NZ      | 2.48                     | 0.40              |
| 24:C2:37:LEU:O     | 24:C2:41:THR:OG1   | 2.32                     | 0.40              |
| 25:S5:36:PHE:HB3   | 25:S5:63:PHE:HB2   | 2.03                     | 0.40              |
| 32:B8:36:MET:HE3   | 32:B8:36:MET:HB2   | 1.90                     | 0.40              |
| 3:s2:52:MET:SD     | 9:2a:295:ARG:NH1   | 2.94                     | 0.40              |
| 7:5a:12:PHE:HE2    | 7:5a:130:ILE:HD13  | 1.87                     | 0.40              |
| 12:s4:151:LYS:HB2  | 12:s4:151:LYS:HE2  | 1.89                     | 0.40              |
| 15:ac:138:LEU:HD12 | 15:ac:138:LEU:HA   | 1.90                     | 0.40              |
| 19:am:102:GLY:HA2  | 19:am:105:THR:HG22 | 2.04                     | 0.40              |
| 28:b5:109:HIS:NE2  | 28:b5:122:ALA:O    | 2.54                     | 0.40              |
| 29:b6:121:ARG:HB2  | 35:b7:40:VAL:HB    | 2.03                     | 0.40              |
| 40:3A:37:THR:OG1   | 40:3A:38:PHE:N     | 2.54                     | 0.40              |
| 40:3A:98:PHE:HB2   | 40:3A:99:LYS:HE3   | 2.02                     | 0.40              |
| 42:3C:3:ASN:O      | 42:3C:7:THR:CB     | 2.69                     | 0.40              |
| 40:3L:136:LEU:HD21 | 41:3M:380:ALA:HA   | 2.04                     | 0.40              |
| 41:3M:43:LEU:HB2   | 41:3M:47:LEU:HB3   | 2.02                     | 0.40              |
| 53:s1:177:ILE:HG13 | 53:s1:179:CYS:HB3  | 2.04                     | 0.40              |
| 54:s7:113:ASP:OD2  | 54:s7:116:ARG:N    | 2.51                     | 0.40              |
| 54:s7:207:GLN:NE2  | 55:s8:176:SER:O    | 2.49                     | 0.40              |
| 7:5:396:ILE:HG21   | 7:5:490:ALA:HB2    | 2.03                     | 0.40              |
| 8:4:22:LYS:O       | 8:4:26:ASN:ND2     | 2.54                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:4:367:LEU:HD12  | 8:4:404:GLY:HA2    | 2.03                     | 0.40              |
| 9:2:178:ILE:HD11  | 9:2:292:PHE:HB2    | 2.02                     | 0.40              |
| 9:2:275:CYS:HB2   | 19:AM:137:PRO:HG2  | 2.03                     | 0.40              |
| 11:A9:55:VAL:HG11 | 13:S6:43:TYR:HB2   | 2.04                     | 0.40              |
| 19:AM:37:SER:HB2  | 19:AM:56:VAL:HA    | 2.04                     | 0.40              |
| 20:AO:11:PRO:HA   | 20:AO:12:PRO:HD3   | 1.96                     | 0.40              |
| 20:AO:23:ARG:HE   | 20:AO:23:ARG:HB2   | 1.75                     | 0.40              |
| 33:B4:48:LEU:HD23 | 33:B4:48:LEU:HA    | 1.98                     | 0.40              |
| 33:B4:85:LYS:HA   | 33:B4:85:LYS:HD3   | 1.93                     | 0.40              |
| 34:B9:47:ARG:NH2  | 60:B9:201:EHZ:O1   | 2.46                     | 0.40              |
| 37:AN:92:ARG:HD3  | 55:S8:200:GLU:HG2  | 2.03                     | 0.40              |
| 3:s2:115:LEU:O    | 54:s7:138:THR:OG1  | 2.38                     | 0.40              |
| 5:6a:17:LEU:HD21  | 5:6a:95:GLY:HA3    | 2.03                     | 0.40              |
| 5:6a:66:VAL:HA    | 5:6a:69:TYR:HB2    | 2.04                     | 0.40              |
| 8:4a:245:ARG:HD2  | 8:4a:245:ARG:HA    | 1.76                     | 0.40              |
| 9:2a:55:ALA:HB1   | 9:2a:118:VAL:HA    | 2.04                     | 0.40              |
| 9:2a:116:PRO:HA   | 9:2a:119:THR:HG22  | 2.03                     | 0.40              |
| 11:a9:45:LYS:HG3  | 17:a6:117:ARG:HH21 | 1.86                     | 0.40              |
| 13:s6:72:VAL:HG13 | 13:s6:77:ILE:HD13  | 2.04                     | 0.40              |
| 20:ao:93:GLU:OE1  | 25:s5:92:TYR:OH    | 2.39                     | 0.40              |
| 33:b4:81:ARG:HA   | 33:b4:82:PRO:HD3   | 1.95                     | 0.40              |
| 38:a7:27:ARG:HD2  | 38:a7:31:ILE:HD11  | 2.02                     | 0.40              |
| 40:3A:298:ASN:HA  | 40:3A:299:PRO:HD3  | 1.88                     | 0.40              |
| 40:3L:254:SER:OG  | 40:3L:255:ARG:N    | 2.40                     | 0.40              |
| 41:3M:182:TYR:OH  | 41:3M:333:SER:O    | 2.37                     | 0.40              |
| 42:3N:256:TYR:HB3 | 43:3O:199:TYR:HD2  | 1.86                     | 0.40              |
| 42:3N:375:LYS:HB2 | 42:3N:375:LYS:HE2  | 1.84                     | 0.40              |
| 1:3:45:SER:OG     | 1:3:46:SER:N       | 2.54                     | 0.40              |
| 2:S3:115:ALA:HB2  | 2:S3:127:ILE:HD13  | 2.04                     | 0.40              |
| 3:S2:316:PHE:O    | 55:S8:35:THR:OG1   | 2.39                     | 0.40              |
| 4:1:129:LEU:HD12  | 4:1:129:LEU:HA     | 1.91                     | 0.40              |
| 8:4:373:ILE:HA    | 8:4:376:MET:HB3    | 2.03                     | 0.40              |
| 11:A9:311:GLU:HA  | 11:A9:312:PRO:HD3  | 1.96                     | 0.40              |
| 1:3a:67:LEU:HG    | 6:4l:65:VAL:HG22   | 2.02                     | 0.40              |
| 4:1a:294:LEU:HD12 | 4:1a:294:LEU:HA    | 1.89                     | 0.40              |
| 5:6a:110:ASP:OD1  | 5:6a:110:ASP:N     | 2.51                     | 0.40              |
| 8:4a:6:LEU:HD21   | 26:b1:22:PHE:HD2   | 1.86                     | 0.40              |
| 9:2a:248:LEU:HD12 | 9:2a:293:TYR:HB3   | 2.03                     | 0.40              |
| 15:ab:136:GLU:H   | 15:ab:136:GLU:HG3  | 1.71                     | 0.40              |
| 15:ab:137:LYS:HE3 | 15:ab:137:LYS:HB3  | 1.95                     | 0.40              |
| 20:ao:105:LYS:HE2 | 20:ao:105:LYS:HB2  | 1.90                     | 0.40              |

*Continued on next page...*

Continued from previous page...

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:b4:15:PRO:HG2   | 33:b4:18:LEU:HD12  | 2.04                     | 0.40              |
| 40:3A:332:ALA:HA   | 40:3A:337:LEU:HD13 | 2.04                     | 0.40              |
| 42:3N:181:PHE:HA   | 42:3N:184:ILE:HG22 | 2.03                     | 0.40              |
| 44:3P:102:SER:OG   | 44:3P:103:SER:N    | 2.54                     | 0.40              |
| 53:S1:282:ASN:ND2  | 53:S1:285:TRP:O    | 2.53                     | 0.40              |
| 53:S1:547:LEU:HD12 | 53:S1:550:ALA:HB3  | 2.03                     | 0.40              |
| 54:S7:158:VAL:HB   | 54:S7:187:VAL:HA   | 2.04                     | 0.40              |
| 52:v2:79:LEU:O     | 52:v2:121:TYR:OH   | 2.38                     | 0.40              |
| 53:s1:374:THR:HG22 | 53:s1:378:GLY:HA3  | 2.03                     | 0.40              |
| 3:S2:383:LYS:NZ    | 3:S2:387:GLU:OE1   | 2.54                     | 0.40              |
| 7:5:139:GLN:HE21   | 7:5:139:GLN:HB3    | 1.75                     | 0.40              |
| 18:A8:68:LEU:O     | 18:A8:72:ARG:HB2   | 2.21                     | 0.40              |
| 29:B6:77:ILE:HG23  | 29:B6:78:PRO:HD3   | 2.03                     | 0.40              |
| 3:s2:41:ILE:HG23   | 10:a1:313:TYR:HB3  | 2.03                     | 0.40              |
| 6:4l:40:LEU:HD21   | 9:2a:71:LEU:HB3    | 2.04                     | 0.40              |
| 7:5a:191:LEU:HD23  | 7:5a:191:LEU:HA    | 1.97                     | 0.40              |
| 7:5a:411:ILE:HA    | 7:5a:414:ILE:HG22  | 2.03                     | 0.40              |
| 8:4a:343:ILE:O     | 8:4a:346:ARG:NE    | 2.52                     | 0.40              |
| 11:a9:247:LYS:HA   | 11:a9:247:LYS:HD2  | 1.84                     | 0.40              |
| 15:ab:82:ARG:NE    | 15:ab:125:GLU:OE2  | 2.46                     | 0.40              |
| 15:ab:106:LYS:HD3  | 15:ab:106:LYS:HA   | 1.95                     | 0.40              |
| 16:a5:60:LYS:HE2   | 16:a5:60:LYS:HB3   | 1.88                     | 0.40              |
| 29:b6:24:LYS:HE2   | 29:b6:24:LYS:HB2   | 1.80                     | 0.40              |
| 35:b7:39:MET:HE2   | 35:b7:39:MET:HB2   | 1.79                     | 0.40              |
| 41:3B:138:LEU:HD13 | 41:3B:238:LEU:HD23 | 2.03                     | 0.40              |
| 44:3E:140:MET:HE3  | 42:3N:163:TRP:HE1  | 1.87                     | 0.40              |
| 40:3L:470:ARG:HH22 | 42:3N:20:ASP:HB3   | 1.85                     | 0.40              |
| 41:3M:112:VAL:HA   | 41:3M:120:ALA:O    | 2.21                     | 0.40              |
| 51:v1:62:TRP:N     | 51:v1:140:GLU:OE1  | 2.50                     | 0.40              |
| 53:s1:587:ALA:HB3  | 53:s1:592:LYS:HD3  | 2.04                     | 0.40              |

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   | 3     | 111/115 (96%)  | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | 3a    | 109/115 (95%)  | 102 (94%) | 7 (6%)  | 0        | 100         | 100 |
| 2   | S3    | 204/263 (78%)  | 197 (97%) | 7 (3%)  | 0        | 100         | 100 |
| 2   | s3    | 203/263 (77%)  | 188 (93%) | 15 (7%) | 0        | 100         | 100 |
| 3   | S2    | 418/463 (90%)  | 401 (96%) | 17 (4%) | 0        | 100         | 100 |
| 3   | s2    | 416/463 (90%)  | 400 (96%) | 16 (4%) | 0        | 100         | 100 |
| 4   | 1     | 315/318 (99%)  | 294 (93%) | 20 (6%) | 1 (0%)   | 36          | 65  |
| 4   | 1a    | 314/318 (99%)  | 293 (93%) | 20 (6%) | 1 (0%)   | 36          | 65  |
| 5   | 6     | 168/172 (98%)  | 160 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 5   | 6a    | 169/172 (98%)  | 163 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 6   | 4L    | 95/98 (97%)    | 90 (95%)  | 5 (5%)  | 0        | 100         | 100 |
| 6   | 4l    | 95/98 (97%)    | 93 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 7   | 5     | 603/607 (99%)  | 573 (95%) | 28 (5%) | 2 (0%)   | 36          | 65  |
| 7   | 5a    | 603/607 (99%)  | 562 (93%) | 41 (7%) | 0        | 100         | 100 |
| 8   | 4     | 457/459 (100%) | 442 (97%) | 15 (3%) | 0        | 100         | 100 |
| 8   | 4a    | 457/459 (100%) | 439 (96%) | 18 (4%) | 0        | 100         | 100 |
| 9   | 2     | 342/345 (99%)  | 331 (97%) | 11 (3%) | 0        | 100         | 100 |
| 9   | 2a    | 342/345 (99%)  | 330 (96%) | 12 (4%) | 0        | 100         | 100 |
| 10  | AL    | 318/355 (90%)  | 299 (94%) | 19 (6%) | 0        | 100         | 100 |
| 10  | al    | 318/355 (90%)  | 304 (96%) | 14 (4%) | 0        | 100         | 100 |
| 11  | A9    | 340/377 (90%)  | 321 (94%) | 19 (6%) | 0        | 100         | 100 |
| 11  | a9    | 340/377 (90%)  | 326 (96%) | 14 (4%) | 0        | 100         | 100 |
| 12  | S4    | 124/175 (71%)  | 118 (95%) | 6 (5%)  | 0        | 100         | 100 |
| 12  | s4    | 124/175 (71%)  | 122 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 13  | S6    | 93/116 (80%)   | 93 (100%) | 0       | 0        | 100         | 100 |
| 13  | s6    | 93/116 (80%)   | 90 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 14  | A2    | 82/99 (83%)    | 78 (95%)  | 4 (5%)  | 0        | 100         | 100 |
| 14  | a2    | 82/99 (83%)    | 75 (92%)  | 7 (8%)  | 0        | 100         | 100 |
| 15  | AB    | 76/156 (49%)   | 73 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 15  | AC    | 86/156 (55%)   | 84 (98%)  | 2 (2%)  | 0        | 100         | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 15  | ab    | 76/156 (49%)  | 73 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 15  | ac    | 86/156 (55%)  | 82 (95%)  | 4 (5%)  | 0        | 100         | 100 |
| 16  | A5    | 112/116 (97%) | 106 (95%) | 6 (5%)  | 0        | 100         | 100 |
| 16  | a5    | 111/116 (96%) | 108 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 17  | A6    | 110/131 (84%) | 105 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 17  | a6    | 109/131 (83%) | 103 (94%) | 6 (6%)  | 0        | 100         | 100 |
| 18  | A8    | 167/172 (97%) | 159 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 18  | a8    | 168/172 (98%) | 162 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 19  | AM    | 139/142 (98%) | 135 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 19  | am    | 139/142 (98%) | 137 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 20  | AO    | 138/144 (96%) | 135 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 20  | ao    | 138/144 (96%) | 135 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 21  | A1    | 67/70 (96%)   | 65 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 21  | a1    | 67/70 (96%)   | 65 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 22  | A3    | 81/84 (96%)   | 75 (93%)  | 6 (7%)  | 0        | 100         | 100 |
| 22  | a3    | 81/84 (96%)   | 76 (94%)  | 5 (6%)  | 0        | 100         | 100 |
| 23  | C1    | 47/76 (62%)   | 47 (100%) | 0       | 0        | 100         | 100 |
| 23  | c1    | 43/76 (57%)   | 42 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 24  | C2    | 118/120 (98%) | 117 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 24  | c2    | 118/120 (98%) | 114 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 25  | S5    | 103/106 (97%) | 98 (95%)  | 5 (5%)  | 0        | 100         | 100 |
| 25  | s5    | 103/106 (97%) | 100 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 26  | B1    | 54/57 (95%)   | 51 (94%)  | 3 (6%)  | 0        | 100         | 100 |
| 26  | b1    | 54/57 (95%)   | 52 (96%)  | 2 (4%)  | 0        | 100         | 100 |
| 27  | BM    | 96/151 (64%)  | 93 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 27  | bm    | 97/151 (64%)  | 93 (96%)  | 4 (4%)  | 0        | 100         | 100 |
| 28  | B5    | 137/189 (72%) | 132 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 28  | b5    | 136/189 (72%) | 132 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 29  | B6    | 90/127 (71%)  | 89 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 29  | b6    | 86/127 (68%)  | 83 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 30  | B2    | 62/105 (59%)  | 57 (92%)  | 5 (8%)  | 0        | 100         | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 30  | b2    | 61/105 (58%)   | 61 (100%) | 0       | 0        | 100         | 100 |
| 31  | B3    | 68/104 (65%)   | 65 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 31  | b3    | 69/104 (66%)   | 66 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 32  | B8    | 153/186 (82%)  | 143 (94%) | 10 (6%) | 0        | 100         | 100 |
| 32  | b8    | 153/186 (82%)  | 149 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 33  | B4    | 123/129 (95%)  | 121 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 33  | b4    | 123/129 (95%)  | 118 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 34  | B9    | 176/179 (98%)  | 169 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 34  | b9    | 175/179 (98%)  | 168 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 35  | B7    | 112/136 (82%)  | 110 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 35  | b7    | 115/136 (85%)  | 109 (95%) | 6 (5%)  | 0        | 100         | 100 |
| 36  | BL    | 165/176 (94%)  | 159 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 36  | bl    | 167/176 (95%)  | 159 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 37  | AN    | 142/145 (98%)  | 135 (95%) | 7 (5%)  | 0        | 100         | 100 |
| 37  | an    | 142/145 (98%)  | 138 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 38  | A7    | 88/112 (79%)   | 84 (96%)  | 4 (4%)  | 0        | 100         | 100 |
| 38  | a7    | 68/112 (61%)   | 63 (93%)  | 5 (7%)  | 0        | 100         | 100 |
| 39  | V3    | 38/104 (36%)   | 38 (100%) | 0       | 0        | 100         | 100 |
| 39  | v3    | 34/104 (33%)   | 34 (100%) | 0       | 0        | 100         | 100 |
| 40  | 3A    | 443/446 (99%)  | 427 (96%) | 16 (4%) | 0        | 100         | 100 |
| 40  | 3L    | 443/446 (99%)  | 426 (96%) | 17 (4%) | 0        | 100         | 100 |
| 41  | 3B    | 418/439 (95%)  | 405 (97%) | 13 (3%) | 0        | 100         | 100 |
| 41  | 3M    | 418/439 (95%)  | 396 (95%) | 22 (5%) | 0        | 100         | 100 |
| 42  | 3C    | 378/380 (100%) | 366 (97%) | 12 (3%) | 0        | 100         | 100 |
| 42  | 3N    | 378/380 (100%) | 361 (96%) | 17 (4%) | 0        | 100         | 100 |
| 43  | 3D    | 239/241 (99%)  | 230 (96%) | 9 (4%)  | 0        | 100         | 100 |
| 43  | 3O    | 238/241 (99%)  | 229 (96%) | 9 (4%)  | 0        | 100         | 100 |
| 44  | 3E    | 78/196 (40%)   | 76 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 44  | 3P    | 79/196 (40%)   | 73 (92%)  | 6 (8%)  | 0        | 100         | 100 |
| 45  | 3F    | 100/110 (91%)  | 97 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 45  | 3Q    | 97/110 (88%)   | 94 (97%)  | 3 (3%)  | 0        | 100         | 100 |

*Continued on next page...*

Continued from previous page...

