



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 07:34 pm BST

PDB ID : 4V8F  
Title : Crystal structure analysis of ribosomal decoding (near-cognate tRNA-ttyr complex with paromomycin).  
Authors : Jenner, L.; Demeshkina, N.; Yusupov, M.; Yusupova, G.  
Deposited on : 2011-12-07  
Resolution : 3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

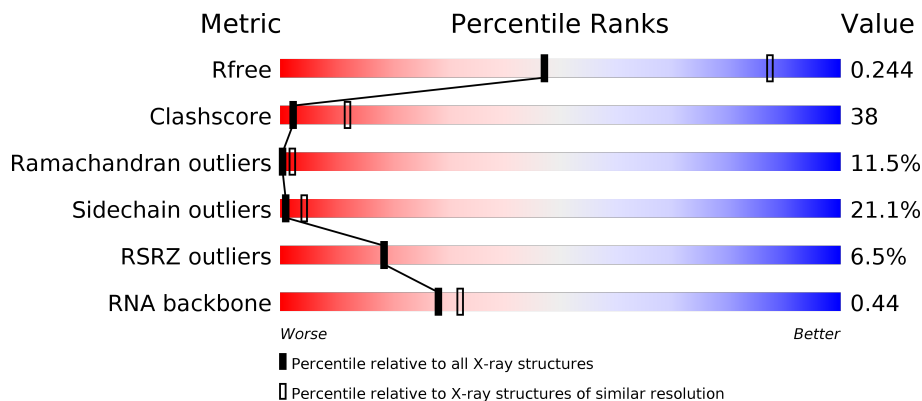
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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.



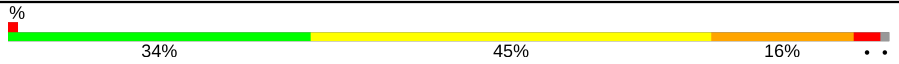

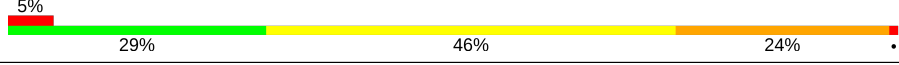
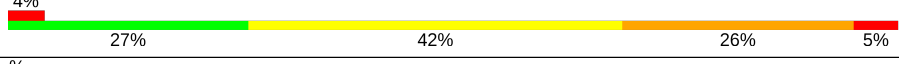
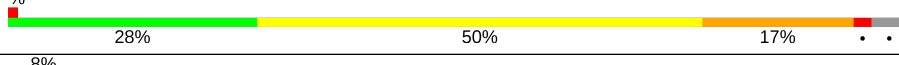
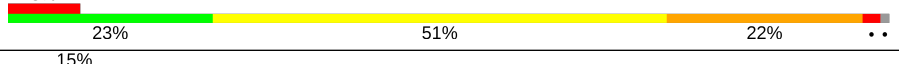
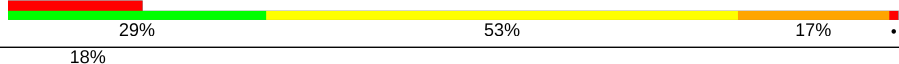
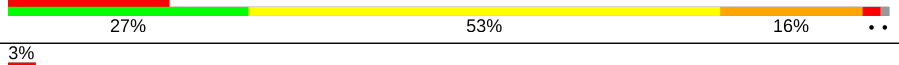
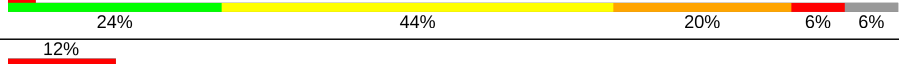
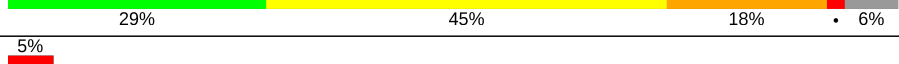
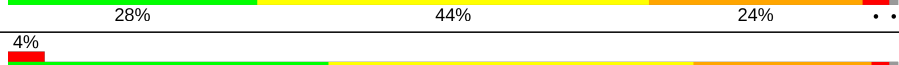
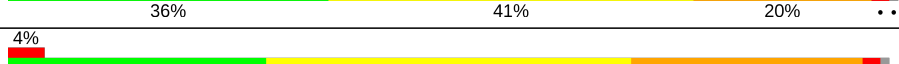
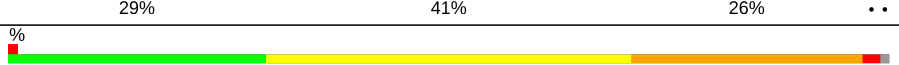
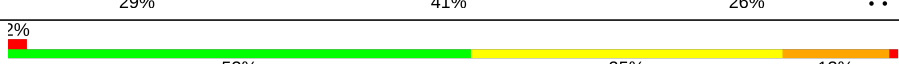
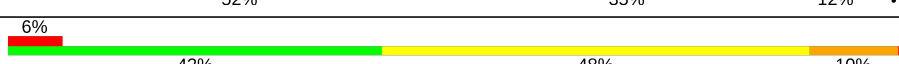
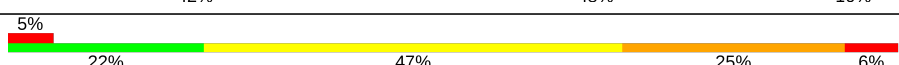
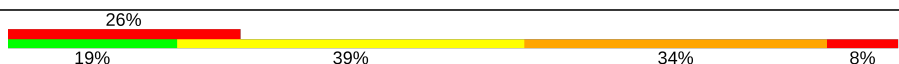
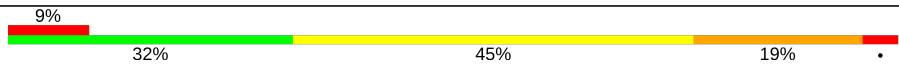
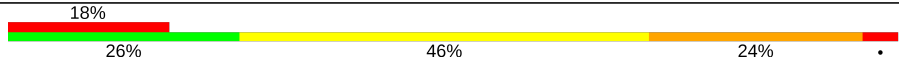
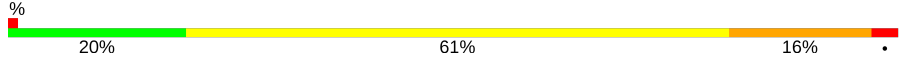
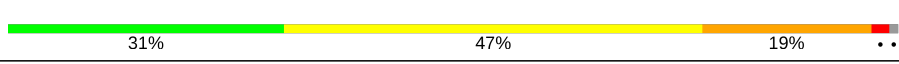
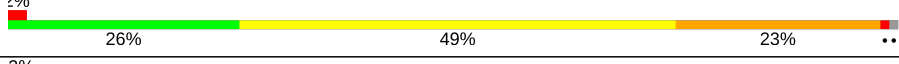
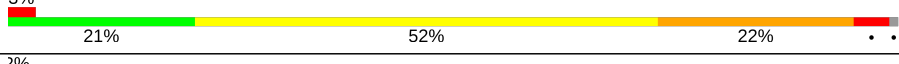
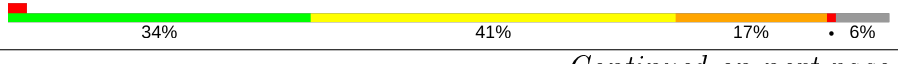

| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 1149 (3.34-3.26)                                      |
| Clashscore            | 141614                      | 1205 (3.34-3.26)                                      |
| Ramachandran outliers | 138981                      | 1183 (3.34-3.26)                                      |
| Sidechain outliers    | 138945                      | 1182 (3.34-3.26)                                      |
| RSRZ outliers         | 127900                      | 1115 (3.34-3.26)                                      |
| RNA backbone          | 3102                        | 1117 (3.70-2.90)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--------------------|
| 1   | AA    | 2912   | <br>28% 49% 21% 2% |
| 1   | DA    | 2912   | <br>27% 50% 21% 2% |
| 2   | AB    | 122    | <br>24% 55% 19% 2% |
| 2   | DB    | 122    | <br>23% 55% 21% 2% |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 3   | AD    | 276    |    |
| 3   | DD    | 276    |    |
| 4   | AE    | 206    |    |
| 4   | DE    | 206    |    |
| 5   | AF    | 210    |    |
| 5   | DF    | 210    |    |
| 6   | AG    | 182    |    |
| 6   | DG    | 182    |    |
| 7   | AH    | 180    |    |
| 7   | DH    | 180    |    |
| 8   | AK    | 148    |    |
| 8   | DK    | 148    |   |
| 9   | AM    | 140    |  |
| 9   | DM    | 140    |  |
| 10  | AN    | 122    |  |
| 10  | DN    | 122    |  |
| 11  | AO    | 150    |  |
| 11  | DO    | 150    |  |
| 12  | AP    | 141    |  |
| 12  | DP    | 141    |  |
| 13  | A0    | 118    |  |
| 13  | D0    | 118    |  |
| 14  | AQ    | 112    |  |
| 14  | DQ    | 112    |  |
| 15  | AR    | 146    |  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15  | DR    | 146    |                  |
| 16  | A1    | 118    |                  |
| 16  | D1    | 118    |                  |
| 17  | A2    | 101    |                  |
| 17  | D2    | 101    |                  |
| 18  | AS    | 113    |                  |
| 18  | DS    | 113    |                  |
| 19  | AT    | 96     |                  |
| 19  | DT    | 96     |                  |
| 20  | AU    | 110    |                  |
| 20  | DU    | 110    |                  |
| 21  | AV    | 206    |                  |
| 21  | DV    | 206    |                  |
| 22  | A3    | 85     |                  |
| 22  | D3    | 85     |                  |
| 23  | AZ    | 98     |                  |
| 23  | DZ    | 98     |                  |
| 24  | AW    | 72     |                  |
| 24  | DW    | 72     |                  |
| 25  | AX    | 60     |                  |
| 25  | DX    | 60     |                  |
| 26  | A4    | 71     |                  |
| 26  | D4    | 71     |                  |
| 27  | A5    | 60     |                  |
| 27  | D5    | 60     |                  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain         |
|-----|-------|--------|--------------------------|
| 28  | A6    | 54     | 83%<br>22% 28% 30% 17%   |
| 28  | D6    | 54     | 72%<br>19% 37% 28% 17%   |
| 29  | A7    | 49     | 33% 49% 10% 8%           |
| 29  | D7    | 49     | 35% 45% 12% 8%           |
| 30  | A8    | 65     | 5%<br>23% 43% 18% 8% 8%  |
| 30  | D8    | 65     | 8%<br>29% 31% 28% 5% 8%  |
| 31  | BA    | 1506   | 20% 58% 21% .            |
| 31  | CA    | 1506   | 24% 55% 20% .            |
| 32  | BE    | 256    | 11%<br>23% 46% 22% . 7%  |
| 32  | CE    | 256    | 25%<br>23% 48% 19% . 7%  |
| 33  | BF    | 239    | 10%<br>28% 44% 13% . 14% |
| 33  | CF    | 239    | 13%<br>24% 45% 16% . 14% |
| 34  | BG    | 208    | %<br>38% 41% 20% .       |
| 34  | CG    | 208    | 2%<br>35% 43% 20% .      |
| 35  | BH    | 162    | 2%<br>31% 44% 17% . 7%   |
| 35  | CH    | 162    | 2%<br>29% 48% 16% . 7%   |
| 36  | BI    | 101    | 25%<br>36% 51% 12% .     |
| 36  | CI    | 101    | 2%<br>41% 51% 8%         |
| 37  | BJ    | 156    | 5%<br>35% 47% 17% .      |
| 37  | CJ    | 156    | 3%<br>38% 48% 12% ..     |
| 38  | BK    | 138    | %<br>30% 54% 16% .       |
| 38  | CK    | 138    | %<br>40% 48% 12%         |
| 39  | BL    | 128    | 3%<br>32% 47% 20% ..     |
| 39  | CL    | 128    | 2%<br>26% 48% 22% . .    |
| 40  | BM    | 105    | 10%<br>32% 50% 12% 6%    |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 40  | CM    | 105    |                  |
| 41  | BN    | 129    |                  |
| 41  | CN    | 129    |                  |
| 42  | BO    | 132    |                  |
| 42  | CO    | 132    |                  |
| 43  | BP    | 126    |                  |
| 43  | CP    | 126    |                  |
| 44  | BQ    | 61     |                  |
| 44  | CQ    | 61     |                  |
| 45  | BR    | 89     |                  |
| 45  | CR    | 89     |                  |
| 46  | BS    | 88     |                  |
| 46  | CS    | 88     |                  |
| 47  | BT    | 105    |                  |
| 47  | CT    | 105    |                  |
| 48  | BU    | 88     |                  |
| 48  | CU    | 88     |                  |
| 49  | BV    | 93     |                  |
| 49  | CV    | 93     |                  |
| 50  | BW    | 106    |                  |
| 50  | CW    | 106    |                  |
| 51  | BX    | 27     |                  |
| 51  | CX    | 27     |                  |
| 52  | BB    | 85     |                  |
| 52  | BD    | 85     |                  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 52  | CB    | 85     |                  |
| 52  | CD    | 85     |                  |
| 53  | BC    | 77     |                  |
| 53  | CC    | 77     |                  |
| 54  | B1    | 16     |                  |
| 54  | C1    | 16     |                  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 55  | MG   | A3    | 101  | -         | -        | -       | X                |
| 55  | MG   | AA    | 3096 | -         | -        | -       | X                |
| 55  | MG   | AA    | 3142 | -         | -        | -       | X                |
| 55  | MG   | AA    | 3215 | -         | -        | -       | X                |
| 55  | MG   | AA    | 3222 | -         | -        | -       | X                |
| 55  | MG   | AA    | 3236 | -         | -        | -       | X                |
| 55  | MG   | AA    | 3245 | -         | -        | -       | X                |
| 55  | MG   | AA    | 3277 | -         | -        | -       | X                |
| 55  | MG   | AA    | 3279 | -         | -        | -       | X                |
| 55  | MG   | AA    | 3291 | -         | -        | -       | X                |
| 55  | MG   | AA    | 3305 | -         | -        | -       | X                |
| 55  | MG   | AA    | 3337 | -         | -        | -       | X                |
| 55  | MG   | BA    | 1615 | -         | -        | -       | X                |
| 55  | MG   | BA    | 1624 | -         | -        | -       | X                |
| 55  | MG   | BA    | 1675 | -         | -        | -       | X                |
| 55  | MG   | BA    | 1699 | -         | -        | -       | X                |
| 55  | MG   | BA    | 1714 | -         | -        | -       | X                |
| 55  | MG   | BB    | 104  | -         | -        | -       | X                |
| 55  | MG   | BB    | 106  | -         | -        | -       | X                |
| 55  | MG   | CA    | 1629 | -         | -        | -       | X                |
| 55  | MG   | CA    | 1641 | -         | -        | -       | X                |
| 55  | MG   | CA    | 1668 | -         | -        | -       | X                |
| 55  | MG   | CA    | 1672 | -         | -        | -       | X                |
| 55  | MG   | CA    | 1674 | -         | -        | -       | X                |
| 55  | MG   | CA    | 1685 | -         | -        | -       | X                |
| 55  | MG   | CA    | 1686 | -         | -        | -       | X                |
| 55  | MG   | CA    | 1699 | -         | -        | -       | X                |

Continued on next page...

*Continued from previous page...*

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 55  | MG   | CA    | 1720 | -         | -        | -       | X                |
| 55  | MG   | CB    | 101  | -         | -        | -       | X                |
| 55  | MG   | CC    | 103  | -         | -        | -       | X                |
| 55  | MG   | CC    | 104  | -         | -        | -       | X                |
| 55  | MG   | DA    | 3048 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3053 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3112 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3145 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3158 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3196 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3201 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3203 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3252 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3295 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3307 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3311 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3320 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3330 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3331 | -         | -        | -       | X                |
| 55  | MG   | DB    | 206  | -         | -        | -       | X                |
| 56  | OHX  | AA    | 3330 | -         | -        | X       | -                |
| 56  | OHX  | AA    | 3365 | -         | -        | X       | -                |
| 56  | OHX  | AA    | 3504 | -         | -        | X       | -                |
| 56  | OHX  | AA    | 3547 | -         | -        | X       | -                |
| 56  | OHX  | BA    | 1785 | -         | -        | X       | -                |
| 56  | OHX  | BA    | 1802 | -         | -        | X       | -                |
| 56  | OHX  | CA    | 1762 | -         | -        | X       | -                |
| 56  | OHX  | CA    | 1798 | -         | -        | X       | -                |
| 56  | OHX  | CC    | 108  | -         | -        | X       | -                |
| 56  | OHX  | D8    | 101  | -         | -        | X       | -                |



## 2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 304031 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 RNA chain called RNA (2912-MER).