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

All (7) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 1     | 91  | MET  |
| 7   | 5     | 433 | THR  |
| 4   | 1a    | 91  | MET  |
| 48  | 3J    | 57  | LYS  |
| 55  | s8    | 152 | CYS  |
| 52  | V2    | 188 | ASN  |
| 7   | 5     | 563 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

All (90) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 3     | 11  | ILE  |
| 2   | S3    | 135 | ARG  |
| 2   | S3    | 168 | GLU  |
| 3   | S2    | 157 | LYS  |
| 3   | S2    | 259 | GLU  |
| 3   | S2    | 298 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | S2    | 450 | ILE  |
| 3   | S2    | 462 | ASP  |
| 4   | 1     | 171 | HIS  |
| 7   | 5     | 30  | ILE  |
| 7   | 5     | 432 | MET  |
| 8   | 4     | 236 | LEU  |
| 8   | 4     | 246 | ILE  |
| 8   | 4     | 285 | LEU  |
| 9   | 2     | 161 | SER  |
| 9   | 2     | 233 | LEU  |
| 9   | 2     | 270 | LEU  |
| 10  | AL    | 61  | THR  |
| 11  | A9    | 353 | LEU  |
| 12  | S4    | 55  | VAL  |
| 13  | S6    | 31  | ILE  |
| 19  | AM    | 14  | ASP  |
| 25  | S5    | 3   | PHE  |
| 26  | B1    | 55  | THR  |
| 32  | B8    | 105 | ILE  |
| 34  | B9    | 134 | ASP  |
| 37  | AN    | 31  | PHE  |
| 2   | s3    | 57  | LEU  |
| 2   | s3    | 93  | ILE  |
| 3   | s2    | 124 | ILE  |
| 3   | s2    | 181 | LEU  |
| 3   | s2    | 409 | VAL  |
| 4   | 1a    | 163 | GLN  |
| 5   | 6a    | 41  | LEU  |
| 5   | 6a    | 159 | LEU  |
| 7   | 5a    | 77  | LYS  |
| 7   | 5a    | 187 | VAL  |
| 7   | 5a    | 210 | LEU  |
| 7   | 5a    | 253 | VAL  |
| 7   | 5a    | 361 | ASN  |
| 8   | 4a    | 245 | ARG  |
| 8   | 4a    | 440 | HIS  |
| 9   | 2a    | 49  | ASN  |
| 9   | 2a    | 232 | LEU  |
| 10  | al    | 199 | LEU  |
| 10  | al    | 237 | ILE  |
| 10  | al    | 256 | LEU  |
| 11  | a9    | 180 | SER  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | a9    | 374 | THR  |
| 13  | s6    | 67  | GLN  |
| 14  | a2    | 38  | VAL  |
| 14  | a2    | 65  | LEU  |
| 15  | ac    | 112 | SER  |
| 17  | a6    | 52  | LEU  |
| 18  | a8    | 135 | ARG  |
| 20  | ao    | 61  | LEU  |
| 20  | ao    | 69  | ILE  |
| 21  | a1    | 38  | VAL  |
| 29  | b6    | 7   | ASP  |
| 34  | b9    | 25  | ARG  |
| 40  | 3A    | 399 | LEU  |
| 41  | 3B    | 388 | THR  |
| 42  | 3C    | 119 | LEU  |
| 42  | 3C    | 232 | ILE  |
| 42  | 3C    | 333 | LEU  |
| 43  | 3D    | 105 | LEU  |
| 44  | 3E    | 96  | VAL  |
| 45  | 3F    | 76  | LEU  |
| 47  | 3H    | 64  | ASP  |
| 40  | 3L    | 379 | LEU  |
| 42  | 3N    | 162 | GLU  |
| 42  | 3N    | 183 | PHE  |
| 42  | 3N    | 335 | LEU  |
| 48  | 3U    | 53  | LEU  |
| 51  | V1    | 45  | LEU  |
| 51  | V1    | 233 | VAL  |
| 51  | V1    | 244 | ASN  |
| 51  | V1    | 410 | ASP  |
| 51  | V1    | 412 | LEU  |
| 52  | V2    | 39  | VAL  |
| 53  | S1    | 96  | VAL  |
| 53  | S1    | 567 | VAL  |
| 54  | S7    | 145 | LEU  |
| 54  | S7    | 202 | LEU  |
| 54  | S7    | 205 | ILE  |
| 55  | S8    | 140 | ARG  |
| 53  | s1    | 154 | LEU  |
| 53  | s1    | 514 | ASN  |
| 54  | s7    | 99  | CYS  |
| 55  | s8    | 130 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (213) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | S3    | 54  | HIS  |
| 2   | S3    | 195 | HIS  |
| 3   | S2    | 36  | GLN  |
| 3   | S2    | 38  | GLN  |
| 3   | S2    | 250 | ASN  |
| 3   | S2    | 306 | GLN  |
| 3   | S2    | 313 | GLN  |
| 3   | S2    | 390 | GLN  |
| 4   | 1     | 93  | HIS  |
| 4   | 1     | 230 | ASN  |
| 6   | 4L    | 50  | ASN  |
| 6   | 4L    | 92  | ASN  |
| 7   | 5     | 31  | ASN  |
| 7   | 5     | 58  | ASN  |
| 7   | 5     | 226 | GLN  |
| 7   | 5     | 321 | GLN  |
| 7   | 5     | 444 | ASN  |
| 7   | 5     | 594 | ASN  |
| 8   | 4     | 83  | HIS  |
| 8   | 4     | 139 | GLN  |
| 8   | 4     | 144 | ASN  |
| 8   | 4     | 304 | GLN  |
| 8   | 4     | 331 | ASN  |
| 8   | 4     | 349 | GLN  |
| 8   | 4     | 390 | ASN  |
| 8   | 4     | 399 | ASN  |
| 9   | 2     | 197 | ASN  |
| 9   | 2     | 289 | ASN  |
| 9   | 2     | 310 | ASN  |
| 10  | AL    | 65  | ASN  |
| 10  | AL    | 176 | GLN  |
| 10  | AL    | 235 | GLN  |
| 11  | A9    | 37  | HIS  |
| 11  | A9    | 38  | HIS  |
| 11  | A9    | 79  | GLN  |
| 11  | A9    | 216 | HIS  |
| 12  | S4    | 51  | GLN  |
| 13  | S6    | 36  | GLN  |
| 14  | A2    | 48  | HIS  |
| 14  | A2    | 50  | ASN  |
| 15  | AB    | 115 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | AB    | 142 | GLN  |
| 18  | A8    | 151 | ASN  |
| 19  | AM    | 79  | GLN  |
| 20  | AO    | 24  | ASN  |
| 20  | AO    | 54  | ASN  |
| 20  | AO    | 137 | ASN  |
| 21  | A1    | 31  | ASN  |
| 21  | A1    | 68  | ASN  |
| 22  | A3    | 52  | ASN  |
| 23  | C1    | 60  | GLN  |
| 24  | C2    | 117 | HIS  |
| 25  | S5    | 29  | ASN  |
| 25  | S5    | 45  | HIS  |
| 25  | S5    | 77  | HIS  |
| 26  | B1    | 45  | GLN  |
| 27  | BM    | 138 | ASN  |
| 27  | BM    | 146 | GLN  |
| 31  | B3    | 39  | GLN  |
| 31  | B3    | 54  | ASN  |
| 32  | B8    | 115 | ASN  |
| 32  | B8    | 132 | HIS  |
| 33  | B4    | 126 | ASN  |
| 34  | B9    | 13  | GLN  |
| 34  | B9    | 139 | GLN  |
| 35  | B7    | 44  | GLN  |
| 35  | B7    | 76  | ASN  |
| 35  | B7    | 110 | GLN  |
| 36  | BL    | 123 | GLN  |
| 36  | BL    | 131 | GLN  |
| 37  | AN    | 91  | HIS  |
| 39  | V3    | 69  | ASN  |
| 1   | 3a    | 108 | GLN  |
| 2   | s3    | 54  | HIS  |
| 2   | s3    | 163 | ASN  |
| 2   | s3    | 179 | ASN  |
| 2   | s3    | 235 | ASN  |
| 3   | s2    | 36  | GLN  |
| 3   | s2    | 88  | HIS  |
| 3   | s2    | 147 | ASN  |
| 3   | s2    | 234 | GLN  |
| 3   | s2    | 313 | GLN  |
| 3   | s2    | 349 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 1a    | 93  | HIS  |
| 4   | 1a    | 138 | GLN  |
| 6   | 4l    | 83  | ASN  |
| 6   | 4l    | 94  | ASN  |
| 6   | 4l    | 97  | GLN  |
| 7   | 5a    | 31  | ASN  |
| 7   | 5a    | 56  | HIS  |
| 7   | 5a    | 57  | ASN  |
| 7   | 5a    | 135 | ASN  |
| 7   | 5a    | 199 | GLN  |
| 7   | 5a    | 295 | GLN  |
| 7   | 5a    | 348 | HIS  |
| 7   | 5a    | 446 | ASN  |
| 7   | 5a    | 506 | ASN  |
| 7   | 5a    | 572 | ASN  |
| 8   | 4a    | 192 | ASN  |
| 8   | 4a    | 374 | ASN  |
| 9   | 2a    | 134 | GLN  |
| 9   | 2a    | 223 | ASN  |
| 9   | 2a    | 309 | ASN  |
| 10  | al    | 71  | ASN  |
| 10  | al    | 79  | GLN  |
| 10  | al    | 132 | GLN  |
| 10  | al    | 142 | GLN  |
| 10  | al    | 175 | ASN  |
| 10  | al    | 286 | GLN  |
| 11  | a9    | 37  | HIS  |
| 11  | a9    | 43  | HIS  |
| 13  | s6    | 36  | GLN  |
| 14  | a2    | 25  | GLN  |
| 14  | a2    | 80  | ASN  |
| 15  | ab    | 115 | GLN  |
| 15  | ac    | 142 | GLN  |
| 19  | am    | 79  | GLN  |
| 20  | ao    | 54  | ASN  |
| 21  | a1    | 31  | ASN  |
| 24  | c2    | 27  | ASN  |
| 24  | c2    | 59  | HIS  |
| 25  | s5    | 7   | GLN  |
| 25  | s5    | 25  | GLN  |
| 27  | bm    | 63  | ASN  |
| 27  | bm    | 146 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | b5    | 124 | ASN  |
| 30  | b2    | 49  | GLN  |
| 30  | b2    | 83  | HIS  |
| 31  | b3    | 27  | GLN  |
| 33  | b4    | 52  | ASN  |
| 33  | b4    | 86  | ASN  |
| 34  | b9    | 12  | HIS  |
| 34  | b9    | 169 | HIS  |
| 35  | b7    | 76  | ASN  |
| 36  | b1    | 107 | GLN  |
| 37  | an    | 21  | HIS  |
| 37  | an    | 73  | ASN  |
| 37  | an    | 120 | ASN  |
| 38  | a7    | 21  | GLN  |
| 38  | a7    | 29  | GLN  |
| 38  | a7    | 51  | ASN  |
| 40  | 3A    | 40  | GLN  |
| 40  | 3A    | 43  | GLN  |
| 40  | 3A    | 86  | ASN  |
| 40  | 3A    | 103 | ASN  |
| 40  | 3A    | 175 | ASN  |
| 40  | 3A    | 207 | ASN  |
| 40  | 3A    | 247 | GLN  |
| 40  | 3A    | 323 | HIS  |
| 40  | 3A    | 375 | GLN  |
| 40  | 3A    | 464 | GLN  |
| 41  | 3B    | 118 | ASN  |
| 41  | 3B    | 139 | ASN  |
| 41  | 3B    | 210 | GLN  |
| 41  | 3B    | 261 | GLN  |
| 41  | 3B    | 303 | ASN  |
| 41  | 3B    | 311 | GLN  |
| 41  | 3B    | 318 | HIS  |
| 42  | 3C    | 15  | ASN  |
| 42  | 3C    | 32  | ASN  |
| 42  | 3C    | 255 | ASN  |
| 42  | 3C    | 263 | ASN  |
| 42  | 3C    | 267 | HIS  |
| 42  | 3C    | 341 | GLN  |
| 42  | 3C    | 345 | HIS  |
| 43  | 3D    | 284 | HIS  |
| 44  | 3E    | 80  | HIS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47  | 3H    | 74  | HIS  |
| 47  | 3H    | 78  | HIS  |
| 40  | 3L    | 175 | ASN  |
| 40  | 3L    | 199 | GLN  |
| 40  | 3L    | 221 | ASN  |
| 41  | 3M    | 34  | GLN  |
| 41  | 3M    | 170 | GLN  |
| 41  | 3M    | 211 | ASN  |
| 41  | 3M    | 236 | GLN  |
| 41  | 3M    | 262 | ASN  |
| 41  | 3M    | 311 | GLN  |
| 43  | 3O    | 155 | GLN  |
| 43  | 3O    | 240 | GLN  |
| 43  | 3O    | 265 | GLN  |
| 44  | 3P    | 135 | GLN  |
| 45  | 3Q    | 57  | ASN  |
| 46  | 3R    | 37  | ASN  |
| 47  | 3S    | 37  | GLN  |
| 49  | 3V    | 16  | ASN  |
| 51  | V1    | 164 | ASN  |
| 51  | V1    | 168 | ASN  |
| 51  | V1    | 281 | HIS  |
| 51  | V1    | 283 | ASN  |
| 52  | V2    | 152 | GLN  |
| 53  | S1    | 101 | ASN  |
| 53  | S1    | 406 | ASN  |
| 53  | S1    | 569 | GLN  |
| 55  | S8    | 172 | ASN  |
| 51  | v1    | 49  | HIS  |
| 51  | v1    | 168 | ASN  |
| 51  | v1    | 283 | ASN  |
| 51  | v1    | 284 | HIS  |
| 51  | v1    | 303 | HIS  |
| 51  | v1    | 418 | GLN  |
| 52  | v2    | 68  | ASN  |
| 52  | v2    | 89  | ASN  |
| 53  | s1    | 101 | ASN  |
| 53  | s1    | 140 | GLN  |
| 53  | s1    | 365 | ASN  |
| 53  | s1    | 384 | ASN  |
| 53  | s1    | 425 | ASN  |
| 53  | s1    | 495 | ASN  |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | s7    | 151 | GLN  |
| 54  | s7    | 166 | ASN  |
| 55  | s8    | 193 | ASN  |
| 55  | s8    | 206 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | 2MR  | s2    | 118 | 3    | 3,4,13       | 0.83 | 0           | 2,4,15      | 1.27 | 0           |
| 3   | 2MR  | S2    | 118 | 3    | 10,12,13     | 2.72 | 3 (30%)     | 5,13,15     | 7.36 | 4 (80%)     |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings |
|-----|------|-------|-----|------|---------|------------|-------|
| 3   | 2MR  | s2    | 118 | 3    | -       | 1/1/2/15   | -     |
| 3   | 2MR  | S2    | 118 | 3    | -       | 4/10/13/15 | -     |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | S2    | 118 | 2MR  | CZ-NE   | 5.73  | 1.46        | 1.34     |
| 3   | S2    | 118 | 2MR  | CZ-NH2  | 5.42  | 1.44        | 1.33     |
| 3   | S2    | 118 | 2MR  | CQ1-NH1 | -2.49 | 1.41        | 1.46     |

All (4) bond angle outliers are listed below:

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

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 4 are monoatomic - leaving 32 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 65  | FES  | S1    | 803 | 53   | 0,4,4        | -    | -           | -           |      |             |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 61  | HEM  | 3C    | 401 | 42   | 50,50,50     | 1.31 | 8 (16%)  | 67,82,82    | 1.62 | 12 (17%) |
| 64  | SF4  | s1    | 801 | 53   | 0,12,12      | -    | -        | -           |      |          |
| 57  | DGT  | AL    | 502 | 56   | 32,33,33     | 0.57 | 0        | 48,52,52    | 0.58 | 0        |
| 64  | SF4  | V1    | 502 | 51   | 0,12,12      | -    | -        | -           |      |          |
| 64  | SF4  | s8    | 301 | 55   | 0,12,12      | -    | -        | -           |      |          |
| 65  | FES  | s1    | 803 | 53   | 0,4,4        | -    | -        | -           |      |          |
| 60  | EHZ  | B9    | 201 | -    | 31,36,37     | 0.20 | 0        | 36,44,47    | 1.04 | 1 (2%)   |
| 57  | DGT  | al    | 502 | -    | 32,33,33     | 0.57 | 0        | 48,52,52    | 0.59 | 0        |
| 63  | FMN  | V1    | 501 | -    | 33,33,33     | 0.30 | 0        | 48,50,50    | 0.48 | 0        |
| 63  | FMN  | v1    | 501 | -    | 33,33,33     | 0.27 | 0        | 48,50,50    | 0.54 | 1 (2%)   |
| 64  | SF4  | s7    | 301 | 54   | 0,12,12      | -    | -        | -           |      |          |
| 60  | EHZ  | a6    | 201 | -    | 31,36,37     | 0.19 | 0        | 36,44,47    | 1.25 | 1 (2%)   |
| 64  | SF4  | S1    | 801 | 53   | 0,12,12      | -    | -        | -           |      |          |
| 62  | HEC  | 3D    | 401 | 43   | 46,50,50     | 2.00 | 9 (19%)  | 58,82,82    | 2.27 | 19 (32%) |
| 58  | NDP  | A9    | 501 | -    | 51,52,52     | 0.32 | 0        | 71,80,80    | 0.42 | 0        |
| 64  | SF4  | S7    | 301 | 54,3 | 0,12,12      | -    | -        | -           |      |          |
| 65  | FES  | V2    | 301 | 52   | 0,4,4        | -    | -        | -           |      |          |
| 64  | SF4  | S1    | 802 | 53   | 0,12,12      | -    | -        | -           |      |          |
| 64  | SF4  | v1    | 502 | 51   | 0,12,12      | -    | -        | -           |      |          |
| 61  | HEM  | 3N    | 402 | 42   | 50,50,50     | 1.37 | 7 (14%)  | 67,82,82    | 1.60 | 15 (22%) |
| 60  | EHZ  | 5a    | 701 | -    | 31,36,37     | 0.25 | 0        | 36,44,47    | 1.14 | 1 (2%)   |
| 64  | SF4  | S8    | 301 | 55   | 0,12,12      | -    | -        | -           |      |          |
| 61  | HEM  | 3C    | 402 | 42   | 50,50,50     | 1.34 | 6 (12%)  | 67,82,82    | 1.62 | 16 (23%) |
| 60  | EHZ  | A6    | 201 | -    | 31,36,37     | 0.20 | 0        | 36,44,47    | 1.26 | 1 (2%)   |
| 61  | HEM  | 3N    | 401 | 42   | 50,50,50     | 1.31 | 6 (12%)  | 67,82,82    | 1.61 | 12 (17%) |
| 65  | FES  | v2    | 301 | 52   | 0,4,4        | -    | -        | -           |      |          |
| 62  | HEC  | 3O    | 401 | 43   | 46,50,50     | 1.92 | 6 (13%)  | 58,82,82    | 1.98 | 12 (20%) |
| 64  | SF4  | s8    | 302 | 55   | 0,12,12      | -    | -        | -           |      |          |
| 64  | SF4  | S8    | 302 | 55   | 0,12,12      | -    | -        | -           |      |          |
| 64  | SF4  | s1    | 802 | 53   | 0,12,12      | -    | -        | -           |      |          |
| 58  | NDP  | a9    | 501 | -    | 51,52,52     | 0.33 | 0        | 71,80,80    | 0.43 | 0        |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 65  | FES  | S1    | 803 | 53   | -       | -          | 0/1/1/1 |
| 61  | HEM  | 3C    | 401 | 42   | -       | 9/14/54/54 | -       |

Continued on next page...

*Continued from previous page...*

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

All (42) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 62  | 3D    | 401 | HEC  | CAC-C3C | 7.33  | 1.58        | 1.35     |
| 62  | 3O    | 401 | HEC  | CAC-C3C | 7.33  | 1.58        | 1.35     |
| 62  | 3O    | 401 | HEC  | CAB-C3B | 6.83  | 1.57        | 1.35     |
| 62  | 3D    | 401 | HEC  | CAB-C3B | 6.70  | 1.56        | 1.35     |
| 61  | 3C    | 402 | HEM  | C4D-ND  | -3.81 | 1.33        | 1.40     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 61  | 3N    | 402 | HEM  | C4D-ND  | -3.62 | 1.34        | 1.40     |
| 61  | 3N    | 401 | HEM  | C4D-ND  | -3.58 | 1.34        | 1.40     |
| 61  | 3C    | 401 | HEM  | C4D-ND  | -3.43 | 1.34        | 1.40     |
| 61  | 3C    | 401 | HEM  | C1B-NB  | -3.43 | 1.34        | 1.40     |
| 62  | 3O    | 401 | HEC  | CBC-CAC | -3.37 | 1.37        | 1.49     |
| 62  | 3D    | 401 | HEC  | CBC-CAC | -3.37 | 1.37        | 1.49     |
| 61  | 3N    | 401 | HEM  | C1B-NB  | -3.32 | 1.34        | 1.40     |
| 61  | 3N    | 402 | HEM  | C1B-NB  | -3.30 | 1.34        | 1.40     |
| 61  | 3C    | 402 | HEM  | C1D-ND  | -3.10 | 1.32        | 1.38     |
| 61  | 3C    | 402 | HEM  | C1C-C2C | -3.00 | 1.39        | 1.45     |
| 61  | 3C    | 402 | HEM  | C1B-NB  | -2.98 | 1.35        | 1.40     |
| 61  | 3N    | 402 | HEM  | C1C-C2C | -2.96 | 1.39        | 1.45     |
| 61  | 3C    | 401 | HEM  | C1D-ND  | -2.85 | 1.33        | 1.38     |
| 61  | 3N    | 401 | HEM  | C1D-ND  | -2.84 | 1.33        | 1.38     |
| 61  | 3N    | 402 | HEM  | C1D-ND  | -2.80 | 1.33        | 1.38     |
| 62  | 3D    | 401 | HEC  | O1A-CGA | 2.74  | 1.31        | 1.22     |
| 61  | 3N    | 401 | HEM  | C1C-C2C | -2.66 | 1.40        | 1.45     |
| 61  | 3N    | 402 | HEM  | C3B-C4B | 2.54  | 1.49        | 1.44     |
| 61  | 3C    | 401 | HEM  | C1C-C2C | -2.43 | 1.40        | 1.45     |
| 62  | 3D    | 401 | HEC  | CMB-C2B | 2.41  | 1.55        | 1.50     |
| 61  | 3N    | 402 | HEM  | FE-NB   | 2.41  | 2.02        | 1.94     |
| 62  | 3O    | 401 | HEC  | CMD-C2D | 2.40  | 1.55        | 1.50     |
| 62  | 3D    | 401 | HEC  | CMA-C3A | 2.39  | 1.55        | 1.50     |
| 62  | 3O    | 401 | HEC  | CBB-CAB | -2.37 | 1.40        | 1.49     |
| 62  | 3D    | 401 | HEC  | CAA-C2A | 2.36  | 1.57        | 1.51     |
| 61  | 3N    | 401 | HEM  | FE-NB   | 2.31  | 2.02        | 1.94     |
| 61  | 3C    | 402 | HEM  | FE-NB   | 2.30  | 2.02        | 1.94     |
| 62  | 3D    | 401 | HEC  | CBB-CAB | -2.28 | 1.41        | 1.49     |
| 62  | 3O    | 401 | HEC  | CMB-C2B | 2.26  | 1.55        | 1.50     |
| 62  | 3D    | 401 | HEC  | CMD-C2D | 2.18  | 1.55        | 1.50     |
| 61  | 3C    | 401 | HEM  | C3C-C4C | -2.16 | 1.42        | 1.46     |
| 61  | 3C    | 402 | HEM  | C4B-NB  | -2.12 | 1.34        | 1.38     |
| 61  | 3C    | 401 | HEM  | FE-NB   | 2.11  | 2.01        | 1.94     |
| 61  | 3C    | 401 | HEM  | FE-ND   | 2.09  | 2.01        | 1.94     |
| 61  | 3N    | 401 | HEM  | FE-ND   | 2.07  | 2.01        | 1.94     |
| 61  | 3C    | 401 | HEM  | C4B-NB  | -2.03 | 1.34        | 1.38     |
| 61  | 3N    | 402 | HEM  | FE-ND   | 2.01  | 2.01        | 1.94     |

All (91) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 62  | 3D    | 401 | HEC  | CBB-CAB-C3B | -8.61 | 110.23      | 127.43   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 62  | 3O    | 401 | HEC  | CBB-CAB-C3B | -7.40 | 112.65      | 127.43   |
| 60  | a6    | 201 | EHZ  | C10-S1-C9   | 7.12  | 122.89      | 101.84   |
| 60  | A6    | 201 | EHZ  | C10-S1-C9   | 6.83  | 122.02      | 101.84   |
| 62  | 3O    | 401 | HEC  | CBC-CAC-C3C | -6.61 | 114.23      | 127.43   |
| 62  | 3D    | 401 | HEC  | CBC-CAC-C3C | -6.54 | 114.37      | 127.43   |
| 60  | 5a    | 701 | EHZ  | C10-S1-C9   | 6.03  | 119.67      | 101.84   |
| 60  | B9    | 201 | EHZ  | C10-S1-C9   | 5.84  | 119.11      | 101.84   |
| 61  | 3N    | 401 | HEM  | CHC-C4B-NB  | 4.69  | 129.47      | 124.42   |
| 61  | 3C    | 401 | HEM  | CHB-C1B-NB  | 4.65  | 130.12      | 124.37   |
| 61  | 3C    | 401 | HEM  | CHC-C4B-NB  | 4.62  | 129.40      | 124.42   |
| 61  | 3C    | 402 | HEM  | CHC-C4B-NB  | 4.61  | 129.39      | 124.42   |
| 61  | 3N    | 402 | HEM  | CHB-C1B-NB  | 4.48  | 129.90      | 124.37   |
| 61  | 3N    | 401 | HEM  | CHB-C1B-NB  | 4.45  | 129.87      | 124.37   |
| 62  | 3D    | 401 | HEC  | CMA-C3A-C4A | -4.18 | 117.37      | 124.73   |
| 61  | 3N    | 402 | HEM  | CHD-C4C-NC  | 4.05  | 128.86      | 124.45   |
| 62  | 3O    | 401 | HEC  | CBD-CAD-C3D | 4.03  | 123.67      | 112.53   |
| 61  | 3N    | 401 | HEM  | CHD-C4C-NC  | 3.87  | 128.66      | 124.45   |
| 61  | 3C    | 402 | HEM  | CHD-C4C-NC  | 3.84  | 128.63      | 124.45   |
| 61  | 3C    | 401 | HEM  | CHD-C4C-NC  | 3.68  | 128.46      | 124.45   |
| 61  | 3C    | 402 | HEM  | CHB-C1B-NB  | 3.67  | 128.91      | 124.37   |
| 62  | 3O    | 401 | HEC  | CMD-C2D-C1D | -3.55 | 120.02      | 125.42   |
| 62  | 3D    | 401 | HEC  | CBD-CAD-C3D | 3.53  | 122.31      | 112.53   |
| 62  | 3D    | 401 | HEC  | CAA-CBA-CGA | 3.52  | 123.00      | 113.67   |
| 61  | 3N    | 402 | HEM  | C4D-ND-C1D  | 3.48  | 109.33      | 105.21   |
| 62  | 3D    | 401 | HEC  | CBA-CAA-C2A | 3.41  | 121.96      | 112.53   |
| 61  | 3C    | 401 | HEM  | C1B-NB-C4B  | 3.23  | 109.03      | 105.21   |
| 62  | 3D    | 401 | HEC  | CMA-C3A-C2A | 3.20  | 134.80      | 126.15   |
| 61  | 3C    | 402 | HEM  | C4D-ND-C1D  | 3.14  | 108.92      | 105.21   |
| 61  | 3C    | 401 | HEM  | CHA-C4D-ND  | 3.08  | 128.18      | 124.37   |
| 61  | 3C    | 402 | HEM  | CHD-C1D-ND  | 3.08  | 127.74      | 124.42   |
| 61  | 3C    | 402 | HEM  | C1B-NB-C4B  | 2.99  | 108.75      | 105.21   |
| 62  | 3D    | 401 | HEC  | C3D-C4D-ND  | -2.99 | 106.83      | 110.15   |
| 62  | 3O    | 401 | HEC  | O1D-CGD-CBD | -2.96 | 113.71      | 123.09   |
| 61  | 3N    | 402 | HEM  | C1B-NB-C4B  | 2.89  | 108.62      | 105.21   |
| 61  | 3N    | 401 | HEM  | CHA-C4D-ND  | 2.85  | 127.89      | 124.37   |
| 62  | 3O    | 401 | HEC  | CMD-C2D-C3D | 2.82  | 131.61      | 125.62   |
| 62  | 3D    | 401 | HEC  | CHD-C4C-C3C | 2.81  | 129.95      | 125.21   |
| 61  | 3N    | 401 | HEM  | C4B-C3B-C2B | -2.76 | 104.74      | 107.28   |
| 62  | 3D    | 401 | HEC  | O1D-CGD-CBD | -2.76 | 114.34      | 123.09   |
| 61  | 3N    | 401 | HEM  | C1B-NB-C4B  | 2.75  | 108.46      | 105.21   |
| 61  | 3C    | 401 | HEM  | CHD-C1D-ND  | 2.74  | 127.38      | 124.42   |
| 61  | 3N    | 401 | HEM  | C4D-ND-C1D  | 2.73  | 108.44      | 105.21   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 61  | 3N    | 401 | HEM  | CHD-C1D-ND  | 2.72  | 127.34      | 124.42   |
| 62  | 3D    | 401 | HEC  | CMB-C2B-C1B | -2.71 | 121.29      | 125.42   |
| 63  | v1    | 501 | FMN  | C4'-C3'-C2' | -2.71 | 109.06      | 113.57   |
| 61  | 3C    | 401 | HEM  | C4D-ND-C1D  | 2.71  | 108.41      | 105.21   |
| 61  | 3N    | 402 | HEM  | CHC-C4B-NB  | 2.70  | 127.33      | 124.42   |
| 61  | 3N    | 401 | HEM  | CHA-C1A-NA  | 2.70  | 128.75      | 123.86   |
| 62  | 3D    | 401 | HEC  | CMD-C2D-C1D | -2.70 | 121.31      | 125.42   |
| 61  | 3C    | 402 | HEM  | C3B-C4B-NB  | -2.67 | 107.55      | 109.47   |
| 61  | 3N    | 401 | HEM  | C3B-C2B-C1B | 2.67  | 108.42      | 106.41   |
| 61  | 3C    | 401 | HEM  | CHA-C1A-NA  | 2.63  | 128.64      | 123.86   |
| 61  | 3C    | 402 | HEM  | C1C-CHC-C4B | -2.58 | 120.54      | 126.02   |
| 62  | 3D    | 401 | HEC  | CHA-C1A-NA  | -2.56 | 121.66      | 124.45   |
| 61  | 3N    | 402 | HEM  | CHB-C1B-C2B | -2.54 | 119.73      | 126.95   |
| 61  | 3N    | 402 | HEM  | C3B-C4B-NB  | -2.49 | 107.68      | 109.47   |
| 62  | 3D    | 401 | HEC  | CAA-C2A-C3A | 2.49  | 132.53      | 127.87   |
| 62  | 3O    | 401 | HEC  | CHD-C4C-C3C | 2.48  | 129.38      | 125.21   |
| 61  | 3C    | 402 | HEM  | CBB-CAB-C3B | -2.48 | 115.16      | 127.53   |
| 61  | 3C    | 401 | HEM  | CHB-C1B-C2B | -2.47 | 119.92      | 126.95   |
| 62  | 3D    | 401 | HEC  | CMB-C2B-C3B | 2.46  | 132.34      | 126.55   |
| 62  | 3O    | 401 | HEC  | CMB-C2B-C1B | -2.42 | 121.73      | 125.42   |
| 61  | 3N    | 402 | HEM  | CHD-C1D-ND  | 2.40  | 127.00      | 124.42   |
| 61  | 3C    | 402 | HEM  | C2A-C1A-NA  | -2.40 | 107.49      | 110.15   |
| 62  | 3O    | 401 | HEC  | CAD-C3D-C2D | 2.38  | 132.41      | 127.07   |
| 61  | 3N    | 402 | HEM  | C3B-C2B-C1B | 2.36  | 108.19      | 106.41   |
| 61  | 3C    | 402 | HEM  | C4A-CHB-C1B | -2.36 | 120.69      | 126.25   |
| 61  | 3N    | 402 | HEM  | C4A-CHB-C1B | -2.36 | 120.70      | 126.25   |
| 62  | 3D    | 401 | HEC  | C4D-ND-C1D  | 2.34  | 109.64      | 105.82   |
| 62  | 3O    | 401 | HEC  | CAD-C3D-C4D | -2.32 | 120.40      | 124.94   |
| 61  | 3N    | 402 | HEM  | C4B-C3B-C2B | -2.32 | 105.14      | 107.28   |
| 61  | 3C    | 401 | HEM  | C3B-C4B-NB  | -2.31 | 107.81      | 109.47   |
| 61  | 3N    | 401 | HEM  | CHB-C1B-C2B | -2.30 | 120.42      | 126.95   |
| 61  | 3N    | 402 | HEM  | CHA-C1A-NA  | 2.26  | 127.95      | 123.86   |
| 61  | 3C    | 401 | HEM  | C1C-CHC-C4B | -2.25 | 121.23      | 126.02   |
| 62  | 3O    | 401 | HEC  | O1A-CGA-CBA | -2.25 | 115.96      | 123.09   |
| 61  | 3N    | 401 | HEM  | C1C-CHC-C4B | -2.22 | 121.30      | 126.02   |
| 61  | 3N    | 402 | HEM  | CHA-C4D-ND  | 2.22  | 127.11      | 124.37   |
| 62  | 3D    | 401 | HEC  | CHD-C4C-NC  | -2.21 | 122.04      | 124.45   |
| 61  | 3C    | 402 | HEM  | CHB-C1B-C2B | -2.20 | 120.68      | 126.95   |
| 61  | 3C    | 402 | HEM  | CHA-C1A-NA  | 2.20  | 127.86      | 123.86   |
| 61  | 3N    | 402 | HEM  | C1C-CHC-C4B | -2.20 | 121.35      | 126.02   |
| 61  | 3C    | 402 | HEM  | CBD-CAD-C3D | 2.19  | 118.58      | 112.53   |
| 62  | 3D    | 401 | HEC  | O2A-CGA-O1A | 2.15  | 128.87      | 123.33   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 61  | 3C    | 401 | HEM  | C4B-C3B-C2B | -2.14 | 105.31      | 107.28   |
| 61  | 3C    | 402 | HEM  | C4C-CHD-C1D | -2.11 | 121.54      | 126.02   |
| 61  | 3N    | 402 | HEM  | C2A-C1A-NA  | -2.10 | 107.82      | 110.15   |
| 62  | 3D    | 401 | HEC  | C2D-C1D-ND  | -2.06 | 106.84      | 110.14   |
| 62  | 3O    | 401 | HEC  | CMB-C2B-C3B | 2.03  | 131.33      | 126.55   |
| 61  | 3C    | 402 | HEM  | CAA-CBA-CGA | -2.02 | 108.32      | 113.67   |

There are no chirality outliers.