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
|     |       |          | Total | C     | N     | O     | P    |         |         |       |
| 1   | AA    | 2912     | 62707 | 27911 | 11722 | 20163 | 2911 | 0       | 0       | 0     |
| 1   | DA    | 2907     | 62607 | 27866 | 11712 | 20123 | 2906 | 0       | 0       | 0     |

There are 14 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference     |
|-------|---------|----------|--------|-----------|---------------|
| AA    | 161     | U        | -      | INSERTION | GB AP008226.1 |
| AA    | 654A    | A        | G      | CONFLICT  | GB AP008226.1 |
| AA    | 654E    | C        | G      | CONFLICT  | GB AP008226.1 |
| AA    | 654P    | G        | C      | CONFLICT  | GB AP008226.1 |
| AA    | 654T    | A        | C      | CONFLICT  | GB AP008226.1 |
| AA    | 1058    | U        | G      | CONFLICT  | GB AP008226.1 |
| AA    | 1080    | A        | C      | CONFLICT  | GB AP008226.1 |
| DA    | 168     | U        | -      | insertion | GB AP008226.1 |
| DA    | 654A    | A        | G      | CONFLICT  | GB AP008226.1 |
| DA    | 654E    | C        | G      | CONFLICT  | GB AP008226.1 |
| DA    | 654P    | G        | C      | CONFLICT  | GB AP008226.1 |
| DA    | 654T    | A        | C      | CONFLICT  | GB AP008226.1 |
| DA    | 1058    | U        | G      | CONFLICT  | GB AP008226.1 |
| DA    | 1080    | A        | C      | CONFLICT  | GB AP008226.1 |

- Molecule 2 is a RNA chain called 5S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
|     |       |          | Total | C    | N   | O   | P   |         |         |       |
| 2   | AB    | 122      | 2617  | 1166 | 486 | 844 | 121 | 0       | 0       | 0     |
| 2   | DB    | 122      | 2617  | 1166 | 486 | 844 | 121 | 0       | 0       | 0     |

- Molecule 3 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | AD    | 272      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2115  | 1335 | 420 | 357 | 3 |         |         |       |
| 3   | DD    | 272      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2115  | 1335 | 420 | 357 | 3 |         |         |       |

- Molecule 4 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | AE    | 205      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1568  | 991 | 300 | 271 | 6 |         |         |       |
| 4   | DE    | 205      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1568  | 991 | 300 | 271 | 6 |         |         |       |

- Molecule 5 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5   | AF    | 202      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1585  | 1011 | 297 | 275 | 2 |         |         |       |
| 5   | DF    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1627  | 1037 | 304 | 283 | 3 |         |         |       |

- Molecule 6 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | AG    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1474  | 942 | 268 | 260 | 4 |         |         |       |
| 6   | DG    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1474  | 942 | 268 | 260 | 4 |         |         |       |

- Molecule 7 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | AH    | 170      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1307  | 829 | 245 | 232 | 1 |         |         |       |
| 7   | DH    | 170      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1307  | 829 | 245 | 232 | 1 |         |         |       |

- Molecule 8 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | AK    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 201 | 208 | 1 |         |         |       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | DK    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 201 | 208 | 1 |         |         |       |

- Molecule 9 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9   | AM    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1104  | 712 | 206 | 182 | 4 |         |         |       |
| 9   | DM    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1104  | 712 | 206 | 182 | 4 |         |         |       |

- Molecule 10 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | AN    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |
| 10  | DN    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |

- Molecule 11 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | AO    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1145  | 712 | 232 | 198 | 3 |         |         |       |
| 11  | DO    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1145  | 712 | 232 | 198 | 3 |         |         |       |

- Molecule 12 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | AP    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 715 | 212 | 188 | 7 |         |         |       |
| 12  | DP    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 715 | 212 | 188 | 7 |         |         |       |

- Molecule 13 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | A0    | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 604 | 203 | 160 | 1 |         |         |       |
| 13  | D0    | 117      | Total | C   | N   | O   |   | 0       | 0       | 0     |
|     |       |          | 960   | 599 | 202 | 159 |   |         |         |       |

- Molecule 14 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
|     |       |          | Total | C   | N   | O   |         |         |       |
| 14  | AQ    | 111      | 882   | 556 | 176 | 150 | 0       | 0       | 0     |
| 14  | DQ    | 111      | 882   | 556 | 176 | 150 | 0       | 0       | 0     |

- Molecule 15 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |         |       |
| 15  | AR    | 137      | 1141  | 710 | 234 | 196 | 1 | 0       | 0       | 0     |
| 15  | DR    | 137      | 1141  | 710 | 234 | 196 | 1 | 0       | 0       | 0     |

- Molecule 16 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |         |       |
| 16  | A1    | 117      | 964   | 610 | 202 | 151 | 1 | 0       | 0       | 0     |
| 16  | D1    | 117      | 964   | 610 | 202 | 151 | 1 | 0       | 0       | 0     |

- Molecule 17 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |         |       |
| 17  | A2    | 101      | 779   | 501 | 142 | 135 | 1 | 0       | 0       | 0     |
| 17  | D2    | 101      | 779   | 501 | 142 | 135 | 1 | 0       | 0       | 0     |

- Molecule 18 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |         |       |
| 18  | AS    | 113      | 900   | 566 | 177 | 155 | 2 | 0       | 0       | 0     |
| 18  | DS    | 113      | 900   | 566 | 177 | 155 | 2 | 0       | 0       | 0     |

- Molecule 19 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 19  | AT    | 92       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 725   | 471 | 131 | 123 |         |         |       |
| 19  | DT    | 92       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 725   | 471 | 131 | 123 |         |         |       |

- Molecule 20 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | AU    | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 785   | 505 | 150 | 125 | 5 |         |         |       |
| 20  | DU    | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 785   | 505 | 150 | 125 | 5 |         |         |       |

- Molecule 21 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21  | AV    | 175      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1397  | 892 | 251 | 251 | 3 |         |         |       |
| 21  | DV    | 179      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1428  | 911 | 255 | 259 | 3 |         |         |       |

- Molecule 22 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22  | A3    | 76       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 607   | 376 | 128 | 102 | 1 |         |         |       |
| 22  | D3    | 77       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 613   | 379 | 129 | 104 | 1 |         |         |       |

- Molecule 23 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 23  | AZ    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 481 | 150 | 131 | 1 |         |         |       |
| 23  | DZ    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 481 | 150 | 131 | 1 |         |         |       |

- Molecule 24 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 24  | AW    | 66       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 558   | 346 | 113 | 98 | 1 |         |         |       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
|     |       |          | Total | C   | N   | O  | S |         |         |       |
| 24  | DW    | 66       | 558   | 346 | 113 | 98 | 1 | 0       | 0       | 0     |

- Molecule 25 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
|     |       |          | Total | C   | N  | O  |         |         |       |
| 25  | AX    | 59       | 469   | 298 | 90 | 81 | 0       | 0       | 0     |
| 25  | DX    | 59       | 469   | 298 | 90 | 81 | 0       | 0       | 0     |

- Molecule 26 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
|     |       |          | Total | C   | N  | O  | S |         |         |       |
| 26  | A4    | 66       | 533   | 335 | 96 | 97 | 5 | 0       | 0       | 0     |
| 26  | D4    | 63       | 515   | 326 | 93 | 91 | 5 | 0       | 0       | 0     |

- Molecule 27 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
|     |       |          | Total | C   | N  | O  | S |         |         |       |
| 27  | A5    | 59       | 459   | 288 | 90 | 76 | 5 | 0       | 0       | 0     |
| 27  | D5    | 59       | 459   | 288 | 90 | 76 | 5 | 0       | 0       | 0     |

- Molecule 28 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
|     |       |          | Total | C   | N  | O  | S |         |         |       |
| 28  | A6    | 45       | 389   | 241 | 79 | 65 | 4 | 0       | 0       | 0     |
| 28  | D6    | 45       | 389   | 241 | 79 | 65 | 4 | 0       | 0       | 0     |

- Molecule 29 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
|     |       |          | Total | C   | N  | O  | S |         |         |       |
| 29  | A7    | 45       | 391   | 240 | 97 | 52 | 2 | 0       | 0       | 0     |
| 29  | D7    | 45       | 391   | 240 | 97 | 52 | 2 | 0       | 0       | 0     |

- Molecule 30 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
|     |       |          | Total | C   | N  | O  | S |         |         |       |
| 30  | A8    | 60       | 480   | 306 | 98 | 74 | 2 | 0       | 0       | 0     |
| 30  | D8    | 60       | 480   | 306 | 98 | 74 | 2 | 0       | 0       | 0     |

- Molecule 31 is a RNA chain called 16S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
|     |       |          | Total | C     | N    | O     | P    |         |         |       |
| 31  | BA    | 1502     | 32284 | 14370 | 5982 | 10431 | 1501 | 0       | 0       | 0     |
| 31  | CA    | 1502     | 32287 | 14370 | 5982 | 10433 | 1502 | 0       | 0       | 0     |

- Molecule 32 is a protein called 30S RIBOSOMAL PROTEIN S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |         |       |
| 32  | BE    | 237      | 1924  | 1228 | 344 | 347 | 5 | 0       | 0       | 0     |
| 32  | CE    | 237      | 1924  | 1228 | 344 | 347 | 5 | 0       | 0       | 0     |

- Molecule 33 is a protein called 30S RIBOSOMAL PROTEIN S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |         |       |
| 33  | BF    | 205      | 1605  | 1011 | 313 | 280 | 1 | 0       | 0       | 0     |
| 33  | CF    | 206      | 1612  | 1016 | 314 | 281 | 1 | 0       | 0       | 0     |

- Molecule 34 is a protein called 30S RIBOSOMAL PROTEIN S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |         |       |
| 34  | BG    | 208      | 1703  | 1066 | 339 | 291 | 7 | 0       | 0       | 0     |
| 34  | CG    | 208      | 1703  | 1066 | 339 | 291 | 7 | 0       | 0       | 0     |

- Molecule 35 is a protein called 30S RIBOSOMAL PROTEIN S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35  | BH    | 151      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1155  | 729 | 218 | 204 | 4 |         |         |       |
| 35  | CH    | 151      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1155  | 729 | 218 | 204 | 4 |         |         |       |

- Molecule 36 is a protein called 30S RIBOSOMAL PROTEIN S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36  | BI    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 843   | 531 | 155 | 154 | 3 |         |         |       |
| 36  | CI    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 843   | 531 | 155 | 154 | 3 |         |         |       |

- Molecule 37 is a protein called 30S RIBOSOMAL PROTEIN S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37  | BJ    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1257  | 781 | 252 | 218 | 6 |         |         |       |
| 37  | CJ    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1257  | 781 | 252 | 218 | 6 |         |         |       |

- Molecule 38 is a protein called 30S RIBOSOMAL PROTEIN S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38  | BK    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1116  | 705 | 215 | 193 | 3 |         |         |       |
| 38  | CK    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1116  | 705 | 215 | 193 | 3 |         |         |       |

- Molecule 39 is a protein called 30S RIBOSOMAL PROTEIN S9.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 39  | BL    | 127      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1010  | 639 | 197 | 174 |         |         |       |
| 39  | CL    | 127      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1010  | 639 | 197 | 174 |         |         |       |

- Molecule 40 is a protein called 30S RIBOSOMAL PROTEIN S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40  | BM    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 801   | 504 | 157 | 139 | 1 |         |         |       |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |         |       |
| 40  | CM    | 99       | 801   | 504 | 157 | 139 | 1 | 0       | 0       | 0     |

- Molecule 41 is a protein called 30S RIBOSOMAL PROTEIN S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |         |       |
| 41  | BN    | 119      | 885   | 549 | 168 | 165 | 3 | 0       | 0       | 0     |
| 41  | CN    | 119      | 885   | 549 | 168 | 165 | 3 | 0       | 0       | 0     |

- Molecule 42 is a protein called 30S RIBOSOMAL PROTEIN S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |         |       |
| 42  | BO    | 125      | 975   | 614 | 196 | 164 | 1 | 0       | 0       | 0     |
| 42  | CO    | 125      | 975   | 614 | 196 | 164 | 1 | 0       | 0       | 0     |

- Molecule 43 is a protein called 30S RIBOSOMAL PROTEIN S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |         |       |
| 43  | BP    | 116      | 928   | 574 | 191 | 161 | 2 | 0       | 0       | 0     |
| 43  | CP    | 117      | 933   | 577 | 192 | 162 | 2 | 0       | 0       | 0     |

- Molecule 44 is a protein called 30S RIBOSOMAL PROTEIN S14.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
|     |       |          | Total | C   | N  | O  | S |         |         |       |
| 44  | BQ    | 58       | 476   | 303 | 99 | 70 | 4 | 0       | 0       | 0     |
| 44  | CQ    | 58       | 476   | 303 | 99 | 70 | 4 | 0       | 0       | 0     |

- Molecule 45 is a protein called 30S RIBOSOMAL PROTEIN S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |         |       |
| 45  | BR    | 88       | 734   | 459 | 147 | 126 | 2 | 0       | 0       | 0     |
| 45  | CR    | 88       | 734   | 459 | 147 | 126 | 2 | 0       | 0       | 0     |

- Molecule 46 is a protein called 30S RIBOSOMAL PROTEIN S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46  | BS    | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 705   | 446 | 140 | 118 | 1 |         |         |       |
| 46  | CS    | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 705   | 446 | 140 | 118 | 1 |         |         |       |

- Molecule 47 is a protein called 30S RIBOSOMAL PROTEIN S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47  | BT    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 834   | 534 | 155 | 143 | 2 |         |         |       |
| 47  | CT    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 834   | 534 | 155 | 143 | 2 |         |         |       |

- Molecule 48 is a protein called 30S RIBOSOMAL PROTEIN S18.

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 48  | BU    | 72       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 591   | 376 | 117 | 98 |         |         |       |
| 48  | CU    | 72       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 591   | 376 | 117 | 98 |         |         |       |

- Molecule 49 is a protein called 30S RIBOSOMAL PROTEIN S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 49  | BV    | 78       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 624   | 398 | 115 | 109 | 2 |         |         |       |
| 49  | CV    | 78       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 624   | 398 | 115 | 109 | 2 |         |         |       |

- Molecule 50 is a protein called 30S RIBOSOMAL PROTEIN S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 50  | BW    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 470 | 162 | 129 | 2 |         |         |       |
| 50  | CW    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 470 | 162 | 129 | 2 |         |         |       |

- Molecule 51 is a protein called 30S RIBOSOMAL PROTEIN THX.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 51  | BX    | 25       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 217   | 134 | 52 | 31 |         |         |       |
| 51  | CX    | 25       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 217   | 134 | 52 | 31 |         |         |       |

- Molecule 52 is a RNA chain called TRNA-TYR.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 52  | BB    | 85       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1814  | 813 | 323 | 592 | 85 | 1 |         |         |       |
| 52  | BD    | 85       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1814  | 813 | 323 | 592 | 85 | 1 |         |         |       |
| 52  | CB    | 85       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1814  | 813 | 323 | 592 | 85 | 1 |         |         |       |
| 52  | CD    | 85       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1814  | 813 | 323 | 592 | 85 | 1 |         |         |       |

- Molecule 53 is a RNA chain called TRNA-FMET.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 53  | BC    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1643  | 732 | 298 | 536 | 77 |         |         |       |
| 53  | CC    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1643  | 732 | 298 | 536 | 77 |         |         |       |

- Molecule 54 is a RNA chain called MRNA.