All (106) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 57  | al    | 502 | DGT  | PB-O3A-PA-O5'   |
| 58  | A9    | 501 | NDP  | C5B-O5B-PA-O3   |
| 58  | A9    | 501 | NDP  | C2N-C3N-C7N-O7N |
| 58  | A9    | 501 | NDP  | C2N-C3N-C7N-N7N |
| 58  | a9    | 501 | NDP  | C5D-O5D-PN-O3   |
| 58  | a9    | 501 | NDP  | C5D-O5D-PN-O1N  |
| 58  | a9    | 501 | NDP  | C5D-O5D-PN-O2N  |
| 58  | a9    | 501 | NDP  | C2D-C1D-N1N-C2N |
| 58  | a9    | 501 | NDP  | C2N-C3N-C7N-N7N |
| 60  | A6    | 201 | EHZ  | O2-C9-S1-C10    |
| 60  | A6    | 201 | EHZ  | C8-C9-S1-C10    |
| 60  | B9    | 201 | EHZ  | O1-C7-C8-C9     |
| 60  | B9    | 201 | EHZ  | O5-C16-C17-C19  |
| 60  | B9    | 201 | EHZ  | O5-C16-C17-C20  |
| 60  | a6    | 201 | EHZ  | O1-C7-C8-C9     |
| 60  | a6    | 201 | EHZ  | O4-C15-C16-O5   |
| 60  | a6    | 201 | EHZ  | C15-C16-C17-C18 |
| 60  | a6    | 201 | EHZ  | C15-C16-C17-C19 |
| 60  | a6    | 201 | EHZ  | C15-C16-C17-C20 |
| 61  | 3C    | 401 | HEM  | C2B-C3B-CAB-CBB |
| 61  | 3C    | 401 | HEM  | C4B-C3B-CAB-CBB |
| 61  | 3C    | 401 | HEM  | C2C-C3C-CAC-CBC |
| 61  | 3C    | 401 | HEM  | C4C-C3C-CAC-CBC |
| 61  | 3C    | 402 | HEM  | C2B-C3B-CAB-CBB |
| 61  | 3C    | 402 | HEM  | C4B-C3B-CAB-CBB |
| 61  | 3C    | 402 | HEM  | C2C-C3C-CAC-CBC |
| 61  | 3C    | 402 | HEM  | C4C-C3C-CAC-CBC |
| 61  | 3N    | 401 | HEM  | C2B-C3B-CAB-CBB |
| 61  | 3N    | 401 | HEM  | C2C-C3C-CAC-CBC |
| 61  | 3N    | 401 | HEM  | C4C-C3C-CAC-CBC |
| 61  | 3N    | 402 | HEM  | C2C-C3C-CAC-CBC |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 61  | 3N    | 402 | HEM  | C4C-C3C-CAC-CBC |
| 62  | 3D    | 401 | HEC  | C1A-C2A-CAA-CBA |
| 62  | 3D    | 401 | HEC  | C3A-C2A-CAA-CBA |
| 63  | V1    | 501 | FMN  | C1'-C2'-C3'-O3' |
| 63  | V1    | 501 | FMN  | C1'-C2'-C3'-C4' |
| 63  | v1    | 501 | FMN  | C5'-O5'-P-O2P   |
| 63  | v1    | 501 | FMN  | C5'-O5'-P-O3P   |
| 60  | 5a    | 701 | EHZ  | C13-C12-N1-C11  |
| 63  | V1    | 501 | FMN  | O2'-C2'-C3'-C4' |
| 61  | 3N    | 402 | HEM  | C2A-CAA-CBA-CGA |
| 60  | 5a    | 701 | EHZ  | O3-C12-N1-C11   |
| 63  | V1    | 501 | FMN  | O2'-C2'-C3'-O3' |
| 58  | a9    | 501 | NDP  | C2D-C1D-N1N-C6N |
| 61  | 3N    | 401 | HEM  | C4B-C3B-CAB-CBB |
| 58  | a9    | 501 | NDP  | O4D-C1D-N1N-C2N |
| 61  | 3C    | 401 | HEM  | C2A-CAA-CBA-CGA |
| 61  | 3N    | 401 | HEM  | C2A-CAA-CBA-CGA |
| 63  | v1    | 501 | FMN  | C5'-O5'-P-O1P   |
| 60  | B9    | 201 | EHZ  | O5-C16-C17-C18  |
| 58  | A9    | 501 | NDP  | O4D-C1D-N1N-C6N |
| 61  | 3C    | 402 | HEM  | C2A-CAA-CBA-CGA |
| 62  | 3D    | 401 | HEC  | C2A-CAA-CBA-CGA |
| 60  | B9    | 201 | EHZ  | C15-C16-C17-C19 |
| 60  | a6    | 201 | EHZ  | C19-C17-C20-O6  |
| 58  | A9    | 501 | NDP  | C2B-O2B-P2B-O1X |
| 62  | 3O    | 401 | HEC  | C4B-C3B-CAB-CBB |
| 57  | AL    | 502 | DGT  | C5'-O5'-PA-O2A  |
| 57  | al    | 502 | DGT  | C5'-O5'-PA-O2A  |
| 60  | a6    | 201 | EHZ  | O5-C16-C17-C20  |
| 62  | 3O    | 401 | HEC  | C2B-C3B-CAB-CBB |
| 62  | 3O    | 401 | HEC  | C2C-C3C-CAC-CBC |
| 63  | V1    | 501 | FMN  | C4'-C5'-O5'-P   |
| 62  | 3O    | 401 | HEC  | C2D-C3D-CAD-CBD |
| 58  | A9    | 501 | NDP  | O4D-C4D-C5D-O5D |
| 58  | a9    | 501 | NDP  | O4B-C4B-C5B-O5B |
| 60  | 5a    | 701 | EHZ  | O5-C16-C17-C19  |
| 58  | A9    | 501 | NDP  | PN-O3-PA-O2A    |
| 62  | 3O    | 401 | HEC  | C4D-C3D-CAD-CBD |
| 60  | A6    | 201 | EHZ  | C10-C11-N1-C12  |
| 60  | a6    | 201 | EHZ  | N2-C15-C16-O5   |
| 60  | B9    | 201 | EHZ  | C21-C1-C2-C3    |
| 61  | 3N    | 401 | HEM  | CAA-CBA-CGA-O1A |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 61  | 3N    | 402 | HEM  | CAD-CBD-CGD-O1D |
| 61  | 3C    | 401 | HEM  | CAD-CBD-CGD-O1D |
| 61  | 3N    | 401 | HEM  | CAA-CBA-CGA-O2A |
| 61  | 3C    | 402 | HEM  | CAA-CBA-CGA-O1A |
| 62  | 3O    | 401 | HEC  | CAD-CBD-CGD-O2D |
| 58  | a9    | 501 | NDP  | PA-O3-PN-O1N    |
| 61  | 3C    | 401 | HEM  | CAD-CBD-CGD-O2D |
| 61  | 3N    | 402 | HEM  | CAD-CBD-CGD-O2D |
| 60  | B9    | 201 | EHZ  | C6-C7-C8-C9     |
| 61  | 3C    | 402 | HEM  | CAA-CBA-CGA-O2A |
| 61  | 3N    | 401 | HEM  | CAD-CBD-CGD-O2D |
| 62  | 3D    | 401 | HEC  | CAD-CBD-CGD-O1D |
| 62  | 3D    | 401 | HEC  | CAA-CBA-CGA-O2A |
| 62  | 3O    | 401 | HEC  | CAD-CBD-CGD-O1D |
| 61  | 3C    | 401 | HEM  | CAA-CBA-CGA-O2A |
| 61  | 3C    | 401 | HEM  | CAA-CBA-CGA-O1A |
| 61  | 3N    | 401 | HEM  | CAD-CBD-CGD-O1D |
| 60  | a6    | 201 | EHZ  | O5-C16-C17-C18  |
| 58  | A9    | 501 | NDP  | PN-O3-PA-O1A    |
| 62  | 3D    | 401 | HEC  | CAD-CBD-CGD-O2D |
| 58  | A9    | 501 | NDP  | C3D-C4D-C5D-O5D |
| 61  | 3N    | 402 | HEM  | CAA-CBA-CGA-O1A |
| 60  | 5a    | 701 | EHZ  | C22-C23-C24-C25 |
| 60  | B9    | 201 | EHZ  | C15-C16-C17-C20 |
| 60  | a6    | 201 | EHZ  | C18-C17-C20-O6  |
| 63  | v1    | 501 | FMN  | N10-C1'-C2'-O2' |
| 61  | 3N    | 402 | HEM  | CAA-CBA-CGA-O2A |
| 62  | 3D    | 401 | HEC  | C4B-C3B-CAB-CBB |
| 62  | 3D    | 401 | HEC  | C4C-C3C-CAC-CBC |
| 62  | 3O    | 401 | HEC  | C4C-C3C-CAC-CBC |
| 62  | 3D    | 401 | HEC  | CAA-CBA-CGA-O1A |
| 58  | a9    | 501 | NDP  | O4D-C4D-C5D-O5D |
| 62  | 3O    | 401 | HEC  | CAA-CBA-CGA-O2A |

There are no ring outliers.

22 monomers are involved in 32 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 65  | S1    | 803 | FES  | 1       | 0            |
| 61  | 3C    | 401 | HEM  | 1       | 0            |
| 64  | s1    | 801 | SF4  | 1       | 0            |
| 57  | AL    | 502 | DGT  | 1       | 0            |

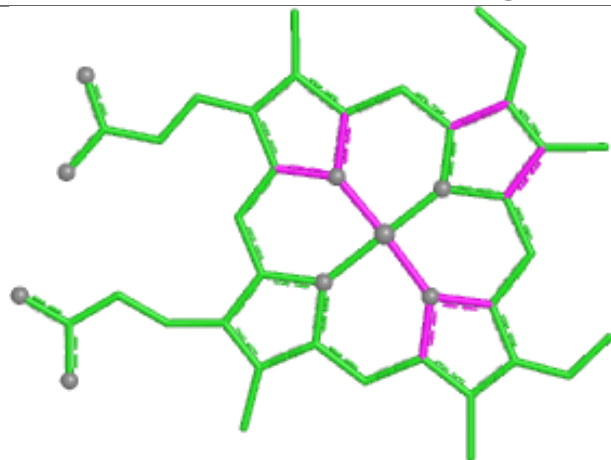
*Continued on next page...*

*Continued from previous page...*

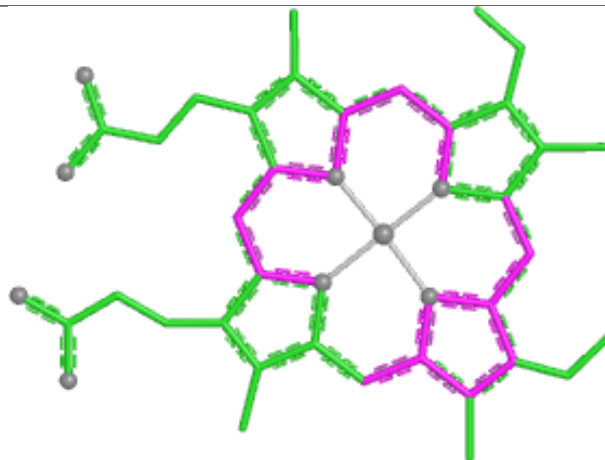
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 64  | V1    | 502 | SF4  | 1       | 0            |
| 64  | s8    | 301 | SF4  | 2       | 0            |
| 65  | s1    | 803 | FES  | 1       | 0            |
| 60  | B9    | 201 | EHZ  | 1       | 0            |
| 63  | V1    | 501 | FMN  | 2       | 0            |
| 64  | s7    | 301 | SF4  | 2       | 0            |
| 64  | S1    | 801 | SF4  | 1       | 0            |
| 62  | 3D    | 401 | HEC  | 3       | 0            |
| 58  | A9    | 501 | NDP  | 3       | 0            |
| 64  | S7    | 301 | SF4  | 3       | 0            |
| 65  | V2    | 301 | FES  | 1       | 0            |
| 64  | v1    | 502 | SF4  | 1       | 0            |
| 61  | 3N    | 402 | HEM  | 1       | 0            |
| 64  | S8    | 301 | SF4  | 1       | 0            |
| 61  | 3N    | 401 | HEM  | 1       | 0            |
| 65  | v2    | 301 | FES  | 1       | 0            |
| 62  | 3O    | 401 | HEC  | 2       | 0            |
| 58  | a9    | 501 | NDP  | 1       | 0            |