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 54  | B1    | 16       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 347   | 156 | 69 | 106 | 16 |         |         |       |
| 54  | C1    | 16       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 347   | 156 | 69 | 106 | 16 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 55  | BA    | 114      | Total | Mg  | 0       | 0       |
|     |       |          | 114   | 114 |         |         |
| 55  | CA    | 121      | Total | Mg  | 0       | 0       |
|     |       |          | 121   | 121 |         |         |
| 55  | AB    | 6        | Total | Mg  | 0       | 0       |
|     |       |          | 6     | 6   |         |         |

*Continued on next page...*

*Continued from previous page...*

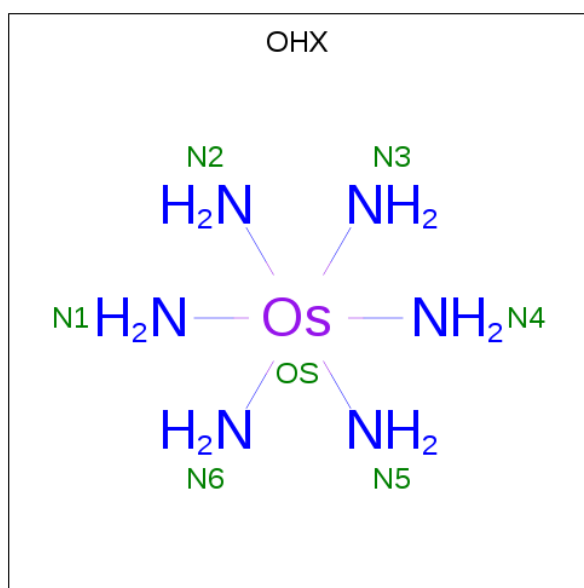
| Mol | Chain | Residues | Atoms               | ZeroOcc | AltConf |
|-----|-------|----------|---------------------|---------|---------|
| 55  | B1    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 55  | C1    | 2        | Total Mg<br>2 2     | 0       | 0       |
| 55  | BB    | 13       | Total Mg<br>13 13   | 0       | 0       |
| 55  | AE    | 3        | Total Mg<br>3 3     | 0       | 0       |
| 55  | BF    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 55  | AA    | 332      | Total Mg<br>332 332 | 0       | 0       |
| 55  | A5    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 55  | D7    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 55  | BC    | 4        | Total Mg<br>4 4     | 0       | 0       |
| 55  | A1    | 2        | Total Mg<br>2 2     | 0       | 0       |
| 55  | CN    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 55  | D0    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 55  | CC    | 7        | Total Mg<br>7 7     | 0       | 0       |
| 55  | DA    | 272      | Total Mg<br>272 272 | 0       | 0       |
| 55  | A0    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 55  | DE    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 55  | CB    | 3        | Total Mg<br>3 3     | 0       | 0       |
| 55  | BS    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 55  | A7    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 55  | D5    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 55  | BD    | 1        | Total Mg<br>1 1     | 0       | 0       |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 55  | AO    | 1        | Total Mg<br>1 1 | 0       | 0       |
| 55  | BW    | 1        | Total Mg<br>1 1 | 0       | 0       |
| 55  | A3    | 1        | Total Mg<br>1 1 | 0       | 0       |
| 55  | AF    | 2        | Total Mg<br>2 2 | 0       | 0       |
| 55  | DB    | 7        | Total Mg<br>7 7 | 0       | 0       |

- Molecule 56 is osmium (III) hexammine (three-letter code: OHX) (formula:  $H_{12}N_6Os$ ).



| Mol | Chain | Residues | Atoms               | ZeroOcc | AltConf |
|-----|-------|----------|---------------------|---------|---------|
| 56  | AA    | 1        | Total N Os<br>7 6 1 | 0       | 0       |
| 56  | AA    | 1        | Total N Os<br>7 6 1 | 0       | 0       |
| 56  | AA    | 1        | Total N Os<br>7 6 1 | 0       | 0       |
| 56  | AA    | 1        | Total N Os<br>7 6 1 | 0       | 0       |
| 56  | AA    | 1        | Total N Os<br>7 6 1 | 0       | 0       |
| 56  | AA    | 1        | Total N Os<br>7 6 1 | 0       | 0       |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
|     |       |          | Total | N | Os |         |         |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
|     |       |          | Total | N | Os |         |         |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |

*Continued on next page...*





*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
|     |       |          | Total | N | Os |         |         |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |

*Continued on next page...*





*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
|     |       |          | Total | N | Os |         |         |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AA    | 1        | 7     | 6 | 1  | 0       | 0       |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 56  | AA    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 56  | AA    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 56  | AA    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 56  | AA    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 56  | AA    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 56  | AA    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 56  | AA    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 56  | AA    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 56  | AA    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 56  | AA    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 56  | AA    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 56  | AA    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 56  | AA    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 56  | AA    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 56  | AA    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 56  | AA    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 56  | AA    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 56  | AA    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 56  | AA    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 56  | AA    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 56  | AA    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 56  | AA    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 56  | AA    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 56  | AA    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

*Continued on next page...*





*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
|     |       |          | Total | N | Os |         |         |
| 56  | AB    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AB    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AB    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AB    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AB    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AB    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AB    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AB    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AB    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AB    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AB    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AB    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AB    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AB    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AB    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AB    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AB    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AE    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AF    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AO    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AO    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | A1    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | A1    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | A3    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | AW    | 1        | 7     | 6 | 1  | 0       | 0       |

*Continued on next page...*





















*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
|     |       |          | Total | N | Os |         |         |
| 56  | CA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | CA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | CA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | CA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | CA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | CA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | CA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | CA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | CA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | CA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | CA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | CA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | CA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | CA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | CA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | CA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | CA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | CA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | CA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | CA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | CK    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | CR    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | CV    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | CB    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | CB    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | CB    | 1        | 7     | 6 | 1  | 0       | 0       |

*Continued on next page...*















*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
|     |       |          | Total | N | Os |         |         |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
|     |       |          | Total | N | Os |         |         |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
|     |       |          | Total | N | Os |         |         |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |

*Continued on next page...*

*Continued from previous page...*

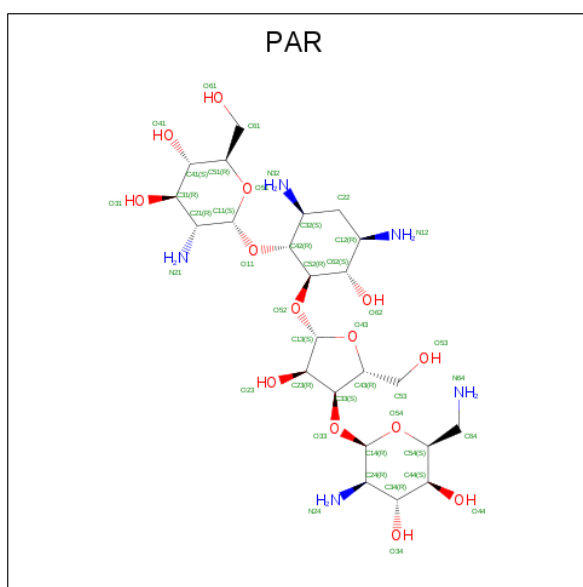
| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
|     |       |          | Total | N | Os |         |         |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DA    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DB    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DB    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DB    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DB    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DB    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DB    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DB    | 1        | 7     | 6 | 1  | 0       | 0       |
| 56  | DB    | 1        | 7     | 6 | 1  | 0       | 0       |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
|     |       |          | Total | N | O |         |         |
| 56  | DB    | 1        | 7     | 6 | 1 | 0       | 0       |
| 56  | DB    | 1        | 7     | 6 | 1 | 0       | 0       |
| 56  | DB    | 1        | 7     | 6 | 1 | 0       | 0       |
| 56  | DB    | 1        | 7     | 6 | 1 | 0       | 0       |
| 56  | DB    | 1        | 7     | 6 | 1 | 0       | 0       |
| 56  | DF    | 1        | 7     | 6 | 1 | 0       | 0       |
| 56  | DO    | 1        | 7     | 6 | 1 | 0       | 0       |
| 56  | D1    | 1        | 7     | 6 | 1 | 0       | 0       |
| 56  | D3    | 1        | 7     | 6 | 1 | 0       | 0       |
| 56  | D5    | 1        | 7     | 6 | 1 | 0       | 0       |
| 56  | D8    | 1        | 7     | 6 | 1 | 0       | 0       |

- Molecule 57 is PAROMOMYCIN (three-letter code: PAR) (formula:  $C_{23}H_{45}N_5O_{14}$ ).



| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---------|---------|
| 57  | BA    | 1        | Total | C  | N | O  | 0       | 0       |
|     |       |          | 42    | 23 | 5 | 14 |         |         |
| 57  | CA    | 1        | Total | C  | N | O  | 0       | 0       |
|     |       |          | 42    | 23 | 5 | 14 |         |         |

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

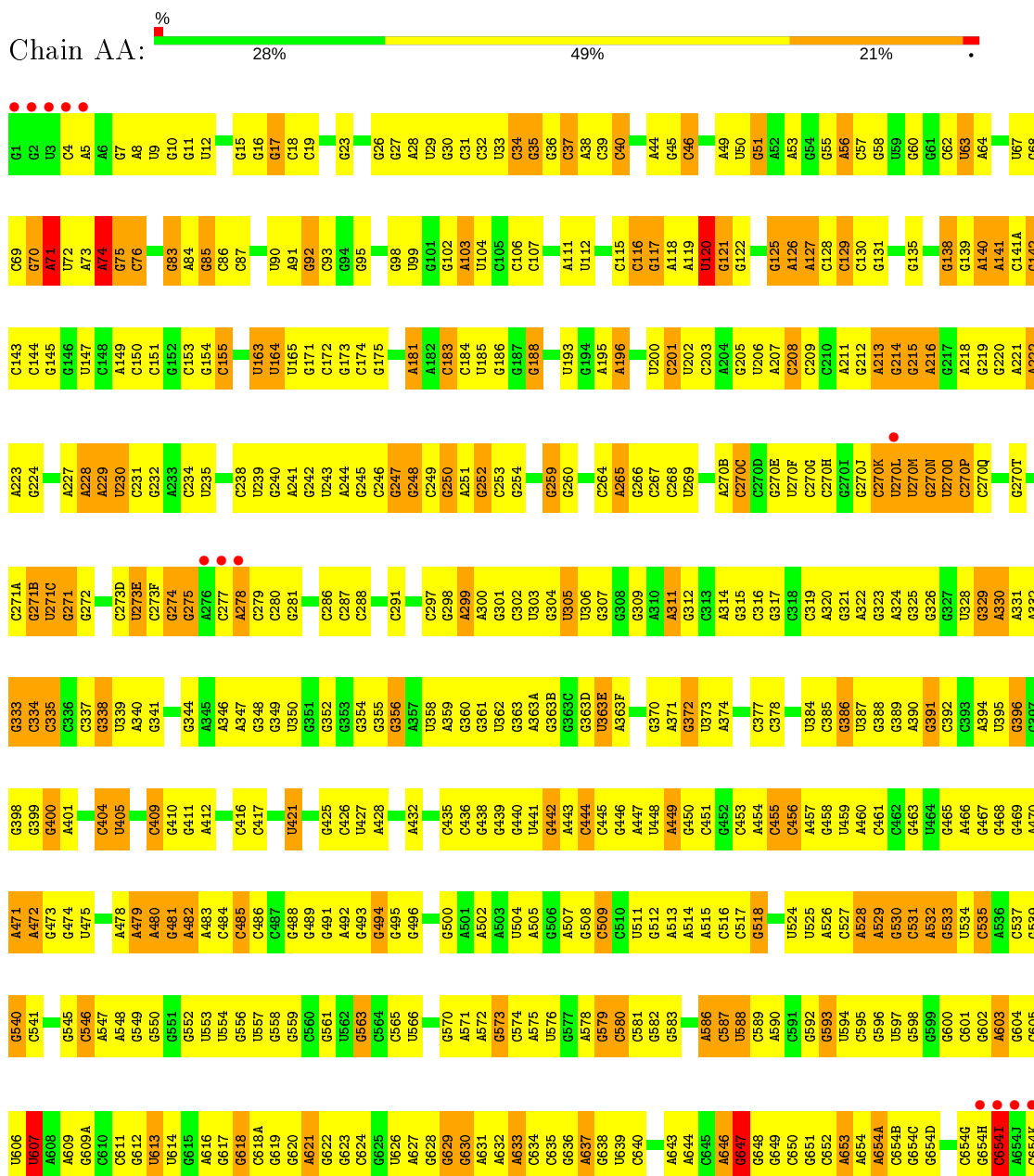
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 58  | BG    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | BQ    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | CQ    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | CG    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |



### 3 Residue-property plots

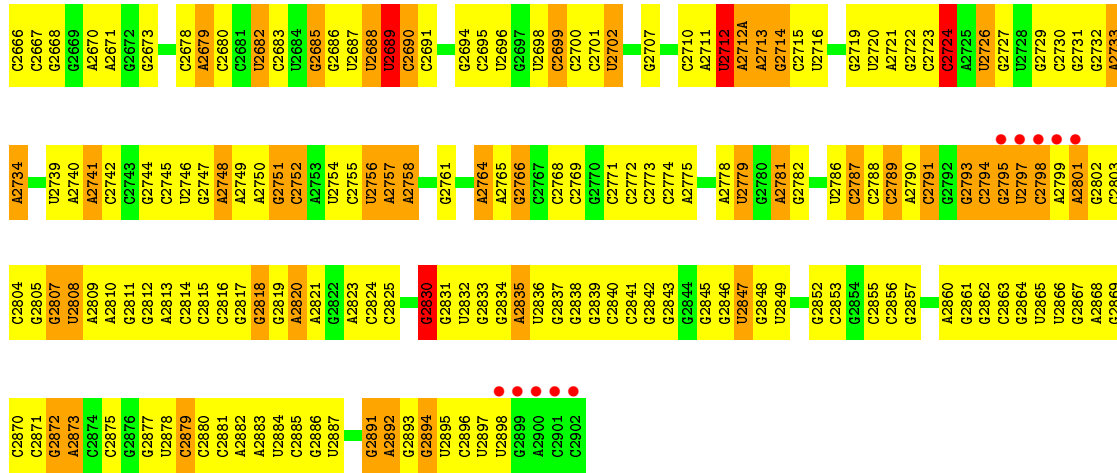
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: RNA (2912-MER)

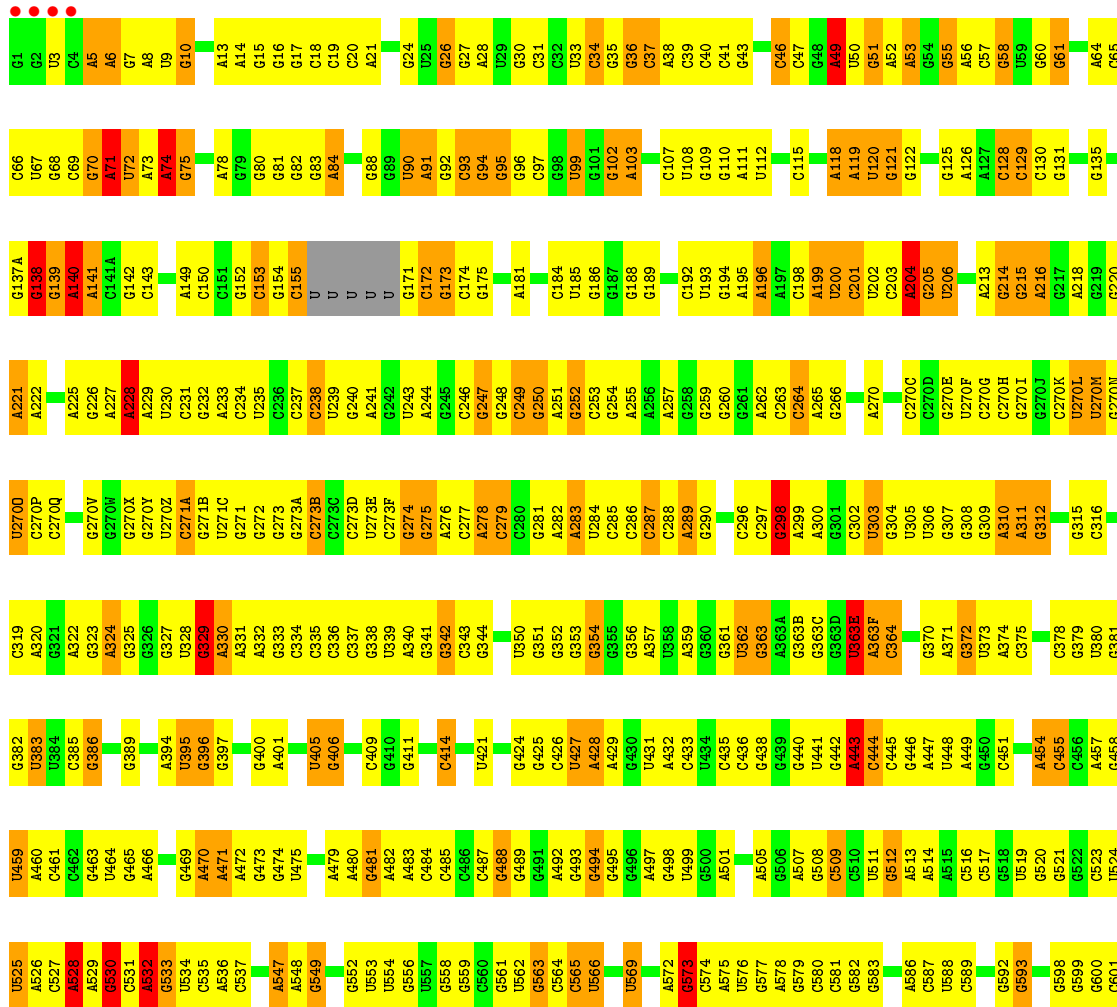








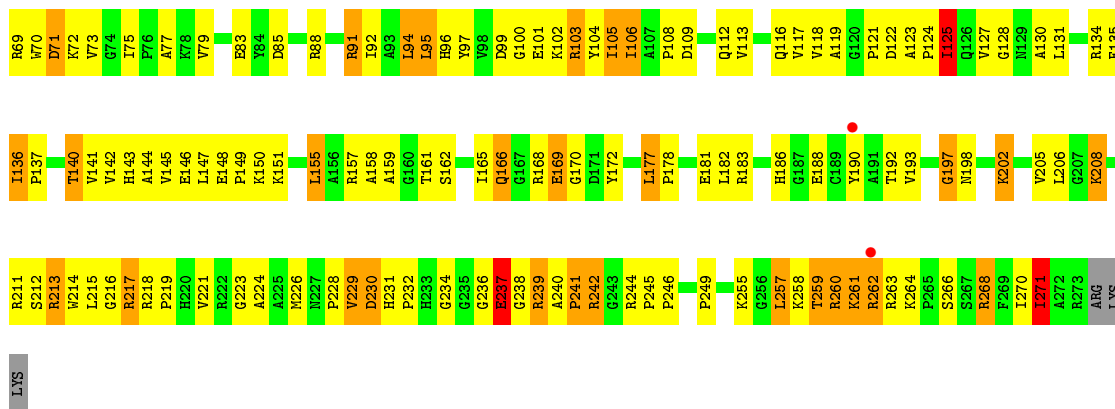
● Molecule 1: RNA (2912-MER)



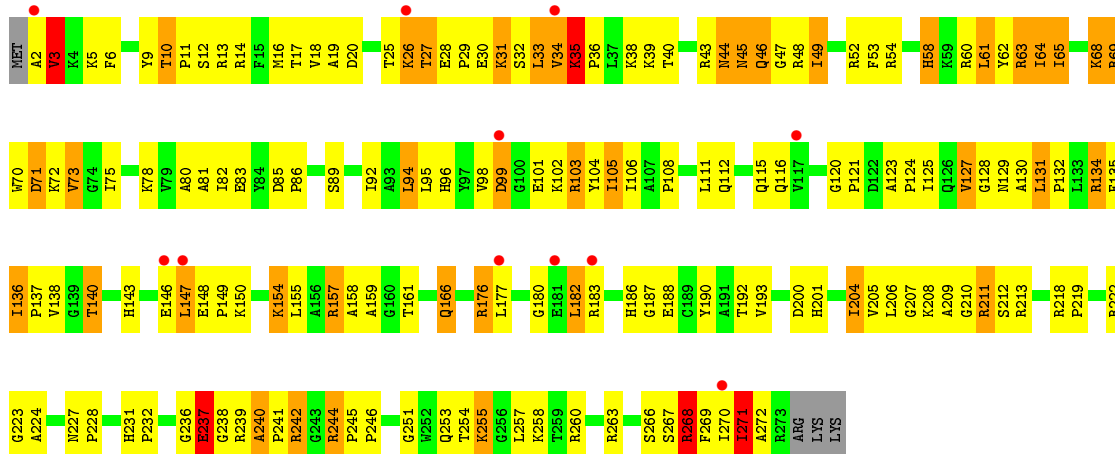
|       |       |       |       |       |       |        |       |       |      |      |      |      |       |       |
|-------|-------|-------|-------|-------|-------|--------|-------|-------|------|------|------|------|-------|-------|
| G1437 | U1438 | A1365 | C1297 | A1220 | C1158 | C1092  | A1029 | G988  | G906 | G845 | A784 | A718 | G664L | G602  |
| G1439 | G1368 | G1368 | C1298 | C1223 | U1189 | G1093  | G1030 | U969  | U907 | C946 | G785 | C719 | C654L | A603  |
| G1440 | G1369 | G1369 | G1299 | G1224 | C1160 | U1094  | G1031 | C970  | A908 | C948 | C786 | C720 | C654N | G604  |
| G1441 | G1370 | C1370 | U1300 | G1225 | C1161 | A1095  | A1032 | C971  | C909 | G848 | U787 | C721 | G654O | C605  |
| G1442 | G1371 | G1371 | A1301 | G1226 | G1163 | A1096  | U1033 | G972  | A910 | A859 | A788 | A722 | G654P | U606  |
| G1443 | U1372 | U1372 | A1302 | A1227 | G1164 | U1097  | G1034 | G973  | A911 | C850 | A789 | G723 | G654Q | U607  |
| A1444 |       |       | C1305 | G1231 | U1165 | A1098  | U1035 | G974  | C912 | U851 | C790 | U724 | G654R | G609A |
| A1445 | A1378 | A1378 | G1306 | G1232 | C1166 | G1099  | G1036 | C974A | C913 | G852 | C791 | G725 | A654S |       |
| A1446 | A1379 | A1379 | G1307 | G1233 | U1101 | G975   | G1039 | G975  | C914 | G853 | C792 | G726 | A654T |       |
| A1447 | G1380 | G1380 | A1308 | G1234 | G1167 | G976   | C1040 | G976  | C915 | G854 | A793 | G727 | A654U | U613  |
| A1448 | G1381 | G1381 | G1309 | U1234 | C1169 | G977   | G1041 | G977  | C916 | G855 | G794 | G728 | A654V | U614  |
| A1449 | G1382 | G1382 | G1310 | G1235 | G1170 | G978   | C1042 | G978  | A917 | C856 | C795 | G729 | A655  | G615  |
| A1450 | C1383 | C1383 | G1311 | G1236 | G1171 | G979   | G1043 | G979  | A918 | C857 | C796 | C730 | A656  | A616  |
| A1451 | A1384 | A1384 | A1237 | A1237 | G1173 | A980   | C1044 | A980  | G919 | U858 | C797 | C731 | G657  | G617  |
| A1452 | G1385 | G1385 | G1312 | G1238 | A1174 | A981   | G1045 | A981  | G920 | G859 | G798 | G732 | G658  | G618  |
| A1453 | C1386 | C1386 | C1314 | G1239 | A1175 | A982   | A1046 | A982  | C921 | U860 | G799 | G733 | C618A | G619  |
|       | G1387 | G1387 | U1315 | U1240 | G1176 | G1110  | G1047 | A984  | U922 | A861 | A734 | A735 | G660  | G620  |
|       | G1388 | G1388 | U1316 | A1241 | A1177 | A1111  | A1048 | C985  | C924 | A863 | A802 | C736 | G662  | A621  |
|       | G1389 | G1389 | A1317 | A1242 | C1178 | G1112  | C1049 | C986  | C925 | G864 | U803 | C737 | G663  | G622  |
|       | A1392 | A1392 | C1318 | G1243 | C1179 | G1113  | A1050 | G987  | A926 | G865 | A804 | G738 | G664  | U626  |
|       | G1393 | G1393 | G1319 | G1244 | U1180 | G1114  | G1051 | A988  | G928 | A866 | G805 | G739 | G665  | A627  |
|       | C1394 | C1394 | A1321 | G1245 | C1181 | G1115  | C1052 | G989  | G929 | U867 | C806 | U740 | G666  | G630  |
|       | G1395 | G1395 | A1322 | A1247 | G1182 | G1116  | A1064 | A990  | U930 | U868 | U807 | G741 | G667  | A631  |
|       | U1396 | U1396 | U1353 | U1249 | G1183 | G1117  | G1055 | C991  | G931 | G870 | G808 | G742 | G668  | G632  |
|       | U1397 | U1397 | G1324 | G1250 | G1184 | G1118  | G1056 | C992  | G932 | A870 | G809 | G743 | G669  | A633  |
|       | G1398 | G1398 | G1325 | C1251 | G1187 | G1119  | A1057 | G993  | A934 | U871 | U810 | G744 | A670  | A634  |
|       | C1399 | C1399 | U1326 | G1252 | U1188 | A1126  | U1058 | C994  | G935 | A872 | U811 | G745 | A671  | A635  |
|       | G1400 | G1400 | G1327 | A1253 | A1189 | A1127  | G1059 | A996  | C936 | G874 | C812 | A746 | C672  | C634  |
|       | A1469 | A1469 | G1328 | A1254 | G1190 | A1128  | U1060 | G997  | U937 | G875 | U813 | U747 | C673  | C635  |
|       | C1404 | C1404 | U1329 | U1255 | G1191 | A1129  | U1061 | C998  | G938 | C876 | C814 | G748 | G674  | G636  |
|       | U1405 | U1405 | C1330 | G1256 | G1192 | U1130  | G1062 | U999  | G939 | U877 | C816 | C749 | A675  | A637  |
|       | A1406 | A1406 | G1331 | G1257 | G1193 | A1131  | G1063 | A1000 | G940 | A878 | C817 | A751 | A676  | G638  |
|       | C1407 | C1407 | U1332 | G1260 | G1194 | A1132  | C1064 | A1001 | G941 | G880 | C818 | A752 | A677  | U639  |
|       | G1408 | G1408 | G1333 | G1261 | U1195 | U1133  | U1065 | G1002 | U942 | G881 | A819 | C753 | C678  | C640  |
|       | C1409 | C1409 | G1334 | G1265 | G1197 | G1136  | A1067 | G1003 | G944 | G882 | A820 | C754 | G684  | G642  |
|       | U1415 | U1415 | G1335 | A1265 | U1198 | G1137  | G1068 | C1005 | A945 | G883 | A824 | G760 | A685  | A643  |
|       | G1416 | G1416 | U1340 | G1266 | U1199 | G1138  | A1069 | C1006 | G946 | C884 | A824 | A761 | G686  | A644  |
|       | C1417 | C1417 | U1341 | U1267 | C1200 | G1139  | A1070 | C1007 | G947 | C885 | A825 | U762 | G687  | C945  |
|       | A1418 | A1418 | A1342 | A1268 | C1201 | C1140  | G1071 | G1011 | G948 | C886 | U826 | G763 | U694  | A646  |
|       | U1419 | U1419 | G1343 | A1269 | C1202 | U1141  | C1072 | U1012 | C949 | A887 | U827 | A764 | G695  | G648  |
|       | U1420 | U1420 | C1344 | G1270 | A1203 | U1142  | A1073 | G950  | G950 | C888 | U828 | G765 | G696  | G649  |
|       | G1421 | G1421 | U1345 | G1271 | U1204 | A1142A | G1074 | C1013 | C951 | C889 | A829 | C766 | C697  | C850  |
|       | G1422 | G1422 | A1349 | A1272 | U1205 | A1143  | C1075 | U1014 | G952 | A890 | G830 | U767 | G698  | G651  |
|       | G1423 | G1423 | G1349 | U1273 | G1206 | G1144  | C1076 | U1015 | G953 | G892 | G831 | G768 | A699  | C652  |
|       | G1424 | G1424 | A1349 | A1274 | G1207 | C1145  | A1077 | G1016 | G954 | C893 | G832 | G769 | G700  | A653  |
|       | G1425 | G1425 | U1352 | G1275 | C1208 | C1146  | U1078 | G1017 | C955 | C894 | U833 | G770 | G701  | G654  |
|       | A1426 | A1426 | G1353 | A1276 | G1209 | C1147  | C1079 | G1018 | G956 | U895 | C834 | U773 | G702  | A654A |
|       | A1427 | A1427 | A1354 | A1278 | A1210 | U1148  | A1080 | U1019 | A957 | A896 | A835 | A774 | G702  | G654A |
|       | C1428 | C1428 | G1355 | G1285 | U1211 | G1149  | U1081 | A1020 | G958 | C997 | G836 | A775 | G709  | C654B |
|       | G1429 | G1429 | A1355 | A1286 | G1212 | C1150  | A1021 | A1021 | A959 | C998 | C837 | G776 | G710  | G654C |
|       | A1430 | A1430 | G1358 | A1287 | A1213 | G1151  | A1085 | G1022 | A960 | C999 | C838 | A777 | G711  | G654D |
|       | U1431 | U1431 | A1359 | G1288 | A1214 | C1152  | A1086 | U1023 | G961 | A900 | U839 | G778 | G712  | C654E |
|       | C1432 | C1432 | A1360 | G1289 | G1215 | C1153  | G1087 | G1024 | G962 | A901 | C840 | U779 | G713  | C654F |
|       | U1433 | U1433 | G1361 | C1290 | G1216 | G1154  | A1088 | G1025 | U963 | C902 | A844 | G780 | G714  | C654G |
|       | A1434 | A1434 | A1362 | C1291 | G1217 | A1155  | G1089 | U1026 | G966 | C903 | G842 | A781 | U714  | G654H |
|       | G1435 | G1435 | C1363 | U1292 | C1218 | A1156  | U1090 | A1027 | G967 | C904 | G843 | A782 | G715  | A654J |
|       | G1436 | G1436 | G1364 | C1293 | G1219 | G1157  | G1091 | A1028 | C967 | U905 | C844 | A783 | G717  | C654K |