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

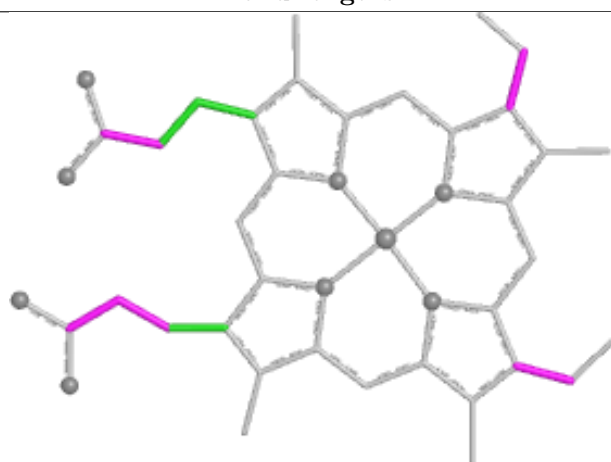
## Ligand HEM 3C 401



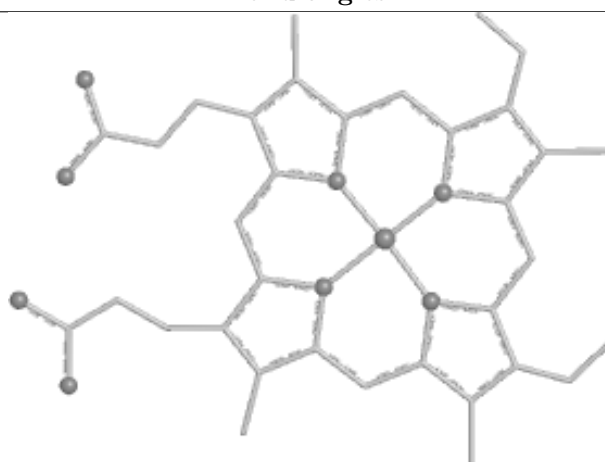
Bond lengths



Bond angles

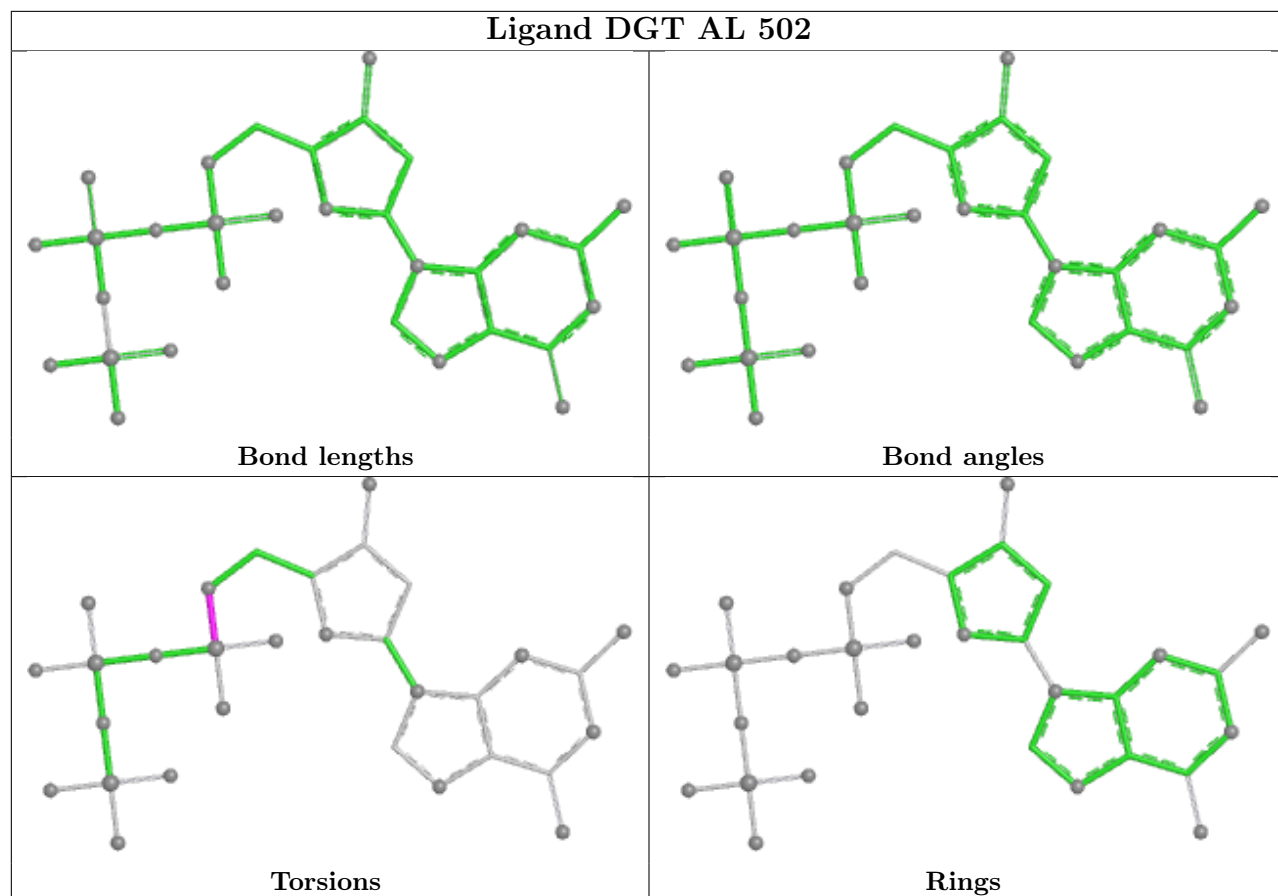


Torsions

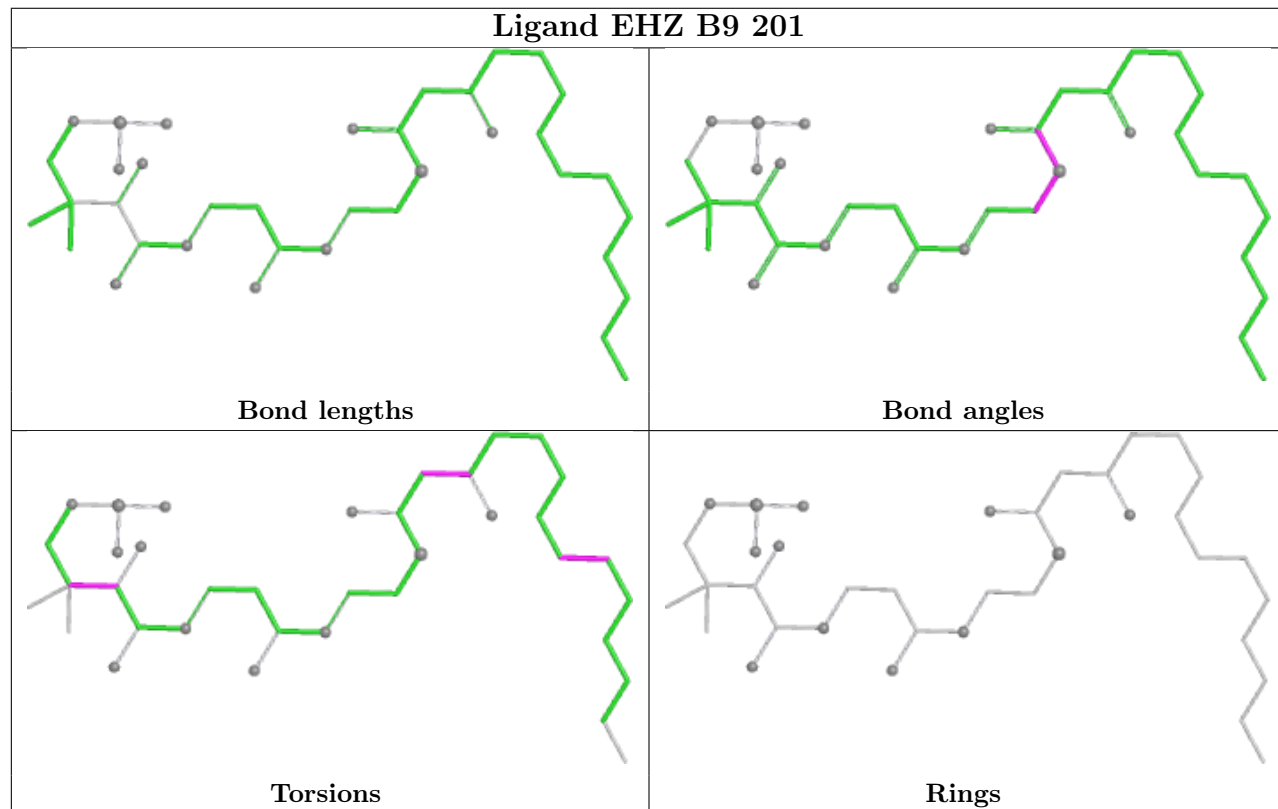


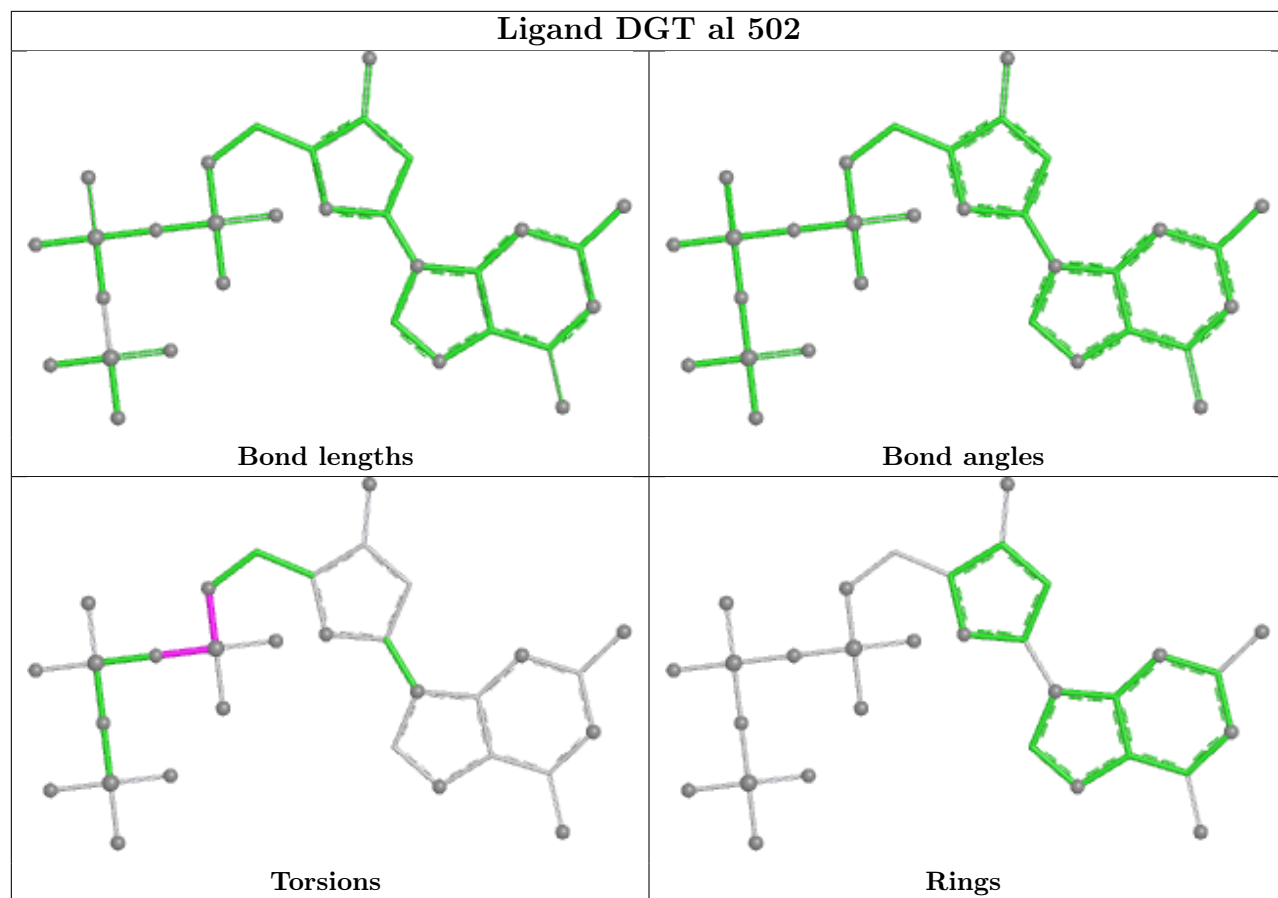
Rings

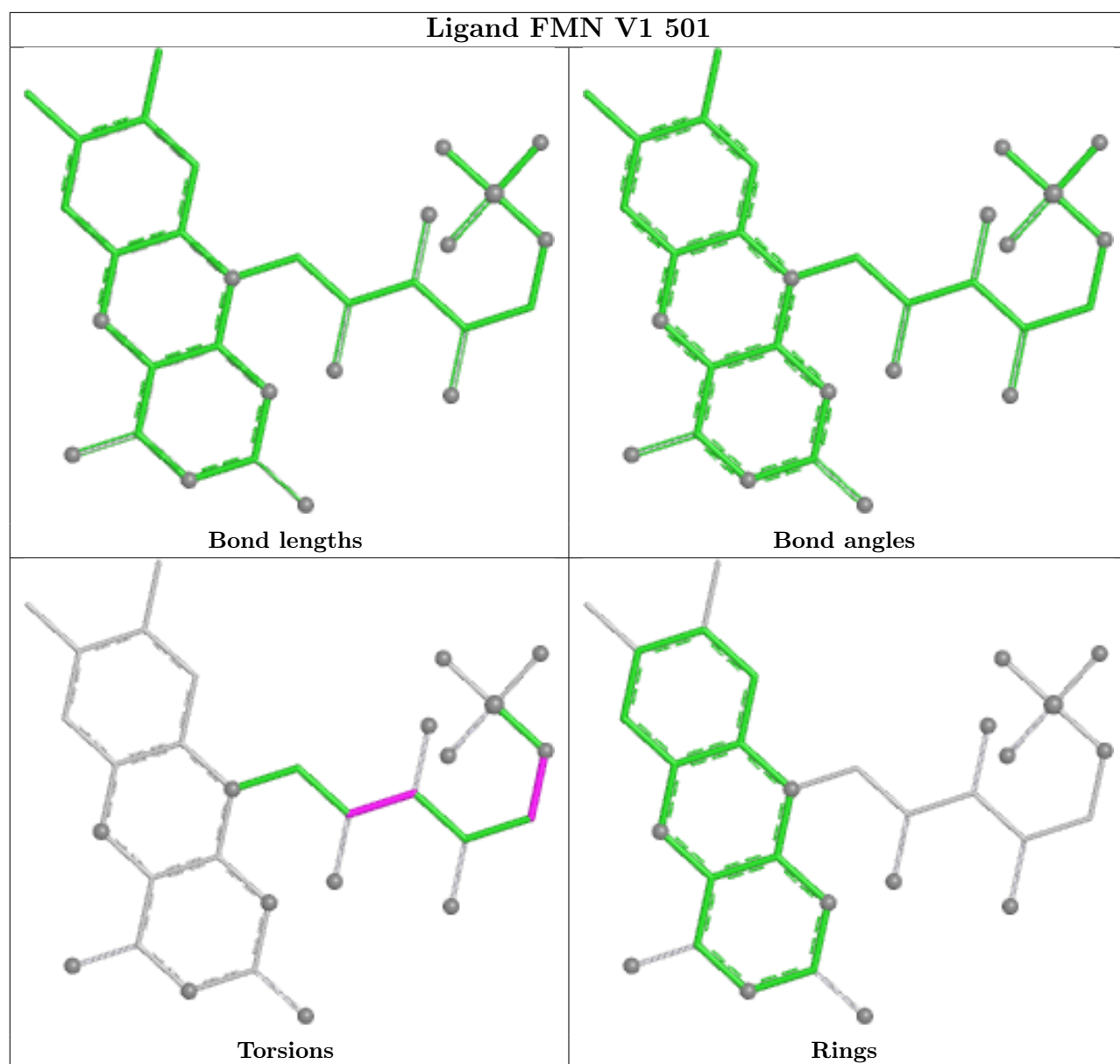
## Ligand DGT AL 502

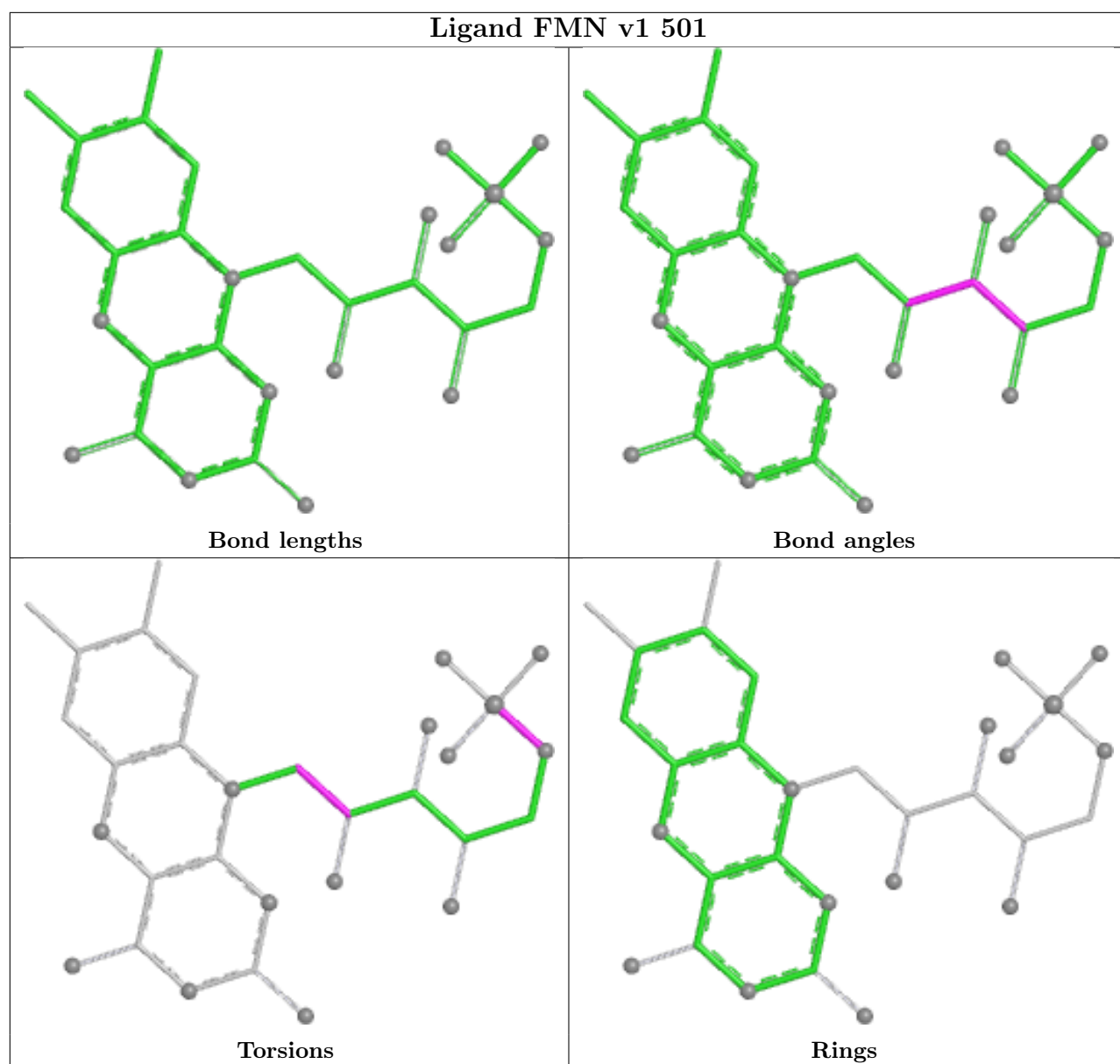


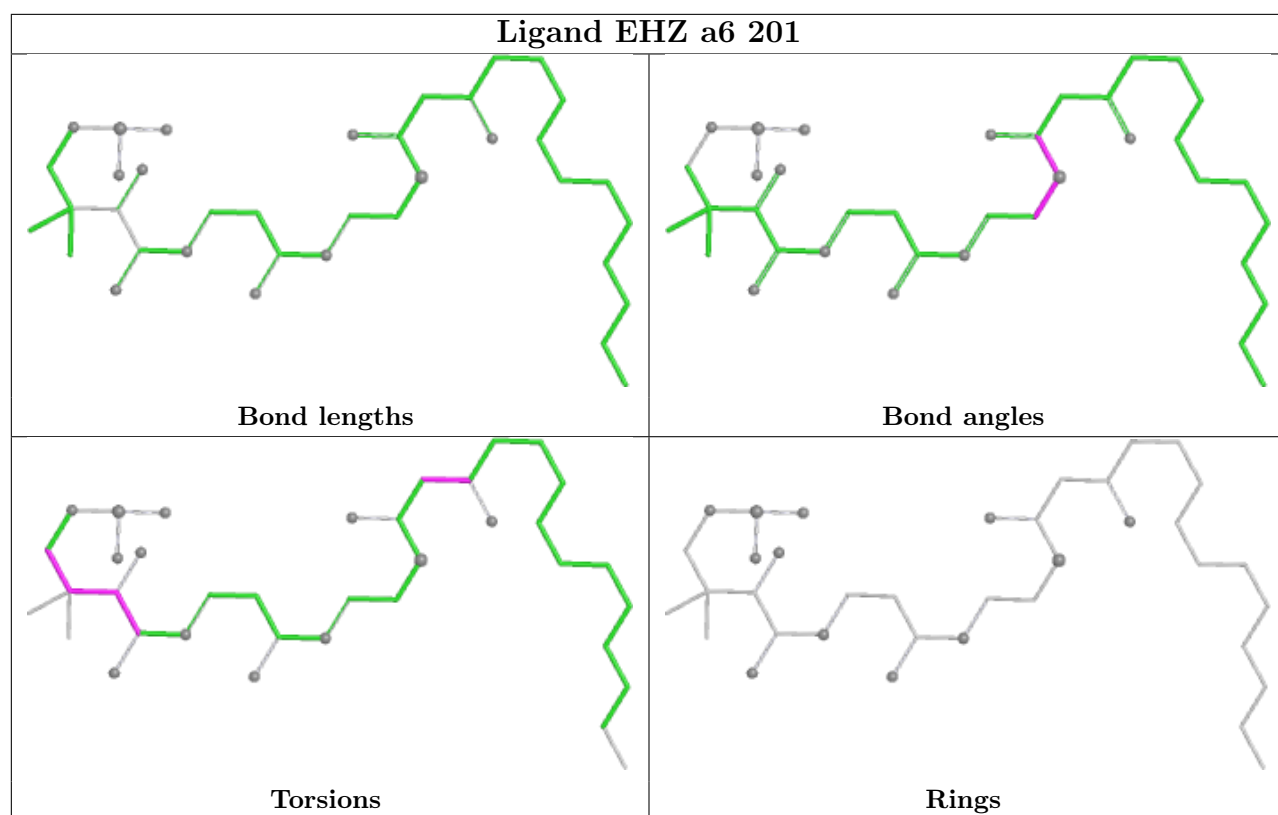
## Ligand EHZ B9 201



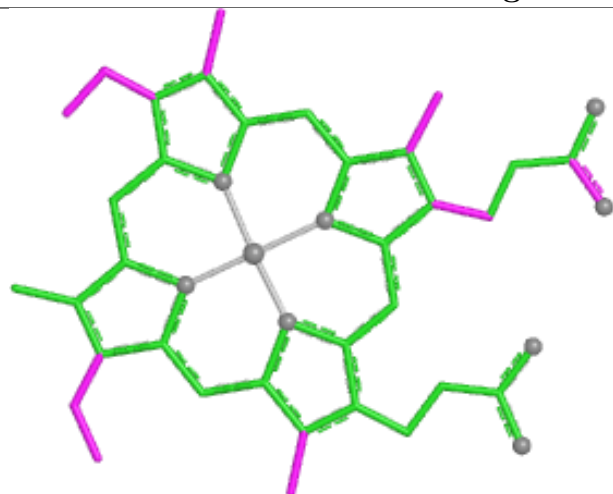




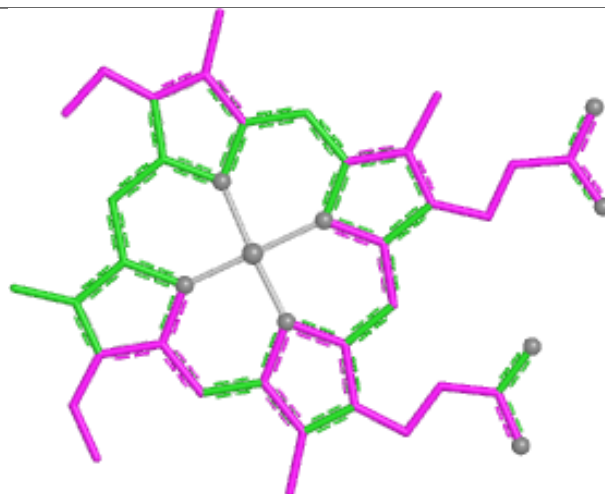




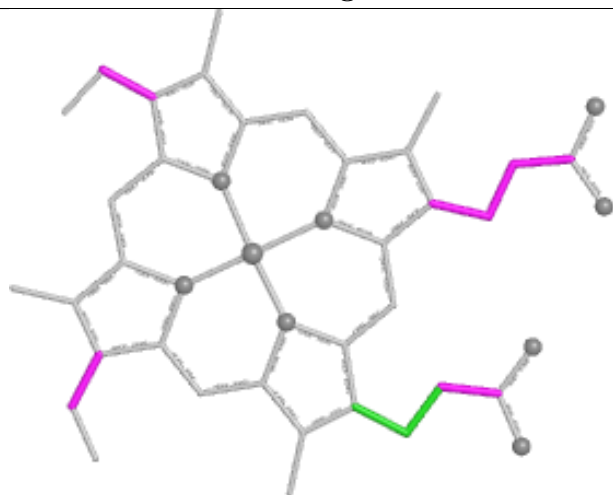
## Ligand HEC 3D 401



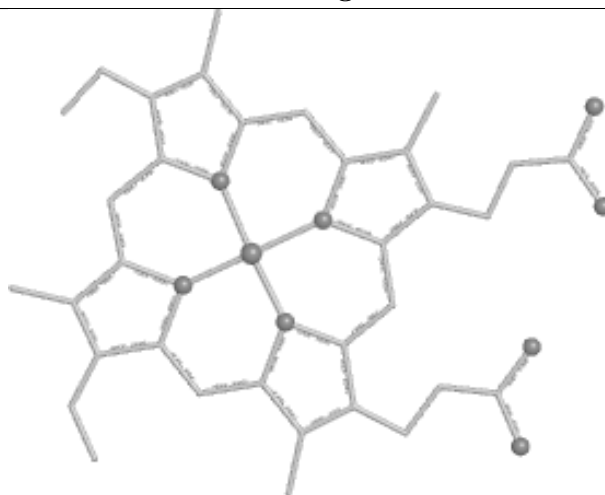
Bond lengths



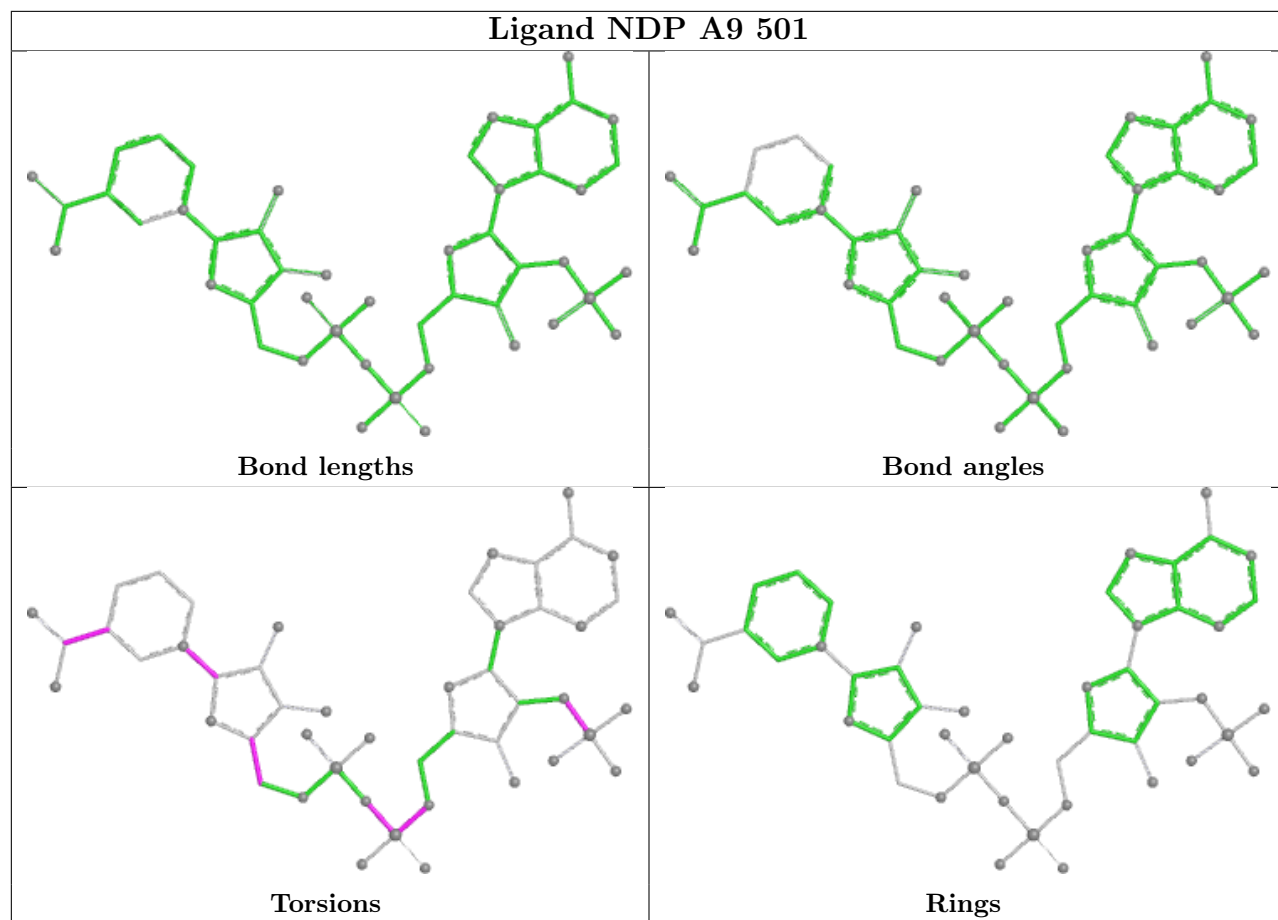
Bond angles