|       |       |       |       |       |       |       |       |       |       |       |       |        |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|--------|
| A2425 | G2358 | G2093 | G2016 | G2094 | G2019 | G1947 | G1882 | G1795 | G1717 | G1643 | G1573 | C1504  |
| A2426 | C2359 | G2094 | G2156 | G2094 | A2019 | G1948 | C1882 | U1796 | G1718 | G1644 | G1574 | C1505  |
| C2427 | A2360 | C2095 | G2157 | C2096 | C2020 | G1949 | A1883 | C1797 | G1725 | C1644 | C1575 | C1506  |
| G2428 | A2361 | G2300 | G2237 | U2096 | G2021 | G1950 | A1884 | G1797 | G1726 | C1645 | C1576 | A1507  |
| A2429 | C2362 | G2301 | G2238 | U2097 | U2022 | U1951 | G1888 | G1800 | U1727 | G1646 | C1577 | A1508  |
| A2430 | G2363 | G2302 | G2239 | U2098 | G2023 | A1952 | A1889 | G1801 | G1728 | G1647 | C1578 | C1509  |
| U2431 | G2365 | G2303 | C2240 | U2099 | G2023 | A1953 | A1890 | A1802 | A1729 | G1648 | U1579 | A1510  |
| A2432 | G2304 | G2304 | G2100 | G2100 | A2031 | G1954 | A1891 | G1807 | U1730 | G1650 | A1579 | A1511  |
| A2433 | A2305 | G2162 | G2101 | G2032 | G2032 | U1955 | C1893 | G1731 | G1731 | G1651 | A1580 | A1512  |
| G2434 | C2306 | G2163 | U2102 | A2033 | A2033 | U1956 | C1894 | A1810 | G1732 | G1652 | G1581 | C1513  |
| A2435 | G2307 | G2164 | G2103 | G2103 | G2034 | C1957 | C1895 | G1811 | G1733 | G1653 | G1582 | C1514  |
| G2436 | G2308 | G2165 | G2104 | G2105 | G2035 | C1961 | C1896 | G1812 | G1734 | A1654 | A1583 | U1514  |
| A2437 | A2309 | G2166 | G2105 | G2106 | G2036 | C1962 | G1897 | G1814 | C1735 | C1657 | A1585 | C1515  |
| A2438 | A2310 | U2167 | G2107 | C2108 | C2039 | C1963 | U1898 | A1815 | C1742 | C1658 | A1586 | U1516  |
| A2439 | A2311 | G2168 | C2107 | C2108 | C2040 | U1963 | U1899 | G1816 | G1743 | U1659 | A1588 | G1517  |
| A2440 | A2312 | A2169 | A2170 | C2108 | C2040 | G1964 | C1899 | G1817 | C1744 | G1660 | C1589 | C1518  |
| C2441 | C2313 | A2170 | C2043 | C2109 | C2043 | U1965 | A1900 | G1818 | G1745 | G1661 | U1590 | G1519  |
| G2442 | C2314 | A2171 | G2046 | G2111 | G2046 | C1966 | C1902 | U1819 | A1749 | C1662 | G1591 | U1520  |
| G2443 | G2315 | U2172 | G2046 | G2112 | G2046 | C1967 | C1903 | U1820 | G1750 | C1663 | C1592 | G1521  |
| G2444 | C2316 | A2173 | G2049 | U2113 | G2049 | G1968 | G1904 | A1821 | G1783 | C1664 | C1593 | U1523  |
| G2445 | C2317 | A2174 | G2050 | G2115 | C2050 | A1969 | C1904 | A1822 | C1784 | A1665 | G1594 | G1524  |
| U2449 | G2318 | C2175 | C2051 | G2116 | A2051 | A1970 | G1906 | G1822 | A1754 | G1666 | G1595 | G1525  |
| A2450 | G2319 | C2176 | G2052 | G2117 | G2052 | A1971 | G1907 | G1826 | G1756 | G1667 | G1526 | G1526  |
| A2451 | A2320 | U2180 | G2053 | A2117 | G2053 | A1972 | G1908 | G1827 | U1757 | A1668 | C1527 | G1527  |
| G2452 | G2321 | G2182 | G2054 | U2118 | A2054 | G1973 | C1908 | C1827 | U1758 | A1669 | C1528 | A1528  |
| A2459 | A2322 | C2183 | A2055 | A2119 | A2055 | C1974 | C1909 | G1828 | G1758 | A1670 | C1529 | A1529  |
| U2460 | G2323 | C2184 | C2056 | G2120 | C2056 | G1980 | A1912 | A1829 | A1759 | C1670 | A1600 | G1530  |
| C2461 | C2324 | G2184 | G2056 | G2121 | G2056 | A1981 | A1913 | A1830 | A1760 | G1671 | G1601 | G1531  |
| U2462 | G2325 | U2122 | A2057 | U2122 | A2057 | C1982 | A1914 | G1831 | C1761 | C1672 | U1602 | C1532  |
| C2463 | C2326 | G2186 | A2058 | G2123 | A2058 | G1983 | A1915 | C1832 | A1762 | G1673 | C1605 | G1533  |
| C2464 | A2327 | G2187 | A2059 | G2124 | A2059 | U1915 | A1916 | U1833 | A1763 | A1676 | G1606 | G1534  |
| G2396 | A2328 | C2188 | A2060 | G2125 | A2060 | G1985 | U1917 | C1837 | G1784 | A1677 | G1607 | U1535  |
| C2465 | A2329 | U2189 | A2061 | A2126 | A2061 | A1986 | A1918 | C1838 | C1785 | G1678 | A1536 | G1536  |
| C2466 | G2330 | G2190 | A2062 | G2127 | A2062 | G1989 | A1919 | G1839 | U1766 | U1679 | A1608 | C1537  |
| C2467 | G2331 | G2191 | C2063 | C2128 | C2063 | C1990 | A1918 | U1680 | A1610 | U1680 | A1609 | G1538  |
| A2469 | G2332 | G2192 | A2064 | G2129 | C2064 | U1991 | A1921 | G1839 | G1770 | G1681 | A1610 | G1539  |
| G2470 | U2333 | G2193 | C2065 | U2130 | C2065 | U1992 | G1923 | U1841 | C1771 | C1611 | C1611 | G1540  |
| C2471 | C2334 | G2196 | C2066 | G2131 | C2066 | G1993 | U1923 | C1842 | G1772 | C1612 | G1612 | C1540  |
| G2472 | A2335 | U2197 | G2067 | U2132 | G2067 | U1994 | C1924 | C1843 | A1773 | G1613 | G1613 | U1941  |
| U2473 | A2336 | G2197 | U2068 | G2133 | U2068 | C1994 | C1925 | U1844 | C1774 | U1688 | A1614 | G1542  |
| C2474 | G2337 | A2198 | G2069 | A2134 | G2069 | U1995 | A1926 | G1845 | U1775 | A1689 | C1615 | A1543  |
| C2475 | G2338 | A2199 | G2070 | A2135 | G2070 | C1996 | A1927 | G1846 | G1776 | A1689 | A1616 | C1544  |
| A2476 | G2339 | C2205 | A2071 | G2136 | A2071 | G1997 | A1928 | G1847 | U1777 | U1693 | C1617 | A1545  |
| C2477 | G2340 | C2206 | G2072 | C2137 | G2072 | G1998 | A1929 | A1847 | U1778 | C1694 | A1618 | A1545A |
| G2478 | G2341 | U2208 | C2073 | C2138 | C2073 | G1999 | A1930 | U1779 | U1779 | G1695 | G1619 | C1546  |
| C2479 | C2342 | C2209 | U2074 | G2139 | U2074 | G2000 | A1931 | U1851 | A1780 | G1696 | G1620 | C1547  |
| G2480 | C2343 | G2210 | U2075 | G2140 | U2075 | A2001 | A1932 | C1781 | C1781 | G1697 | C1625 | C1548  |
| C2481 | U2344 | A2212 | G2076 | G2141 | G2076 | G2002 | A1933 | C1782 | C1782 | A1698 | G1626 | A1553  |
| G2482 | G2345 | G2213 | G2077 | C2142 | G2077 | C2006 | A1936 | G1855 | A1783 | G1699 | G1627 | A1554  |
| C2483 | A2346 | U2213 | U2078 | C2143 | U2078 | G2007 | A1937 | G1857 | A1784 | A1700 | G1627 | G1555  |
| G2484 | C2347 | G2215 | G2080 | U2144 | G2080 | C2007 | A1938 | G1858 | A1785 | A1701 | A1632 | C1556  |
| G2485 | G2348 | G2216 | C2081 | C2145 | C2081 | C2008 | A1939 | G1859 | A1786 | G1705 | A1632 | C1557  |
| C2486 | G2349 | G2217 | A2082 | G2146 | A2082 | G2009 | U1939 | A1859 | A1787 | U1706 | A1634 | A1558  |
| G2487 | G2350 | G2218 | A2083 | C2147 | A2083 | G2009 | U1940 | G1860 | C1788 | U1706 | A1634 | A1558  |
| A2488 | G2351 | G2219 | U2084 | G2148 | U2084 | G2012 | A1941 | G1861 | A1789 | G1709 | G1636 | G1559  |
| G2489 | C2352 | G2224 | G2087 | G2149 | U2087 | A2013 | C1942 | U1864 | C1790 | U1709 | G1636 | A1567  |
| A2490 | G2353 | A2225 | G2088 | U2150 | G2088 | A2014 | C1943 | A1871 | C1790 | C1710 | A1637 | G1568  |
| G2491 | C2354 | G2226 | U2089 | G2151 | U2089 | A2015 | U1944 | A1872 | A1791 | C1711 | A1638 | A1569  |
| U2492 | G2355 | A2227 | U2090 | G2152 | U2090 | U2016 | U1945 | A1873 | A1792 | C1712 | G1639 | G1569  |
| U2493 | U2357 | G2227 | U2092 | G2153 | U2092 | U2017 | U1946 | G1878 | U1794 | U1716 | C1640 | A1570  |

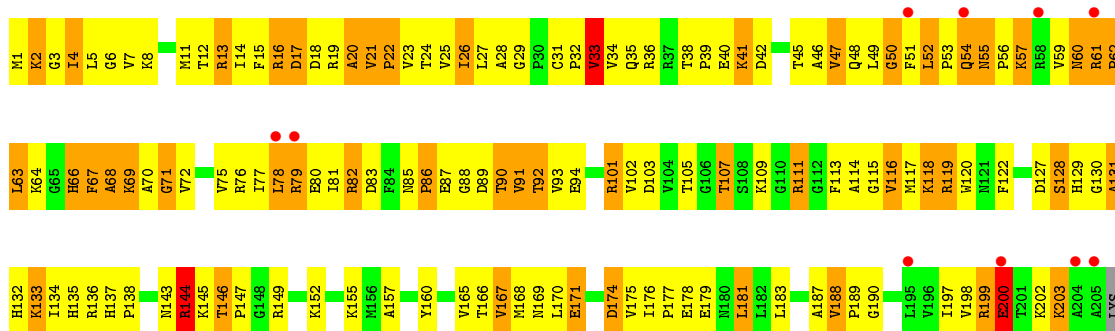




• Molecule 3: 50S ribosomal protein L2



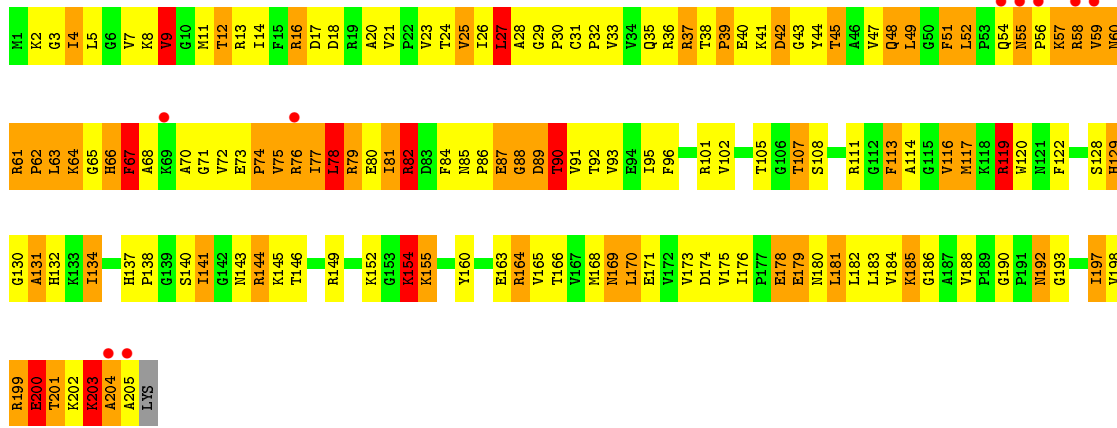
• Molecule 4: 50S ribosomal protein L3



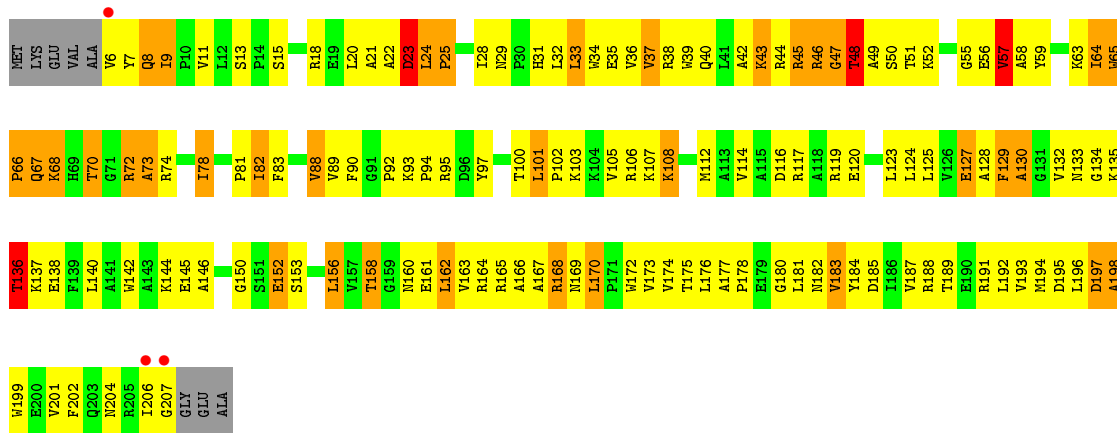
• Molecule 4: 50S ribosomal protein L3



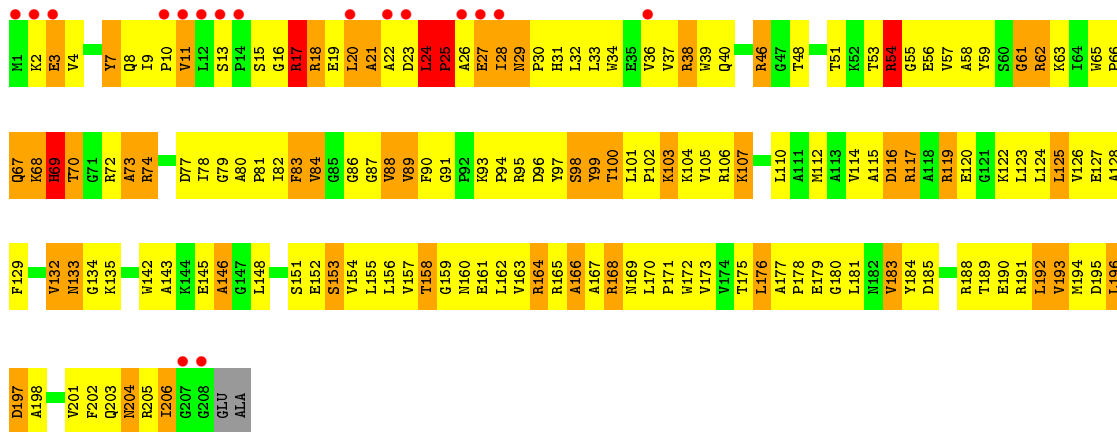




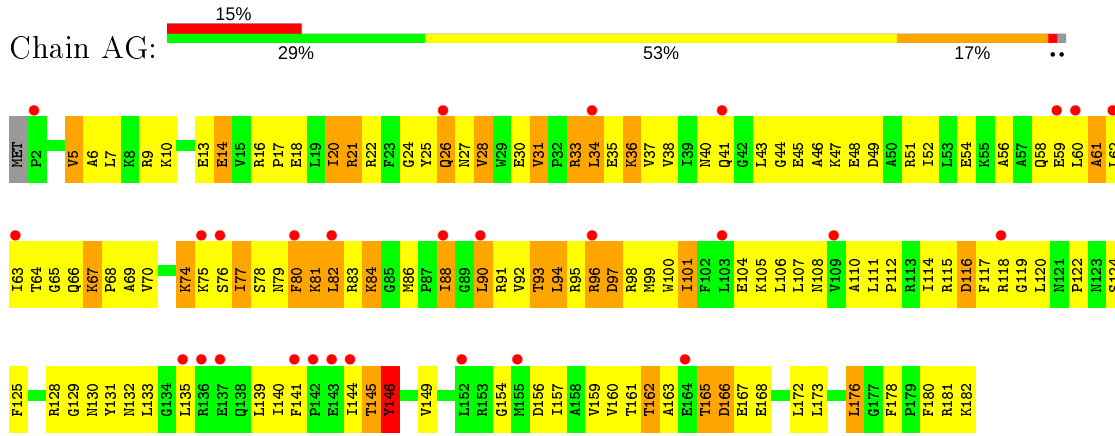
• Molecule 5: 50S ribosomal protein L4



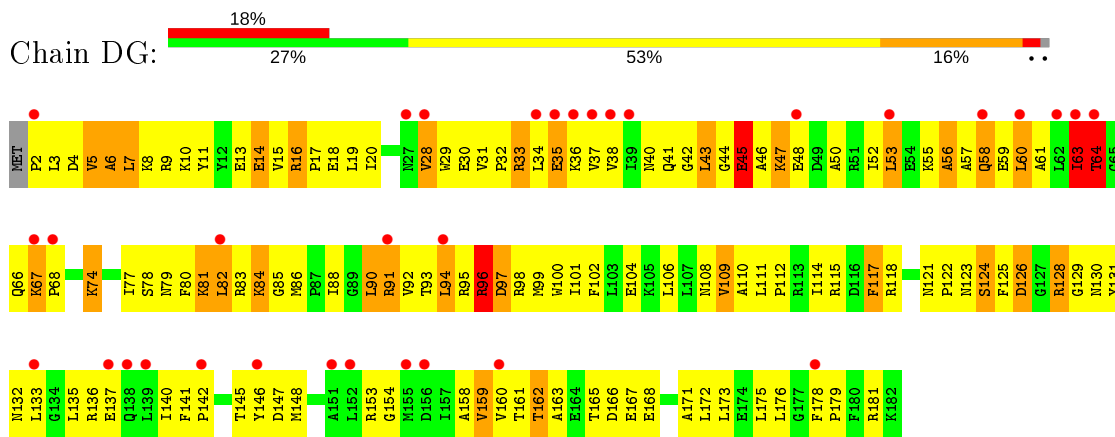
• Molecule 5: 50S ribosomal protein L4



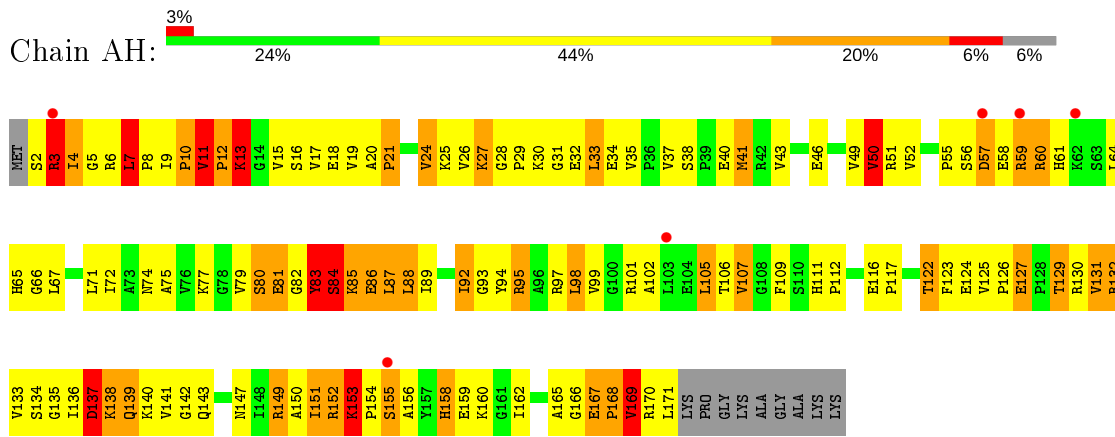
• Molecule 6: 50S ribosomal protein L5



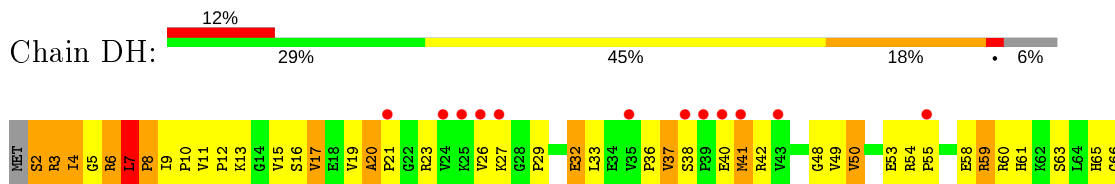
• Molecule 6: 50S ribosomal protein L5

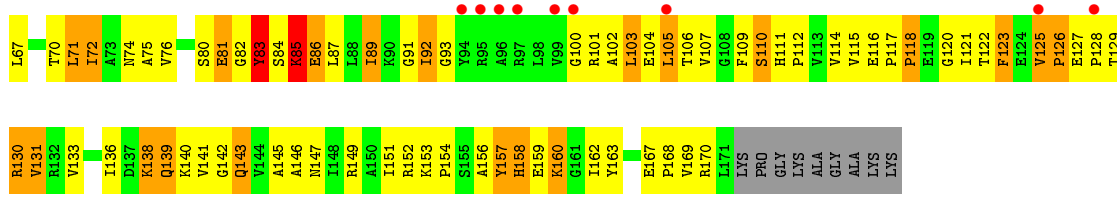


• Molecule 7: 50S ribosomal protein L6

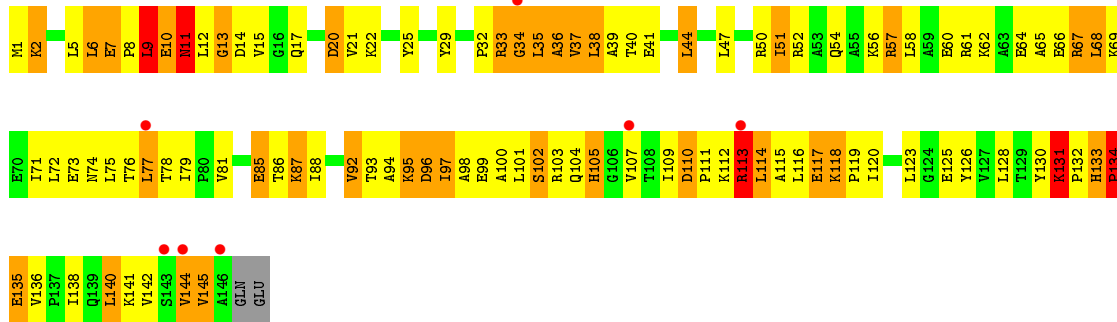


• Molecule 7: 50S ribosomal protein L6

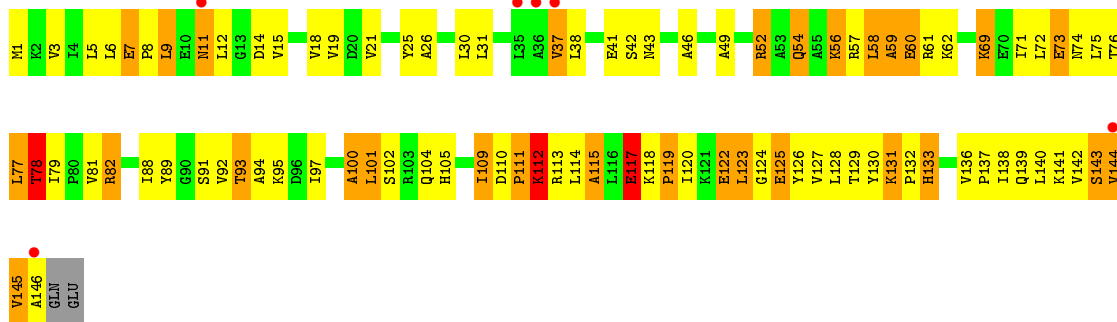




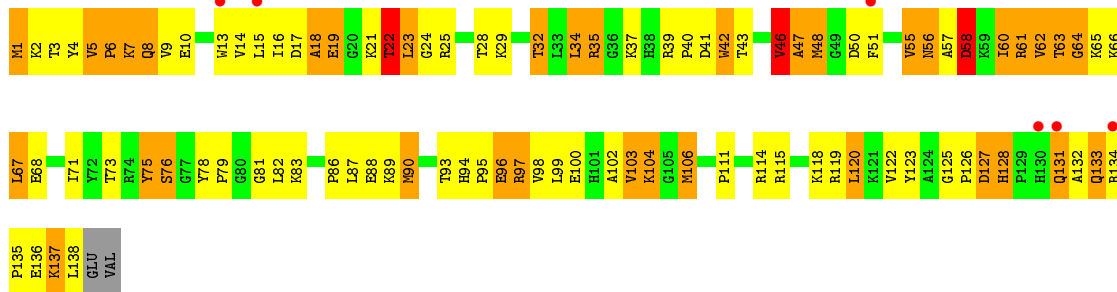
• Molecule 8: 50S ribosomal protein L9



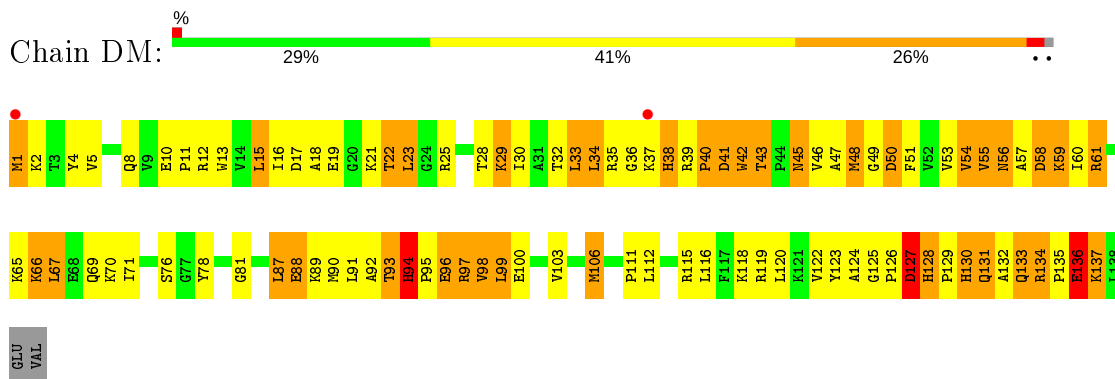
• Molecule 8: 50S ribosomal protein L9



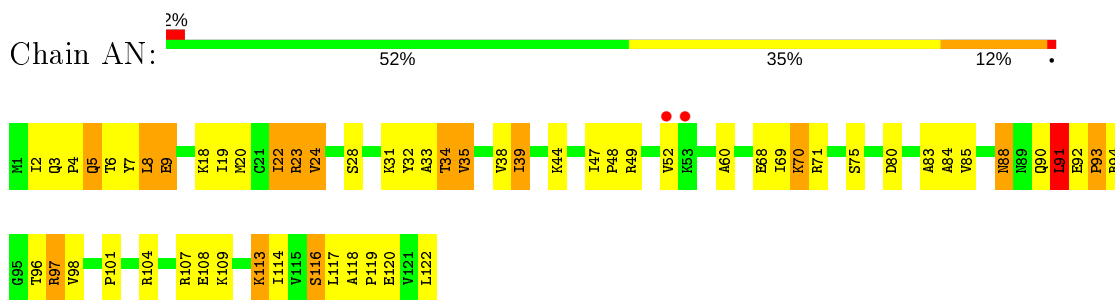
• Molecule 9: 50S ribosomal protein L13



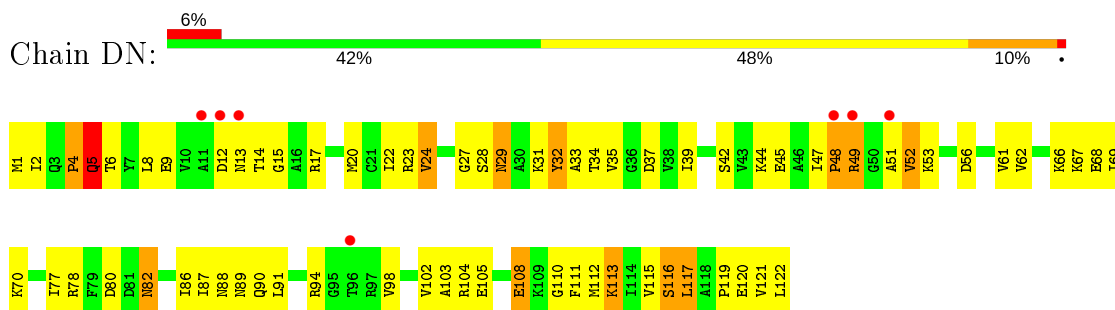
• Molecule 9: 50S ribosomal protein L13



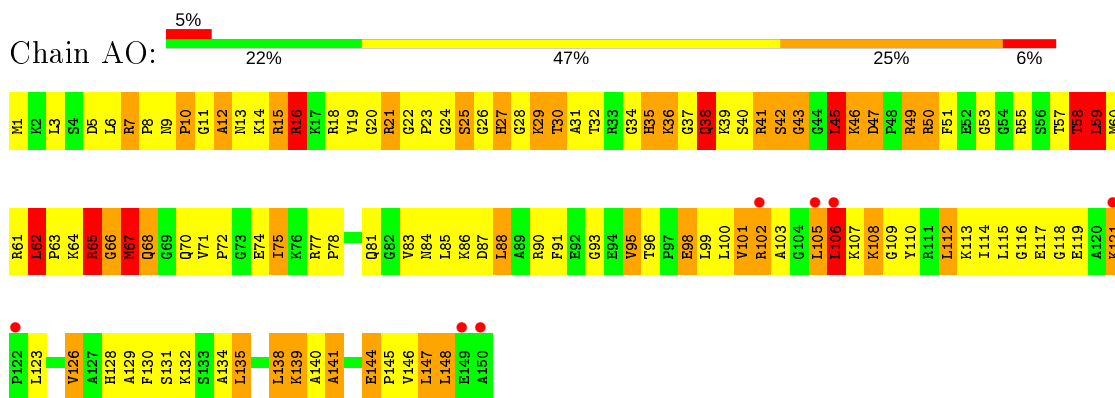
• Molecule 10: 50S ribosomal protein L14



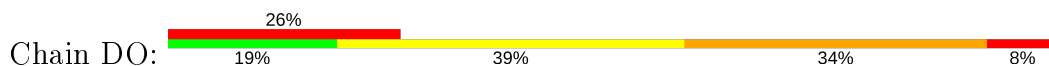
• Molecule 10: 50S ribosomal protein L14

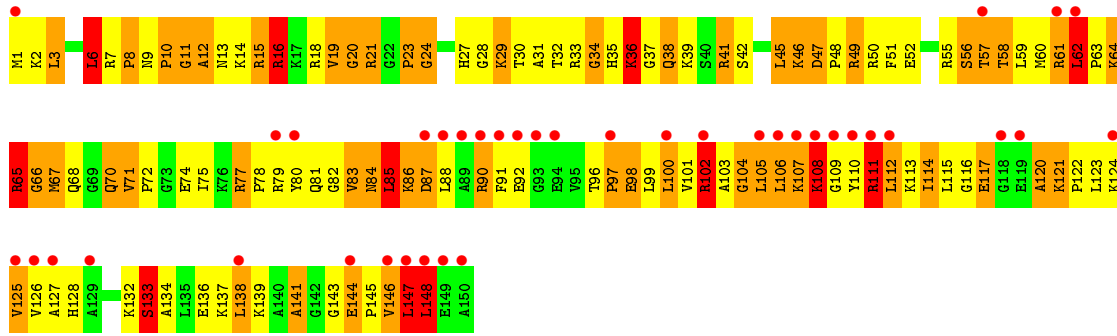


• Molecule 11: 50S ribosomal protein L15

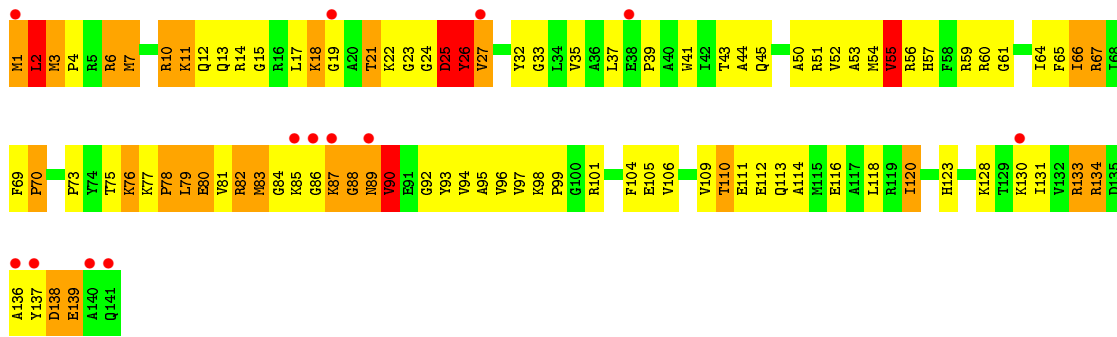
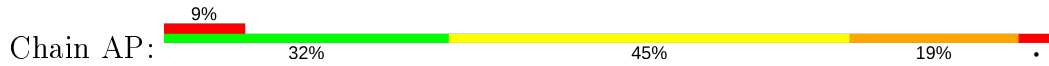


• Molecule 11: 50S ribosomal protein L15

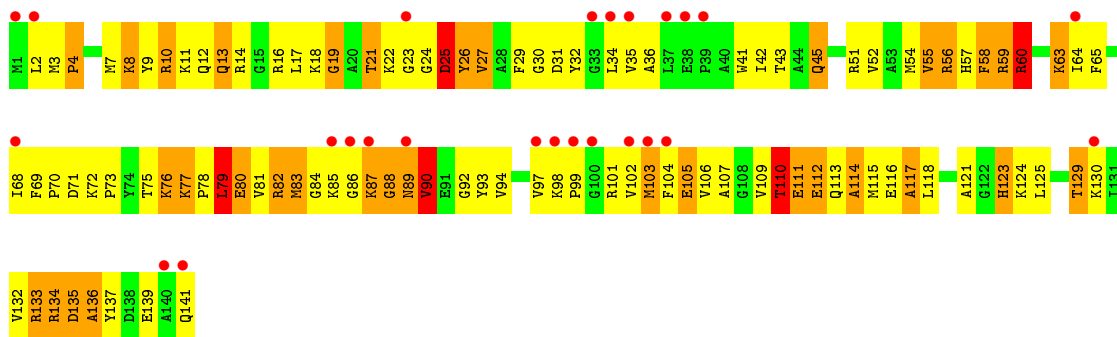




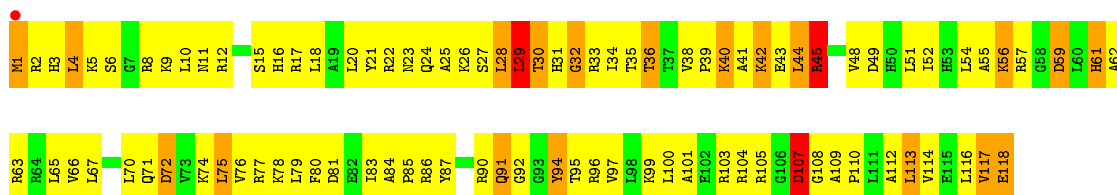
• Molecule 12: 50S ribosomal protein L16



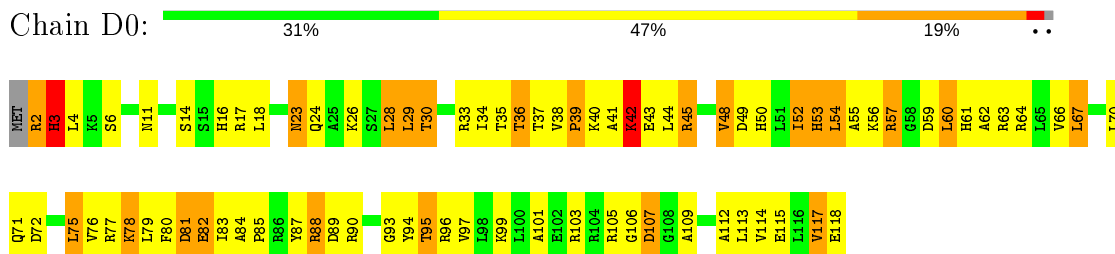
• Molecule 12: 50S ribosomal protein L16



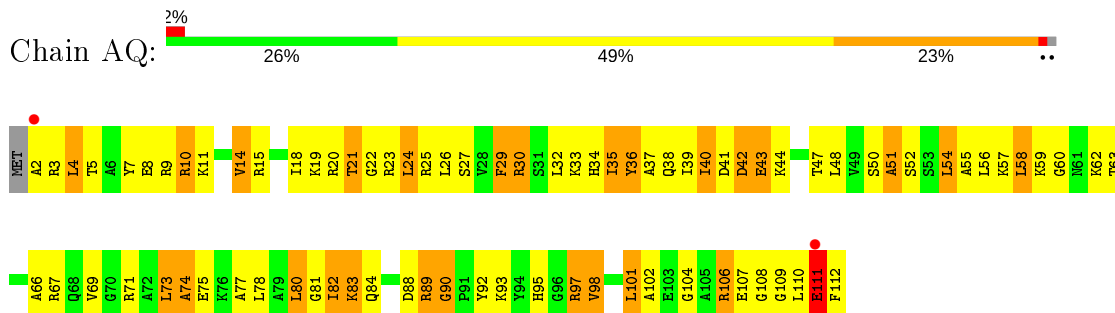
• Molecule 13: 50S ribosomal protein L17