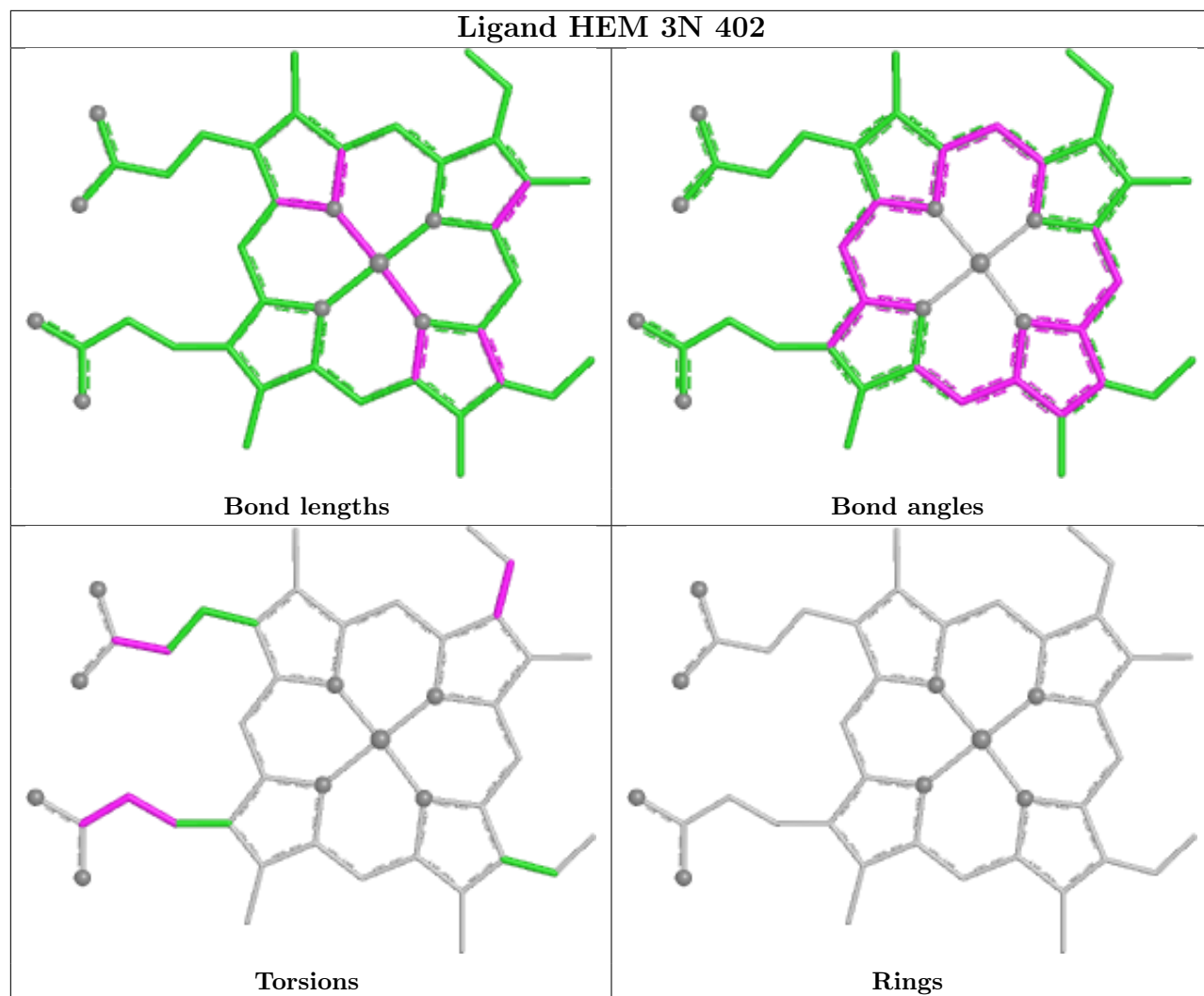
Torsions

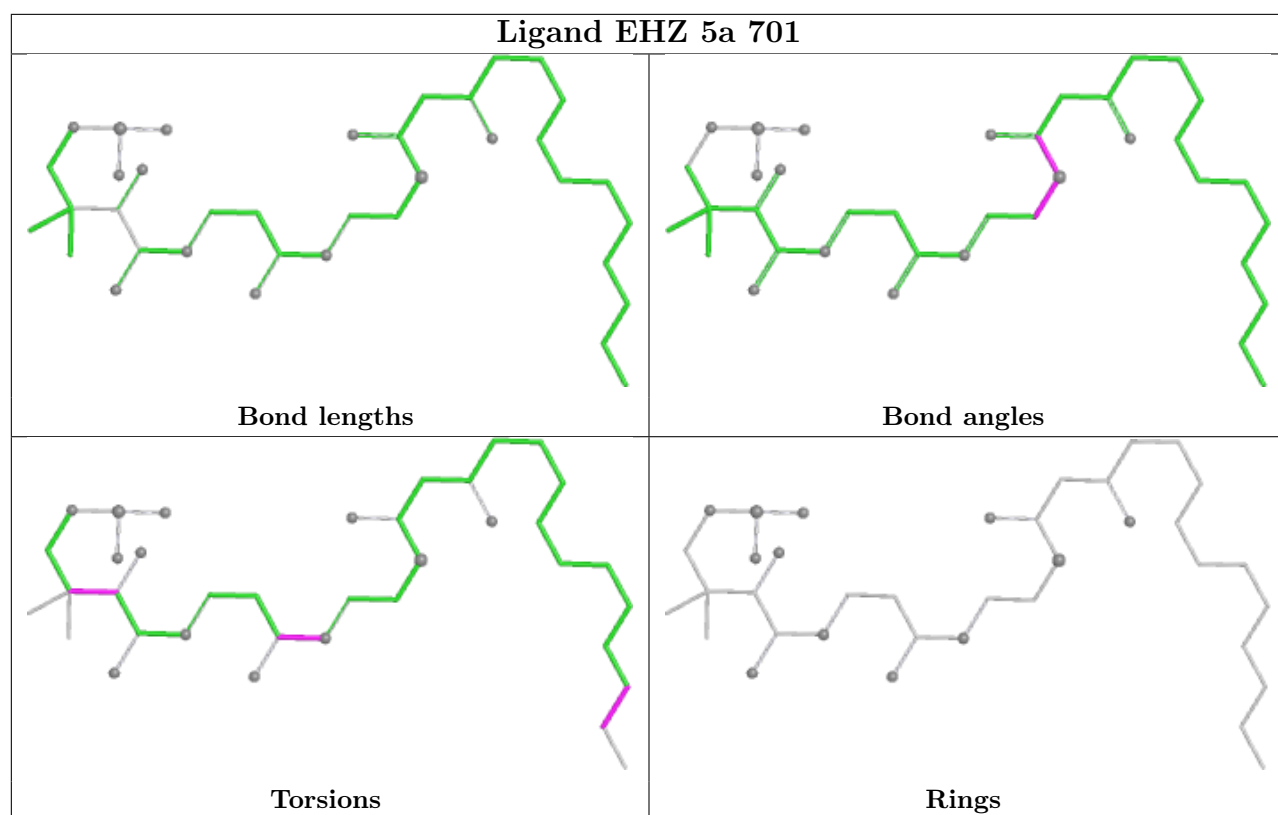


Rings

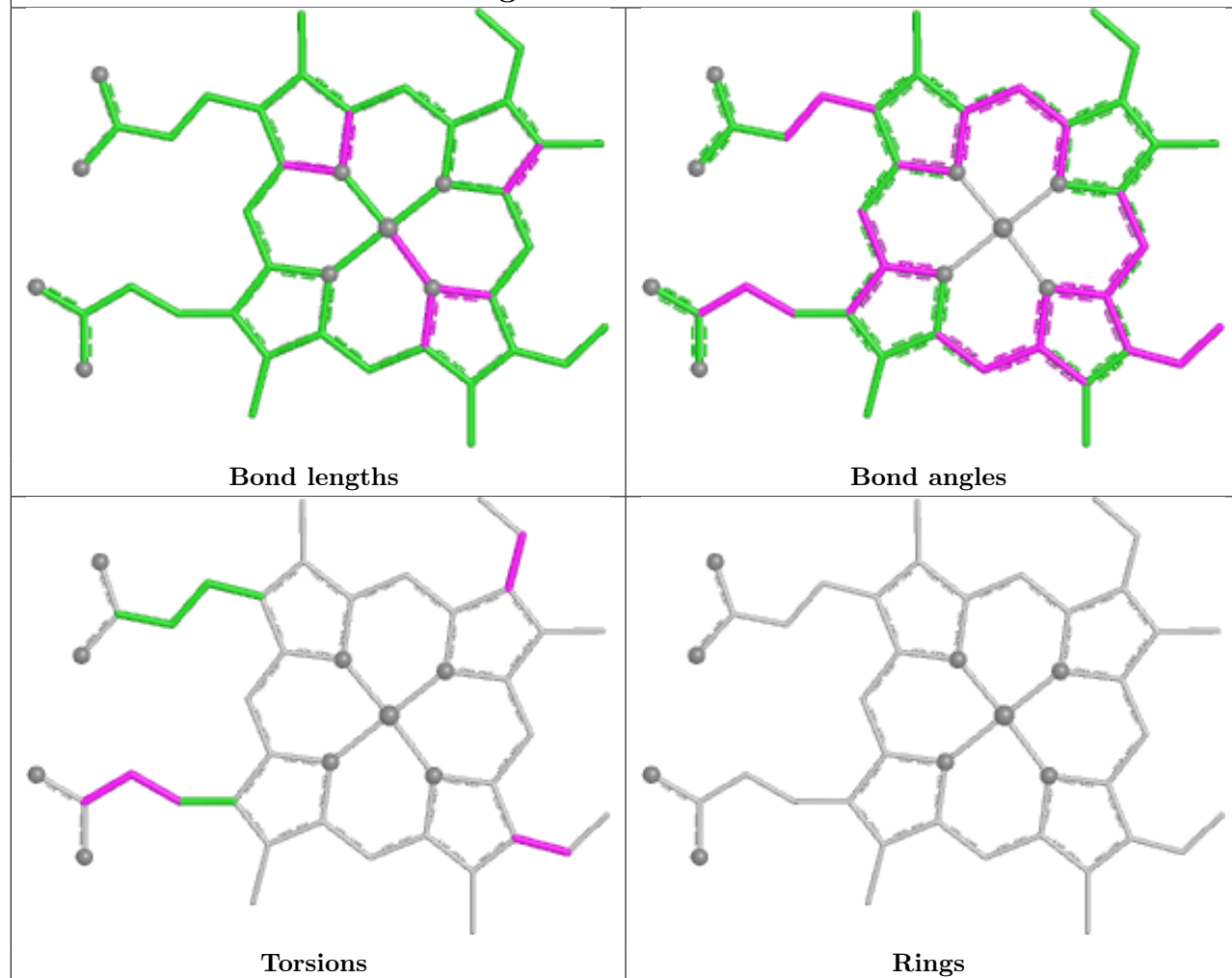


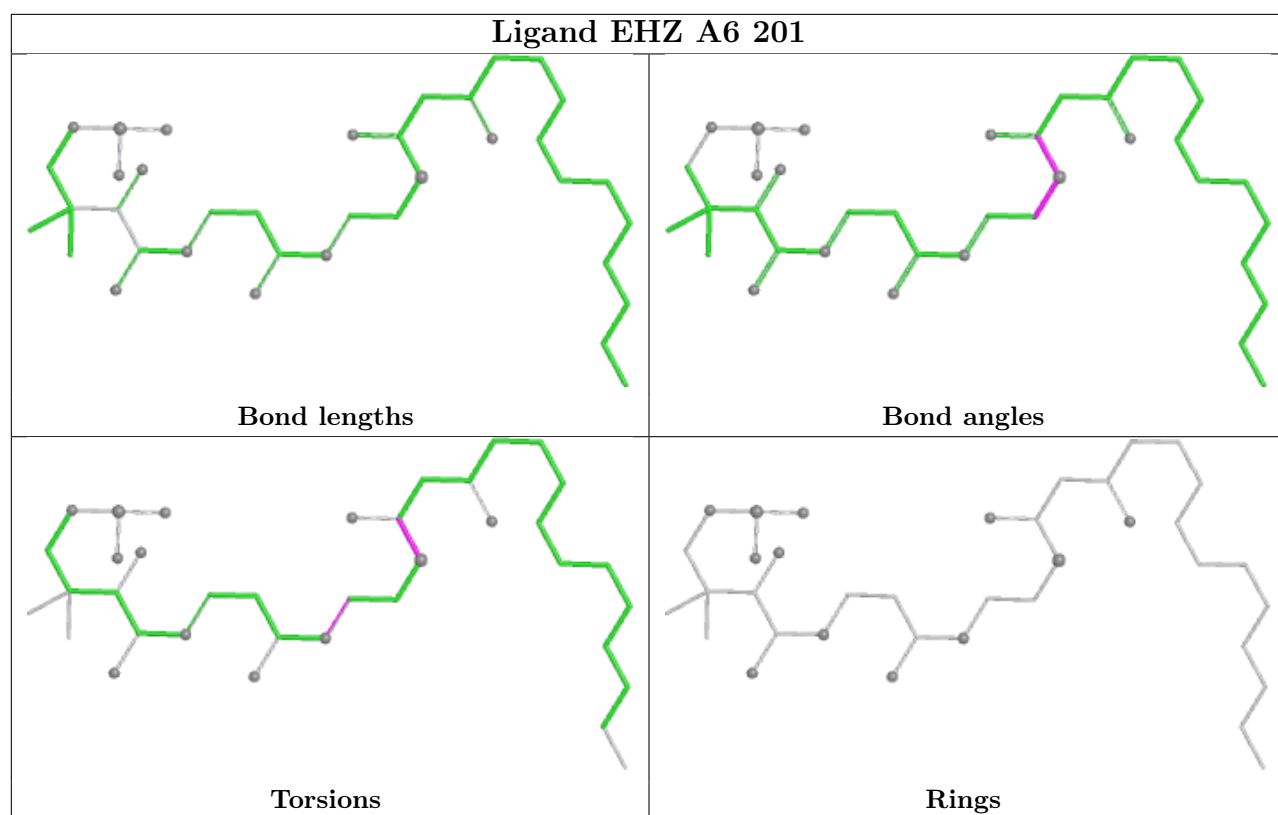
## Ligand HEM 3N 402



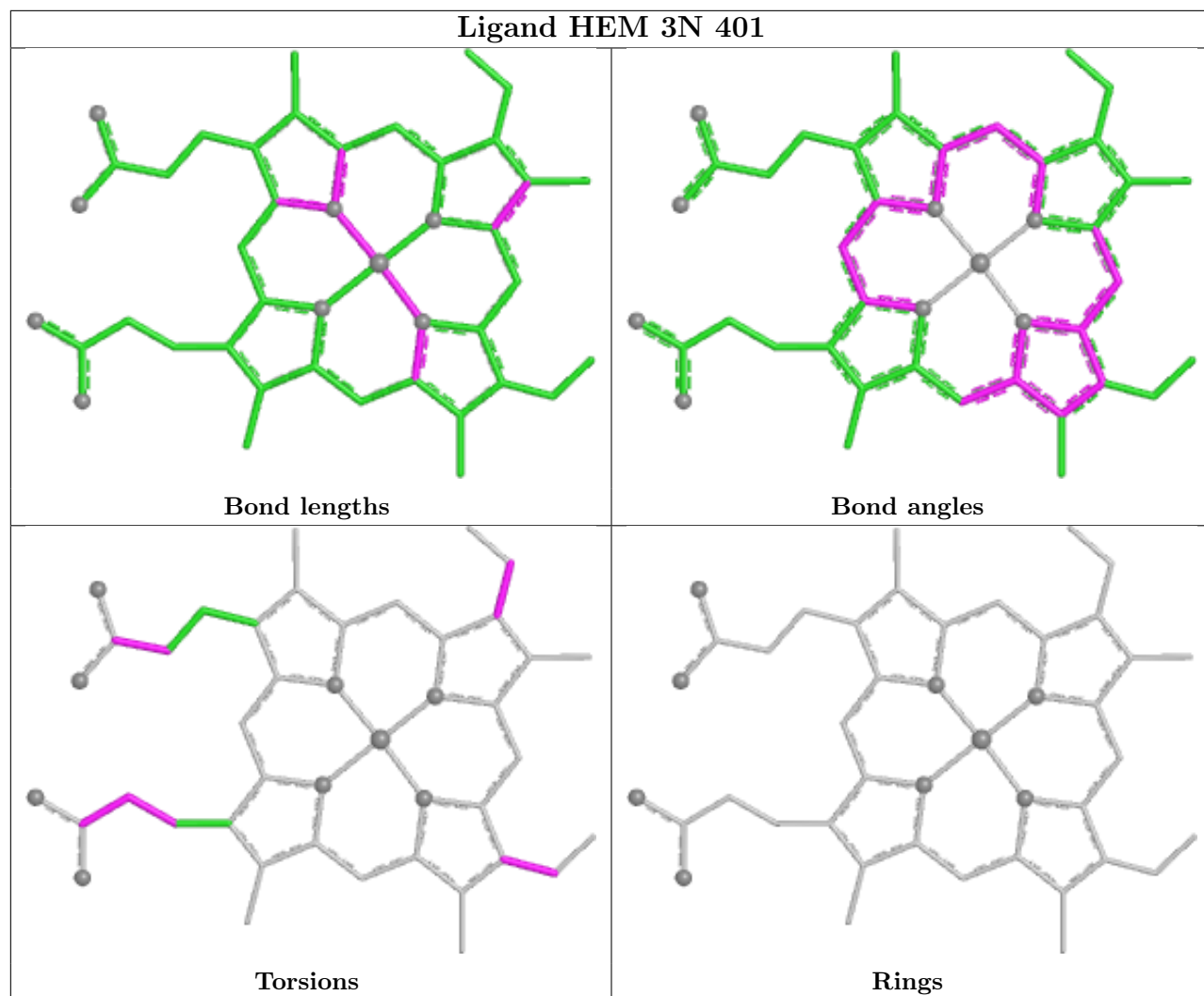


## Ligand HEM 3C 402

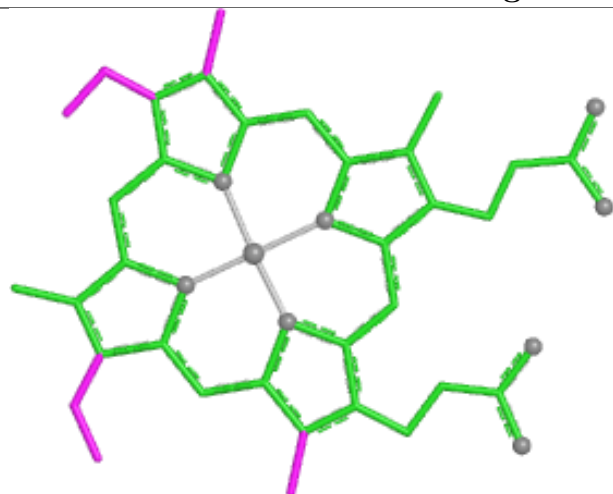




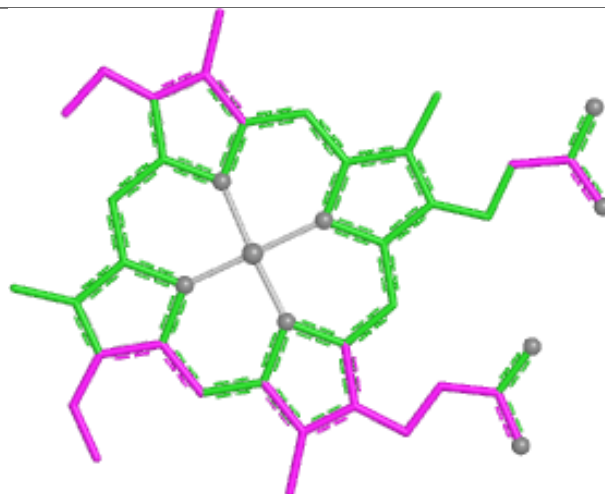
## Ligand HEM 3N 401



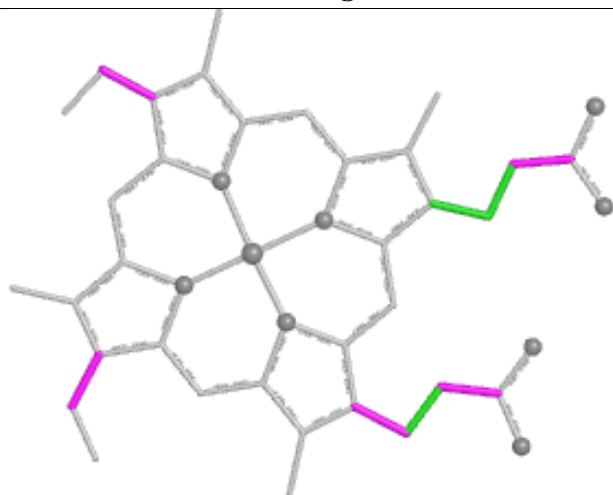
## Ligand HEC 3O 401



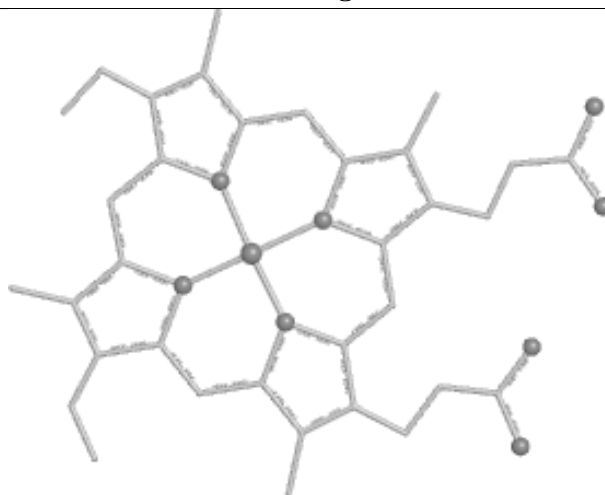
Bond lengths



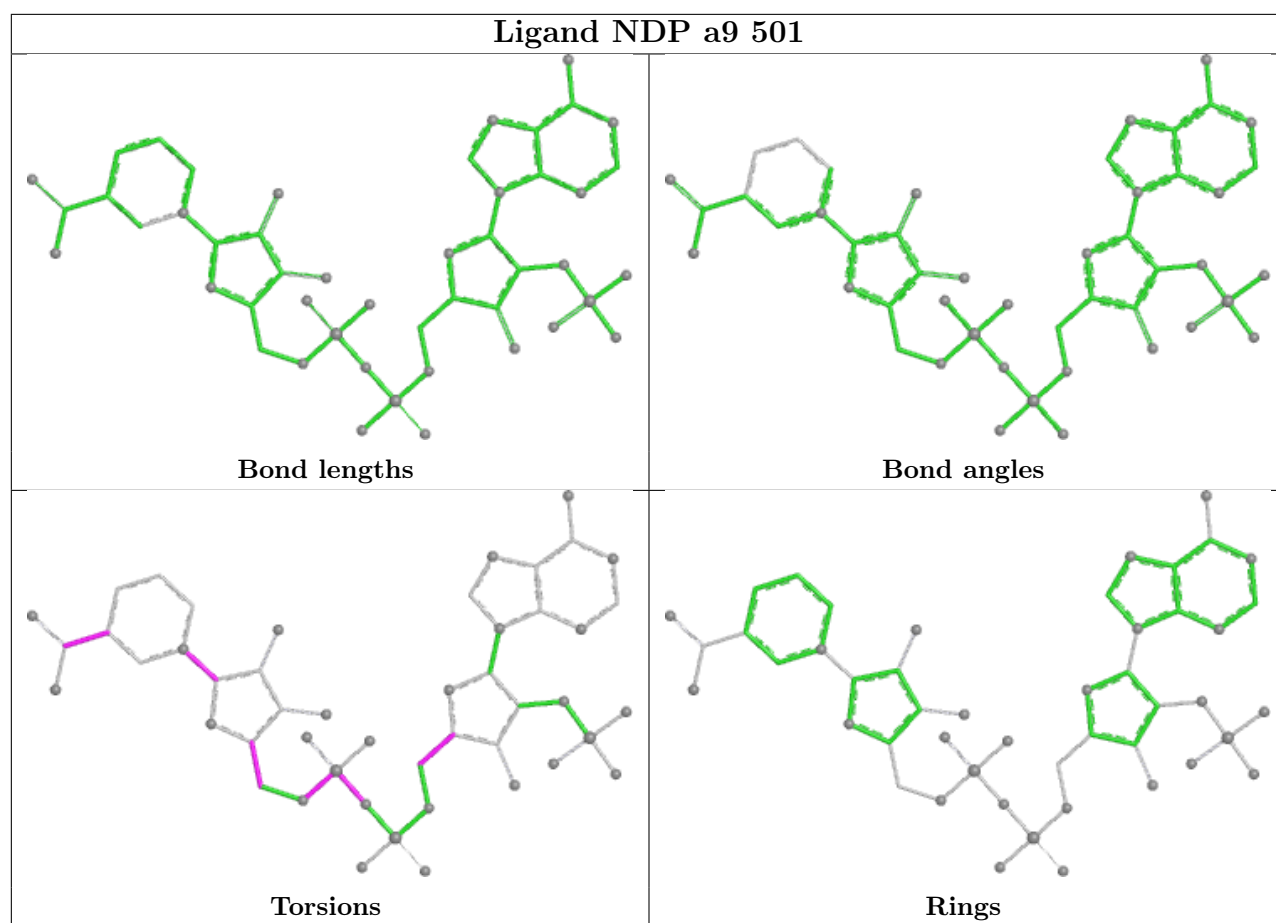
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

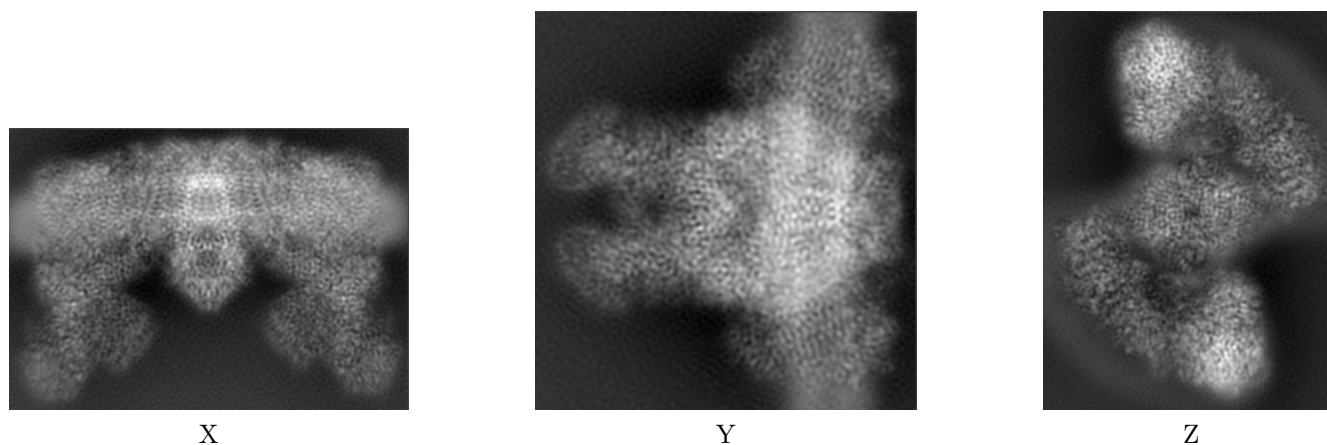
## 6 Map visualisation [i](#)

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

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