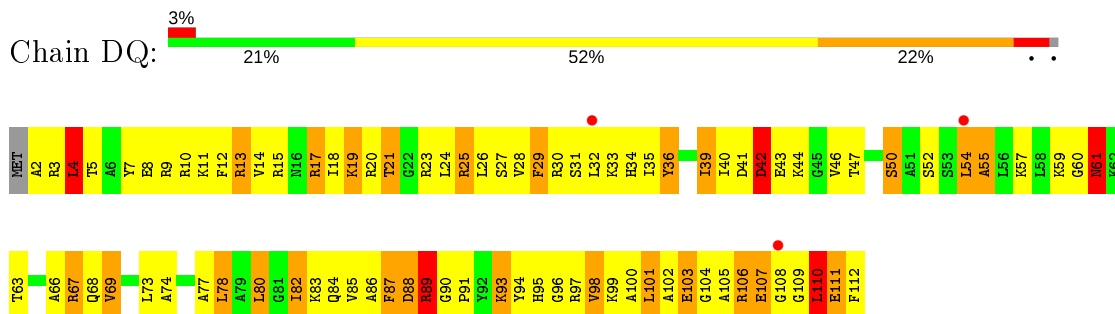
• Molecule 13: 50S ribosomal protein L17



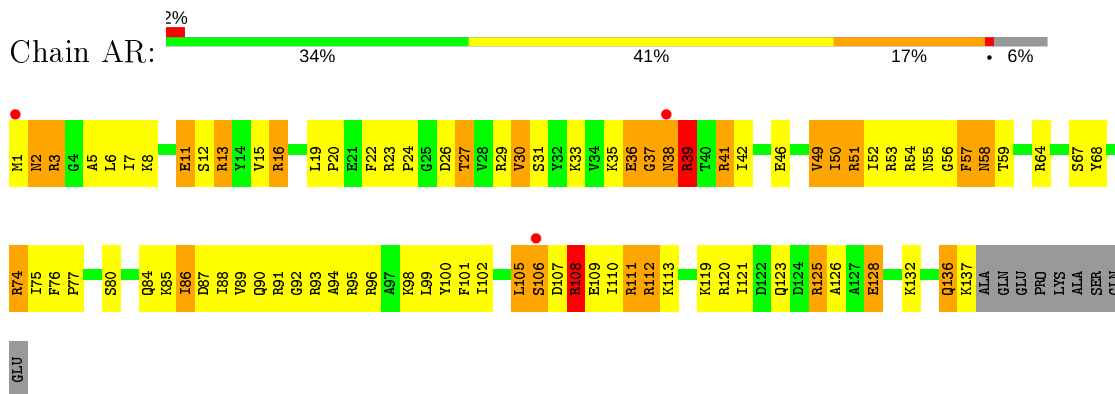
• Molecule 14: 50S ribosomal protein L18



• Molecule 14: 50S ribosomal protein L18

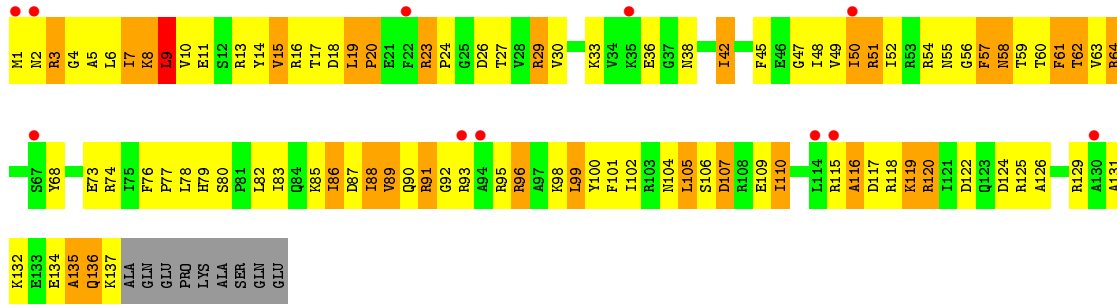


• Molecule 15: 50S ribosomal protein L19

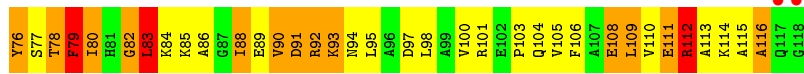
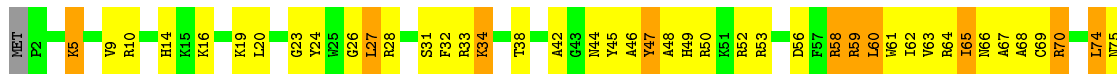


• Molecule 15: 50S ribosomal protein L19

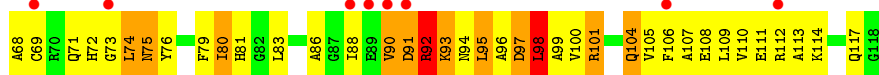
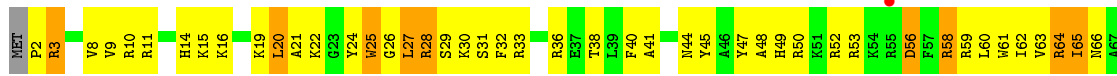




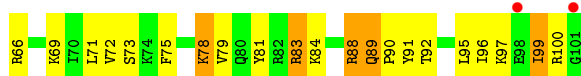
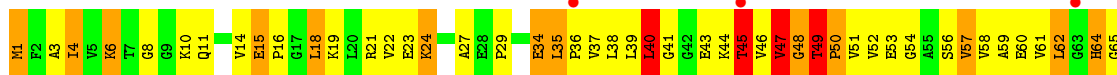
• Molecule 16: 50S ribosomal protein L20



• Molecule 16: 50S ribosomal protein L20

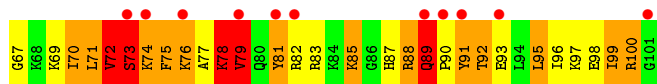


• Molecule 17: 50S ribosomal protein L21

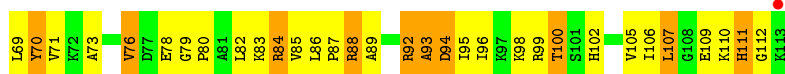


• Molecule 17: 50S ribosomal protein L21

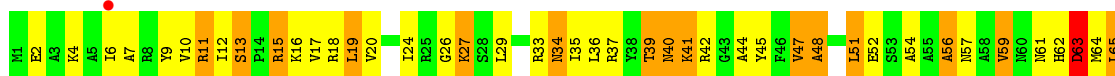




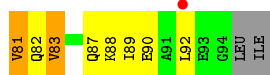
• Molecule 18: 50S ribosomal protein L22



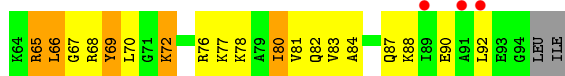
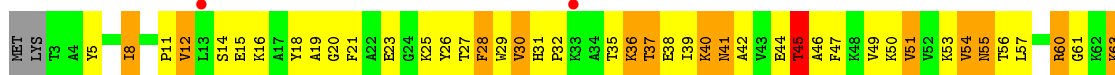
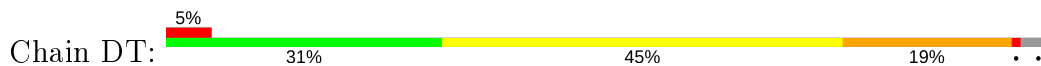
• Molecule 18: 50S ribosomal protein L22



• Molecule 19: 50S ribosomal protein L23



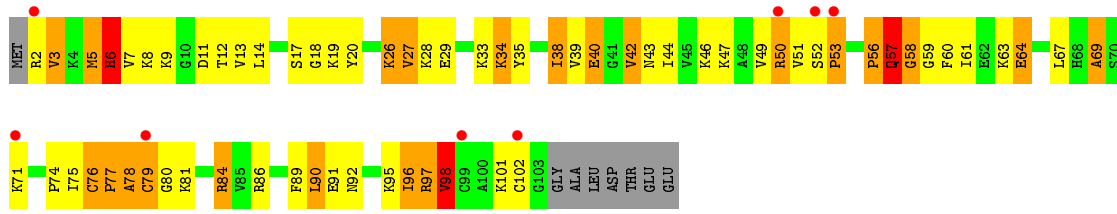
• Molecule 19: 50S ribosomal protein L23



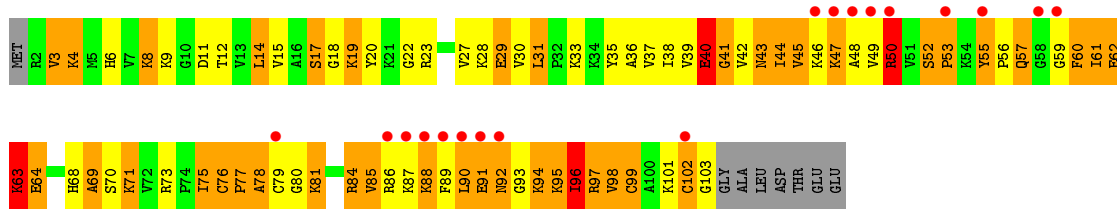
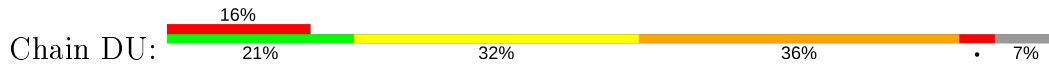
• Molecule 20: 50S ribosomal protein L24



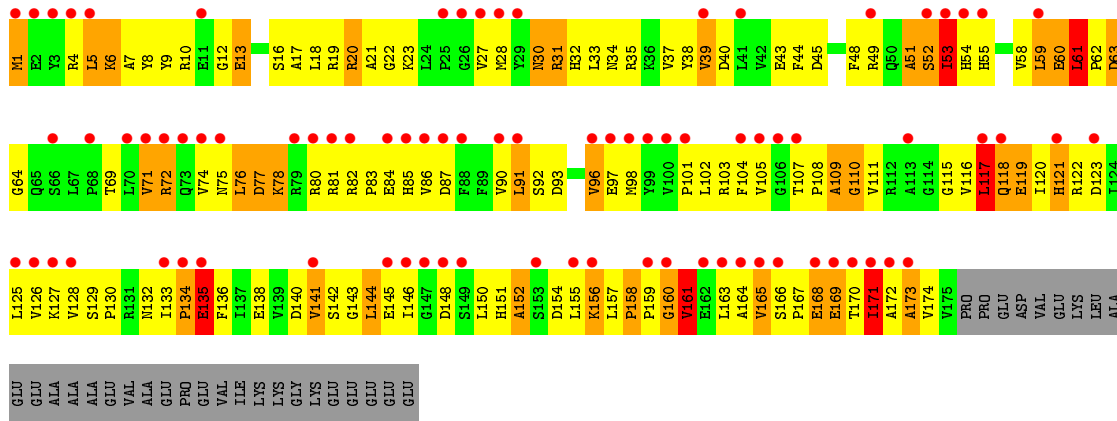
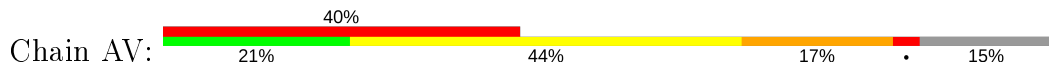




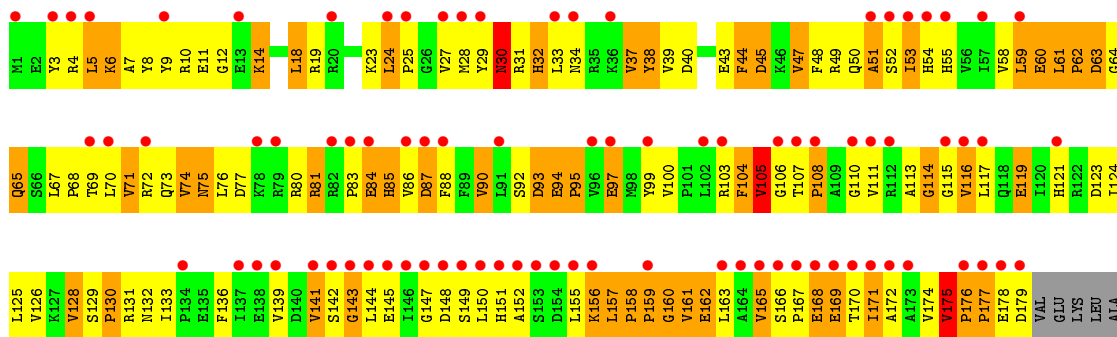
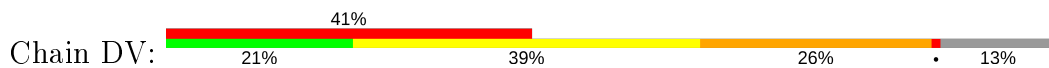
• Molecule 20: 50S ribosomal protein L24



• Molecule 21: 50S ribosomal protein L25



• Molecule 21: 50S ribosomal protein L25



GLU  
GLU  
ALA  
ALA  
ALA  
GLU  
VAL  
ALA  
GLU  
PHE  
GLU  
VAL  
ILE  
LYS  
LYS  
LYS  
LYS  
GLU  
GLU  
GLU  
GLU

- Molecule 22: 50S ribosomal protein L27



MET  
ALA  
HIS  
LYS  
LYS  
GLY  
LEU  
GLY  
SER  
T10  
R11  
R14  
K19  
R20  
V23  
K24  
R25  
Y26  
E27  
G28  
Q29  
A33  
G34  
N35  
I36  
L37  
V38  
R39  
Q40  
R41  
G42  
T43  
R44  
F45  
K46  
P47  
G48  
K49  
N50  
V51  
G52  
M53  
G54  
R55  
D56  
F57  
T58  
L59  
F60  
A61  
L62  
V63  
D64  
G65  
V66  
V67

E68  
F69  
Q70  
D71  
R72  
E73  
R74  
L75  
H80  
V81  
R82  
R83  
L84  
A85

- Molecule 22: 50S ribosomal protein L27



MET  
ALA  
HIS  
LYS  
GLY  
LEU  
GLY  
S9  
T10  
R11  
M12  
G13  
R14  
D15  
S16  
Q17  
A18  
K19  
R20  
L21  
G22  
V23  
K24  
R25  
Y26  
E27  
G28  
V31  
R32  
A33  
G34  
N35  
I36  
L37  
V38  
R39  
Q40  
G42  
T43  
R44  
F45  
K46  
P47  
G48  
K49  
N50  
V51  
G52  
M53  
G54  
R55  
D56  
F57  
T58  
L59  
L62

V63  
D64  
G65  
V66  
V67  
E68  
F69  
Q70  
D71  
R72  
G73  
R74  
L75  
Y78  
V79  
H80  
V81  
R82  
P83  
L84  
A85

- Molecule 23: 50S ribosomal protein L28



MET  
S2  
K3  
V4  
S8  
G9  
K10  
R11  
P12  
M16  
I17  
I18  
Q19  
K23  
R26  
E27  
G28  
G29  
V30  
G31  
K32  
K33  
I37  
R40  
R41  
Q42  
Y43  
P44  
M45  
L46  
R50  
V51  
R52  
V53  
O56  
E57  
I58  
T59  
V62  
S65  
H66  
I67  
P68  
L73  
R76  
A77  
K78  
G79

L80  
K81  
L82  
E83  
G84  
L85  
S86  
P87  
K88  
E89  
I90  
K91  
K92  
E93  
L94  
L95  
K96  
L97  
L98

- Molecule 23: 50S ribosomal protein L28

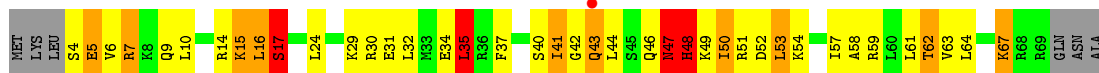


MET  
S2  
K3  
V4  
C5  
E6  
I7  
S8  
R11  
P12  
I13  
M16  
S17  
I18  
Q19  
K23  
R26  
E27  
G28  
G29  
V30  
T35  
G36  
I37  
S38  
K39  
R40  
L46  
Q56  
E57  
I58  
R61  
V62  
H66  
I67  
P68  
R69  
V70  
V74  
E75  
R76  
A77  
K78  
G79  
L80  
L81  
L82  
E83  
G84  
L85