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

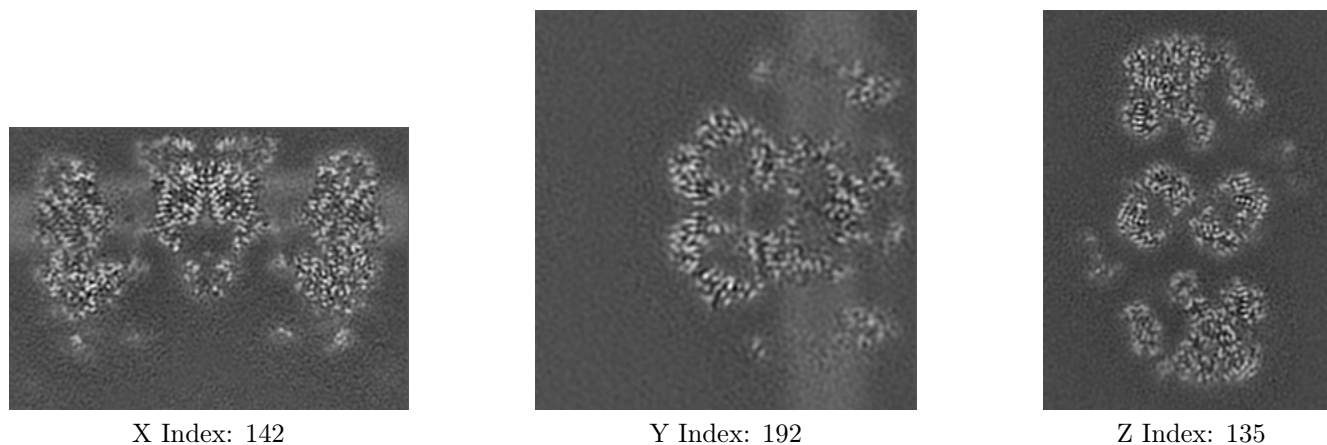
#### 6.1.1 Primary map



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

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

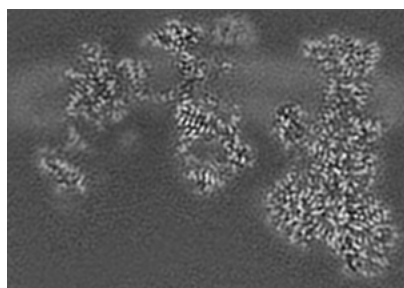
#### 6.2.1 Primary map



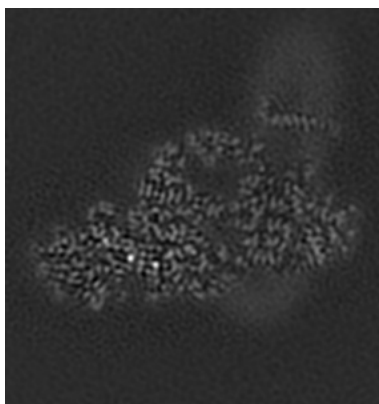
The images above show central slices of the map in three orthogonal directions.

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

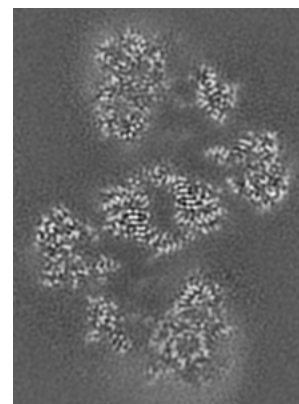
### 6.3.1 Primary map



X Index: 114



Y Index: 323

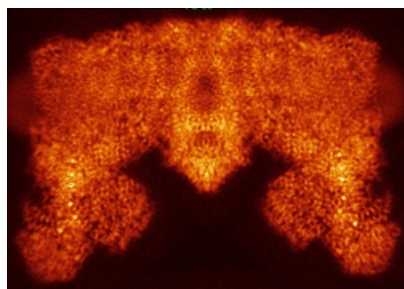


Z Index: 159

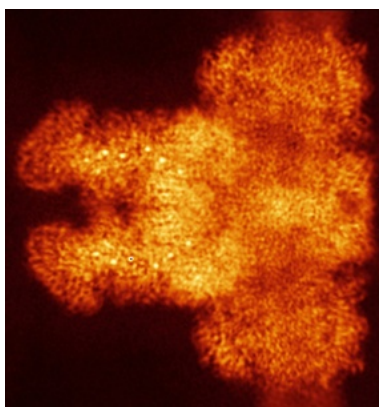
The images above show the largest variance slices of the map in three orthogonal directions.

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

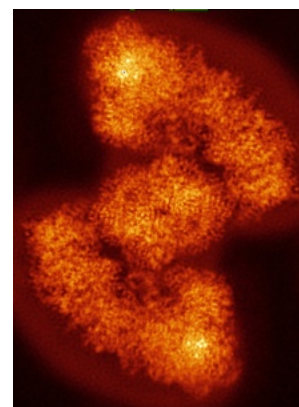
### 6.4.1 Primary map



X



Y

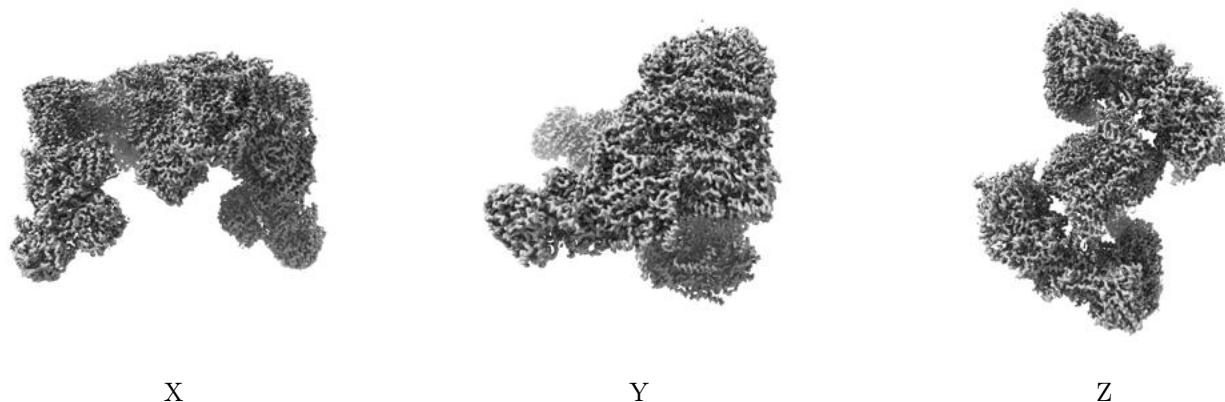


Z

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

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

### 6.5.1 Primary map



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

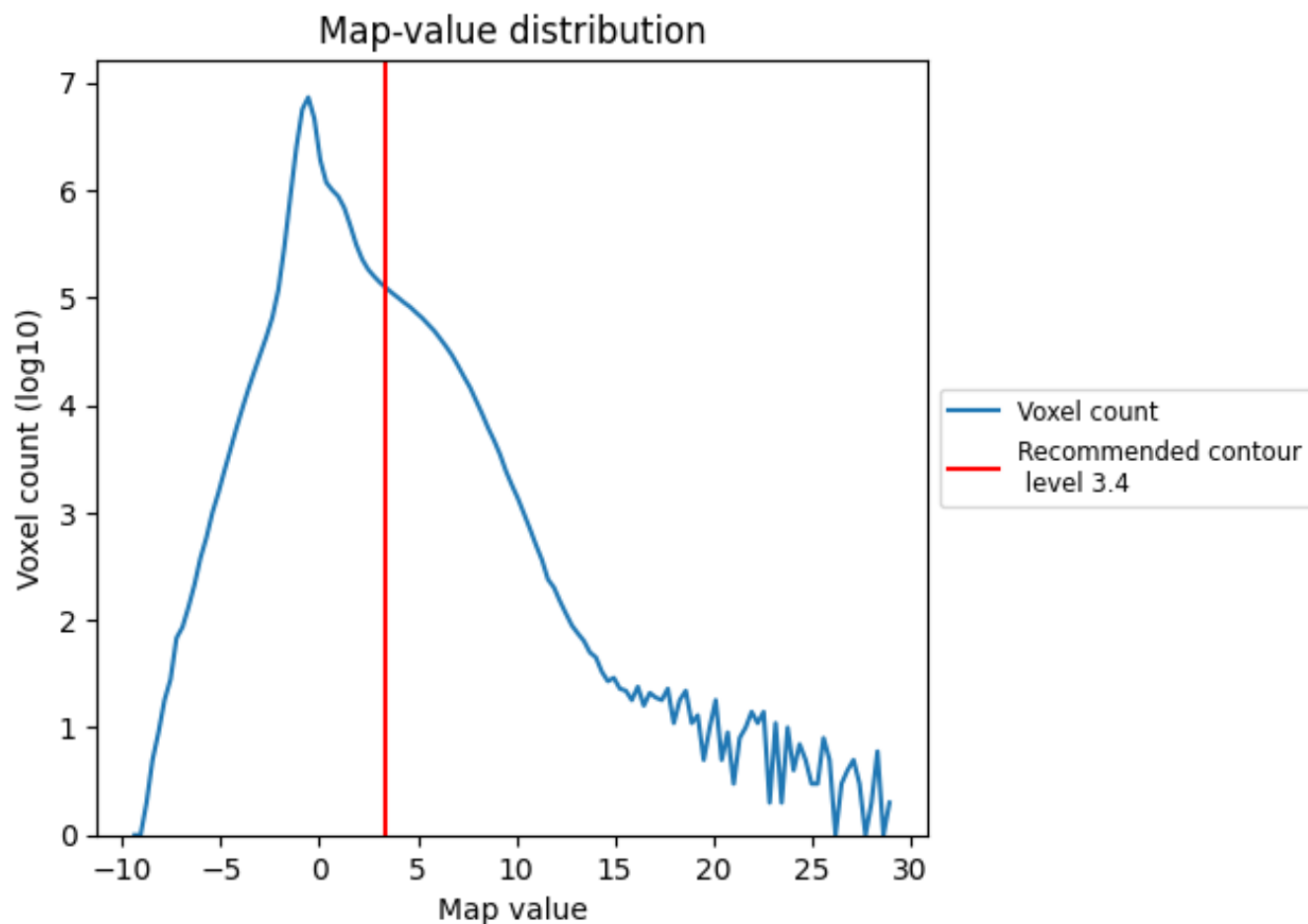
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

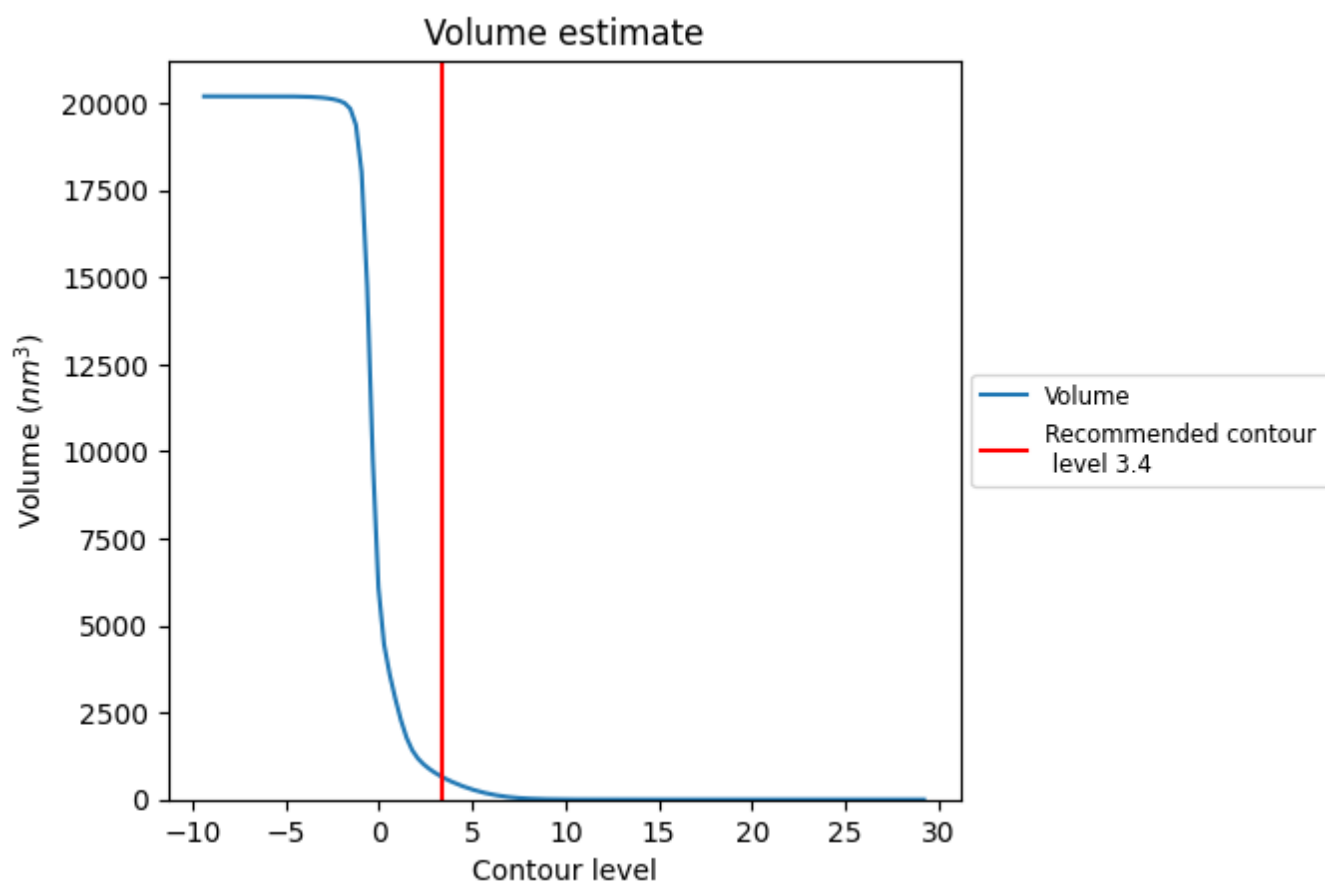
This section contains the results of statistical analysis of the map.

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



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

## 7.2 Volume estimate [i](#)



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

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

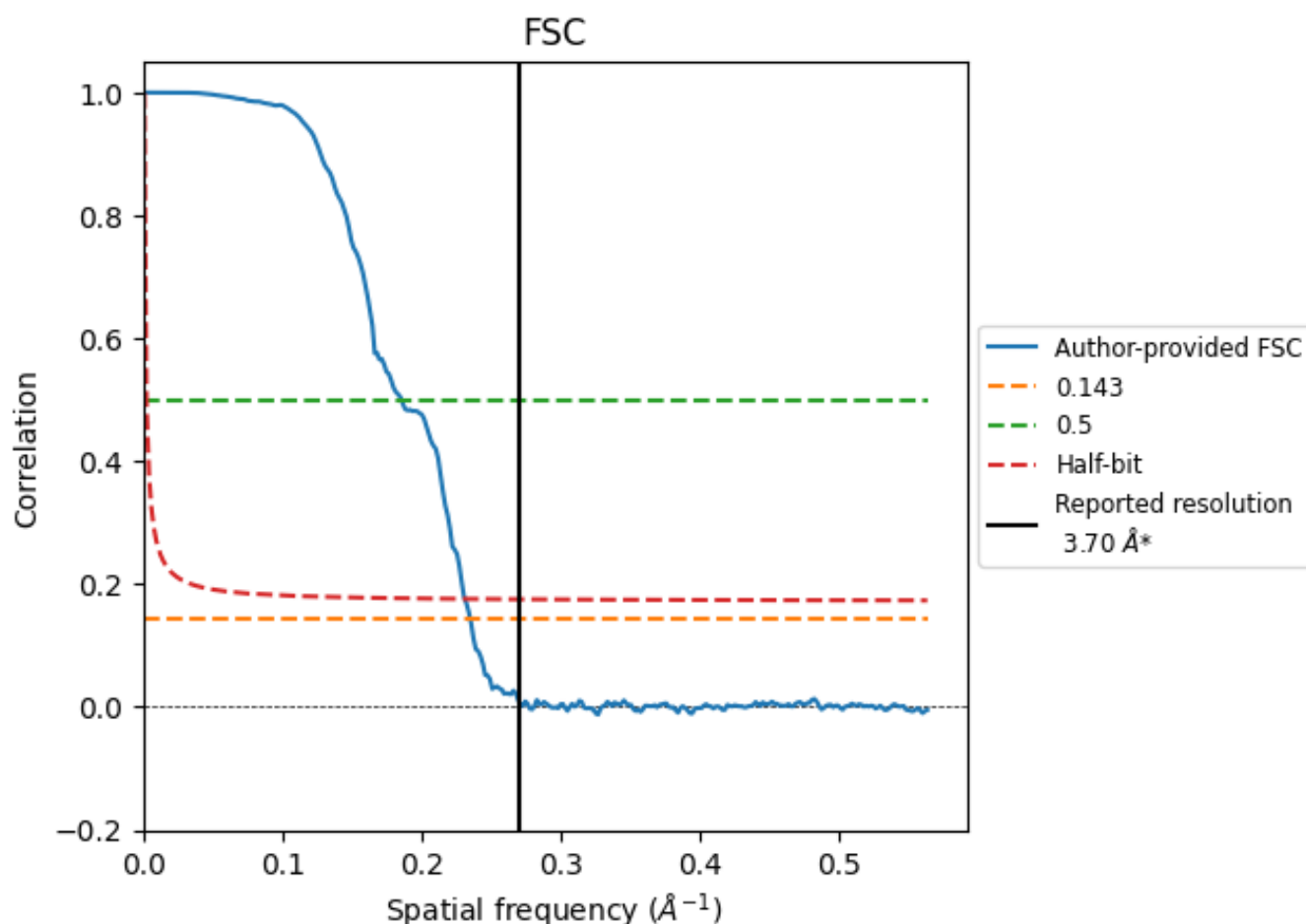
## 7.3 Rotationally averaged power spectrum [i](#)

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

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

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

### 8.1 FSC [i](#)



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

## 8.2 Resolution estimates [i](#)

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

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

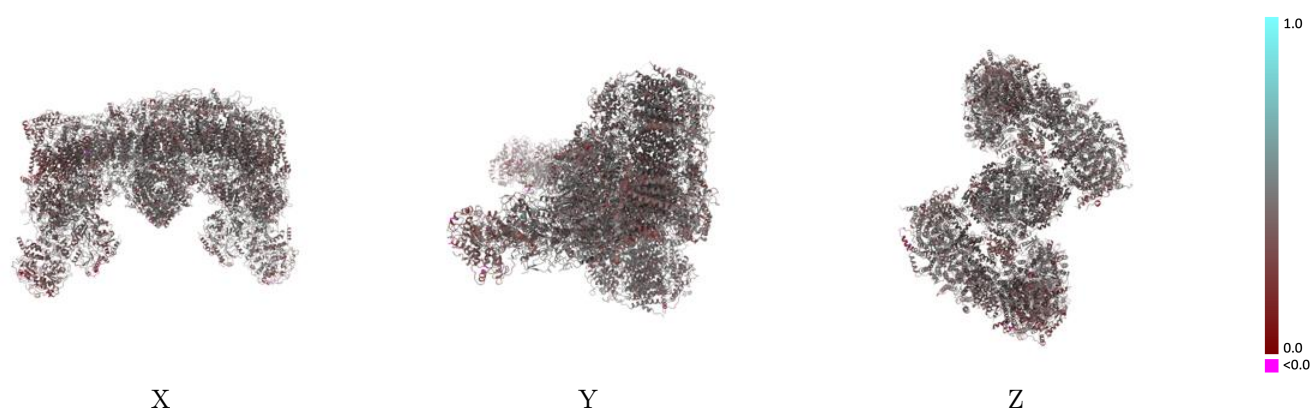
## 9 Map-model fit [i](#)

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

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

This section was not generated.

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

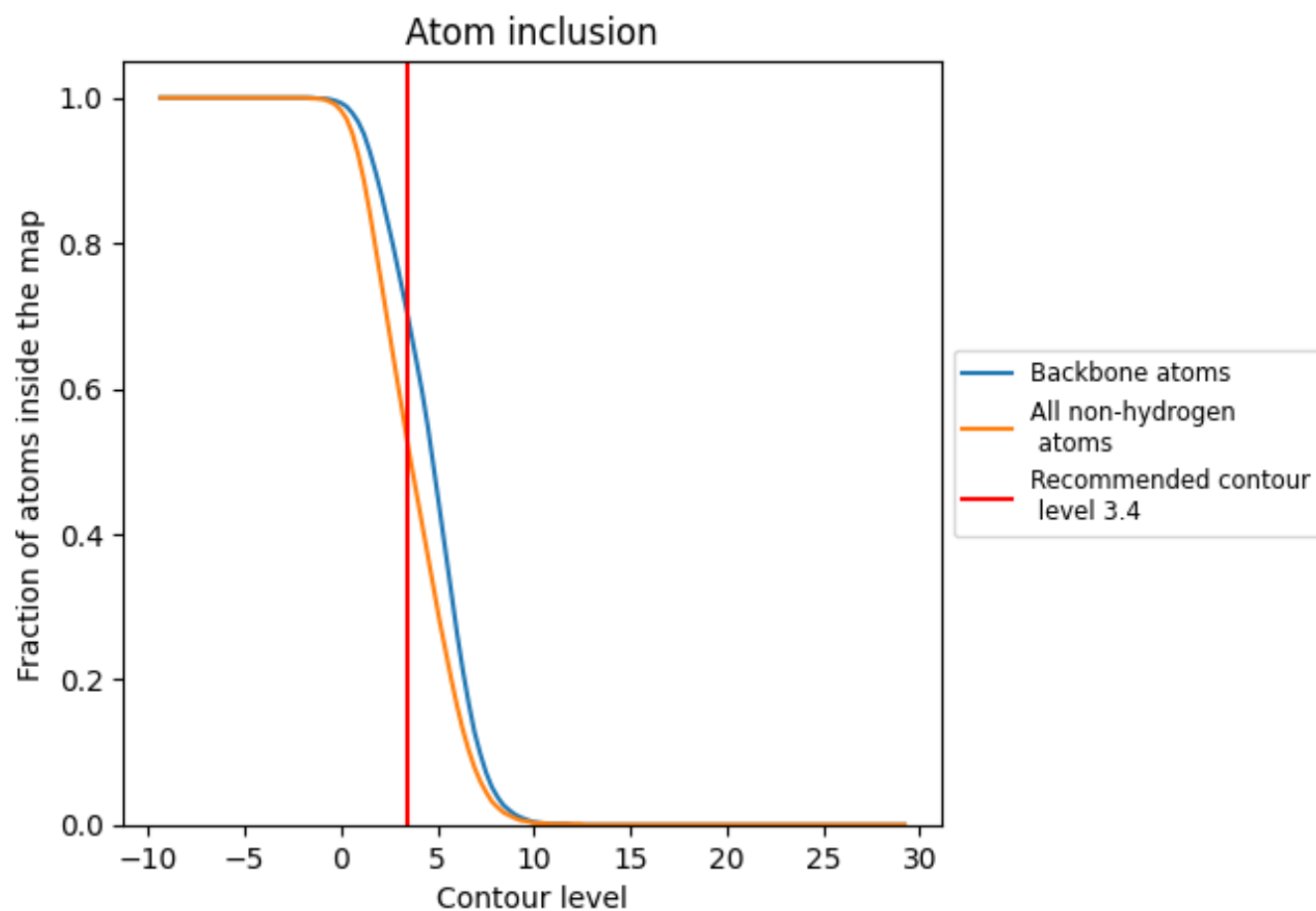


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

## 9.4 Atom inclusion [i](#)



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

## 9.5 Map-model fit summary ⓘ

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

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



*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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