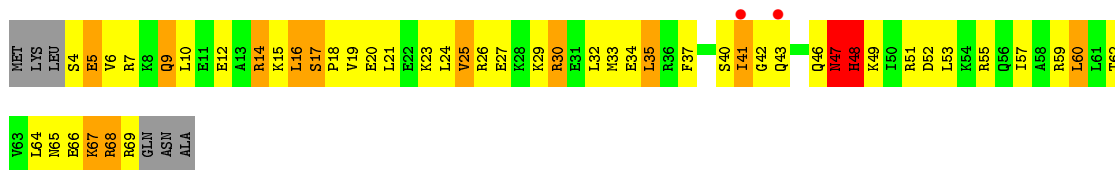
S86  
P87  
K88  
E89  
I90  
K91  
K92  
E93  
L94  
L95  
L98

- Molecule 24: 50S ribosomal protein L29

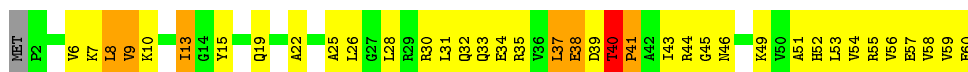




- Molecule 24: 50S ribosomal protein L29



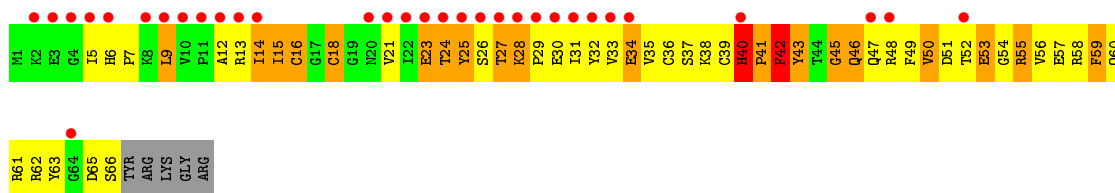
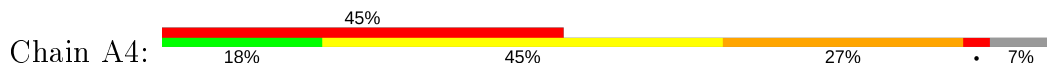
- Molecule 25: 50S ribosomal protein L30



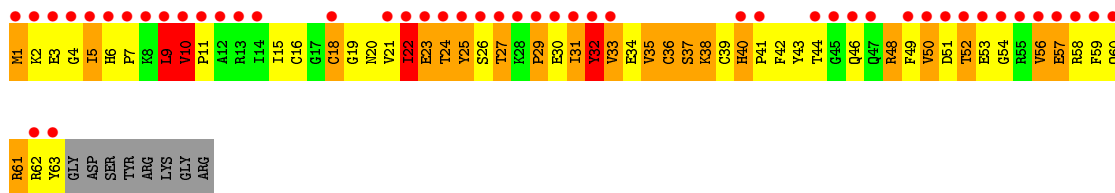
- Molecule 25: 50S ribosomal protein L30



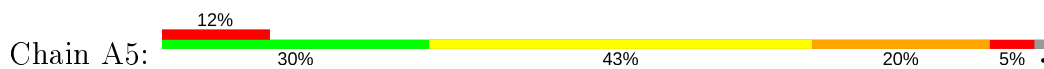
- Molecule 26: 50S ribosomal protein L31



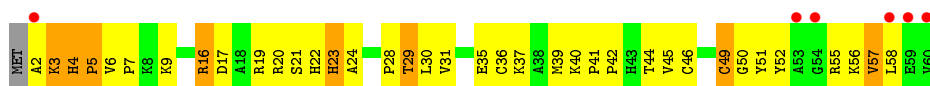
- Molecule 26: 50S ribosomal protein L31



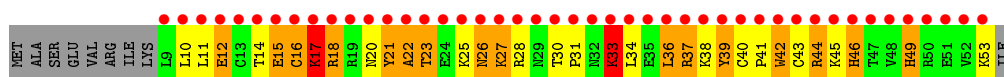
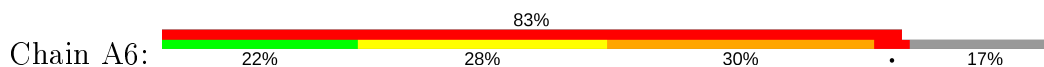
- Molecule 27: 50S ribosomal protein L32



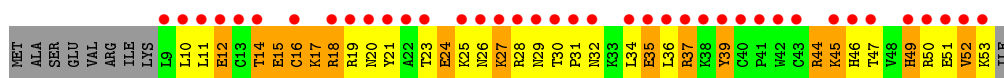
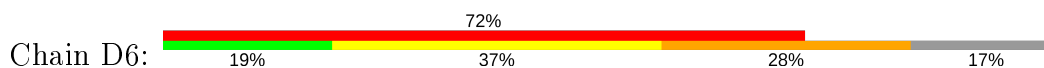
- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



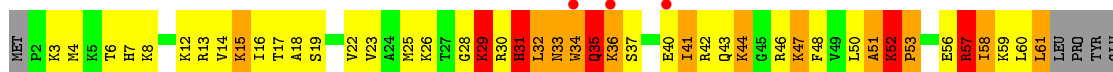
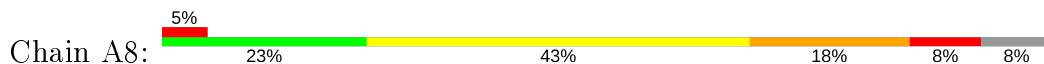
- Molecule 29: 50S ribosomal protein L34



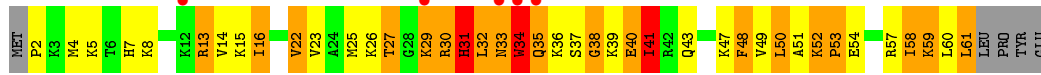
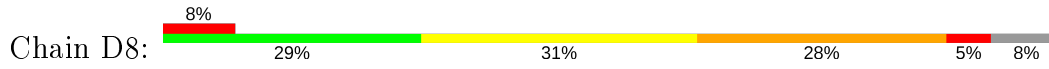
- Molecule 29: 50S ribosomal protein L34



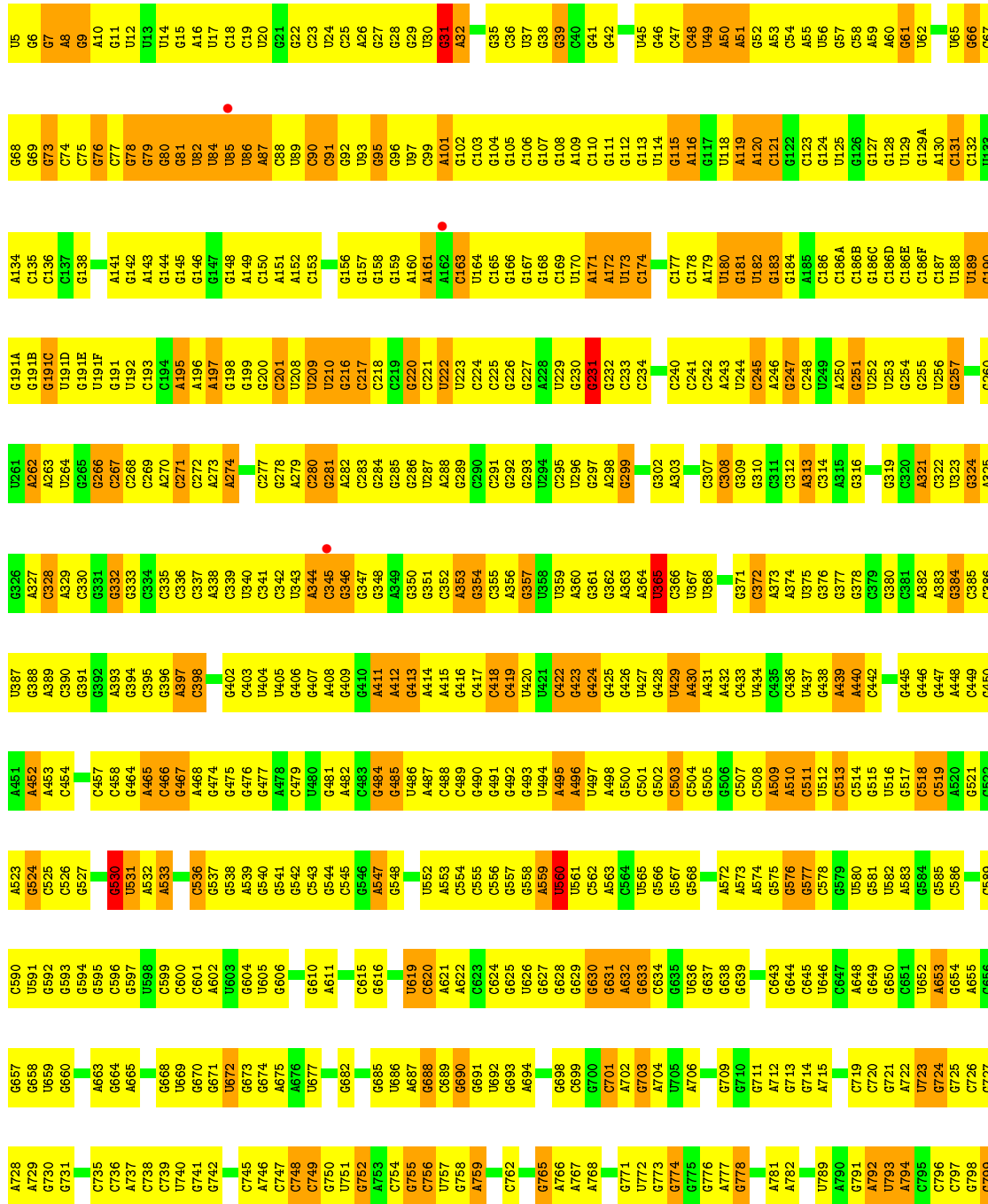
- Molecule 30: 50S ribosomal protein L35

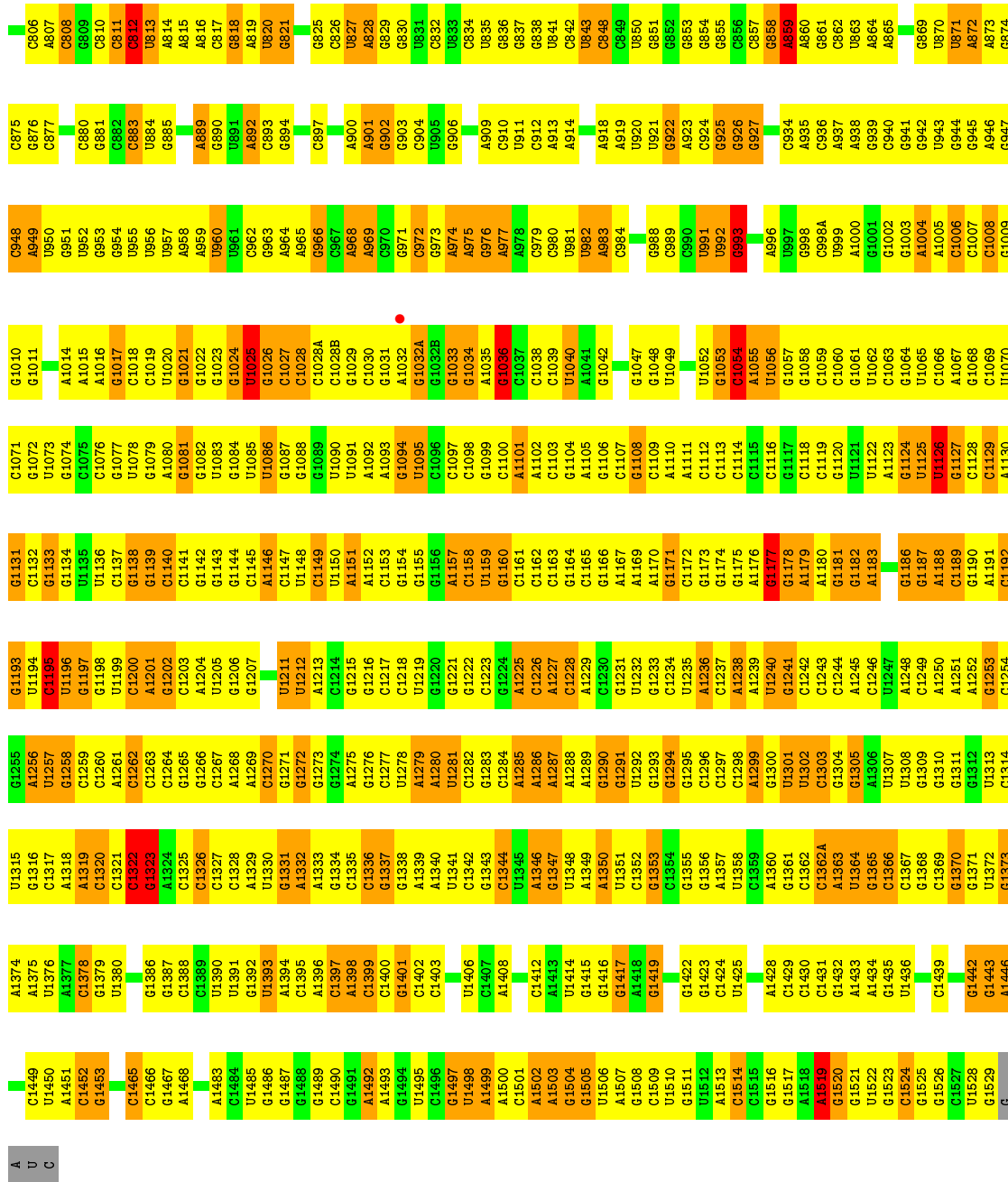


- Molecule 30: 50S ribosomal protein L35



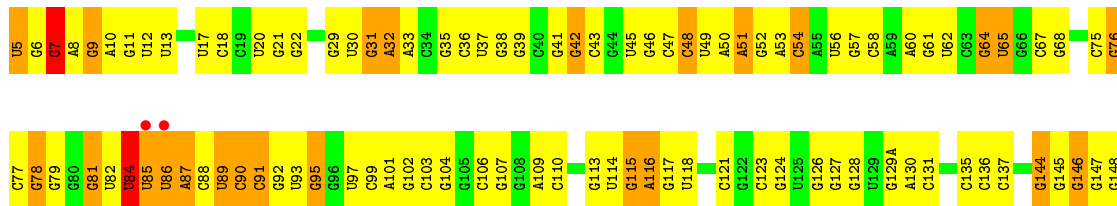
● Molecule 31: 16S ribosomal RNA



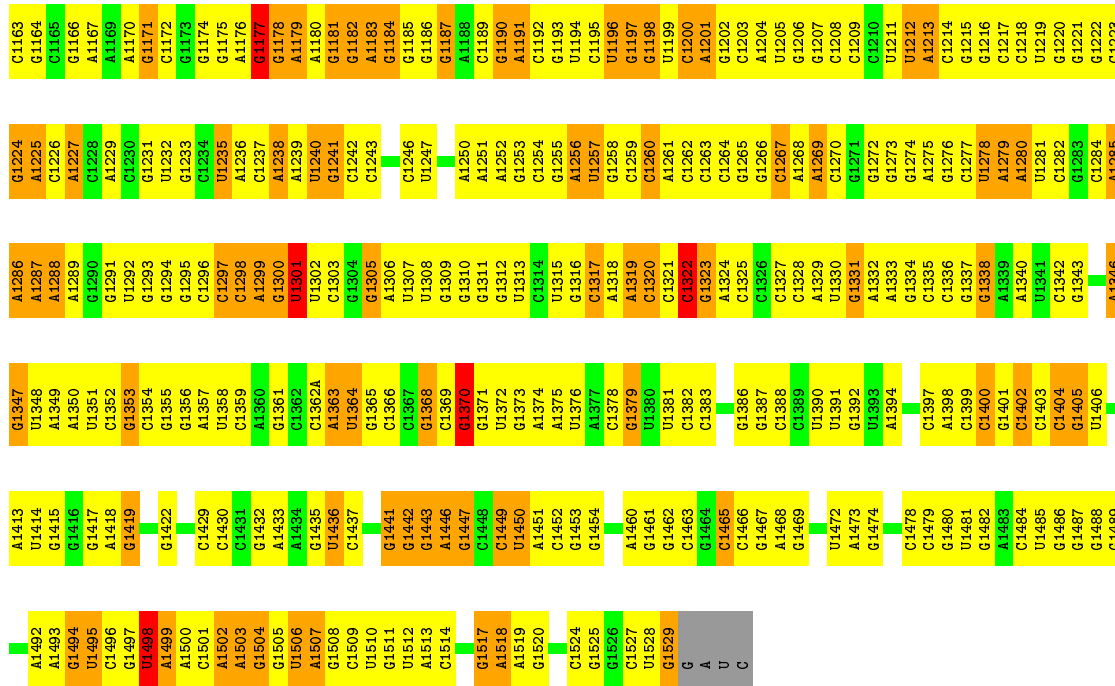


• Molecule 31: 16S ribosomal RNA

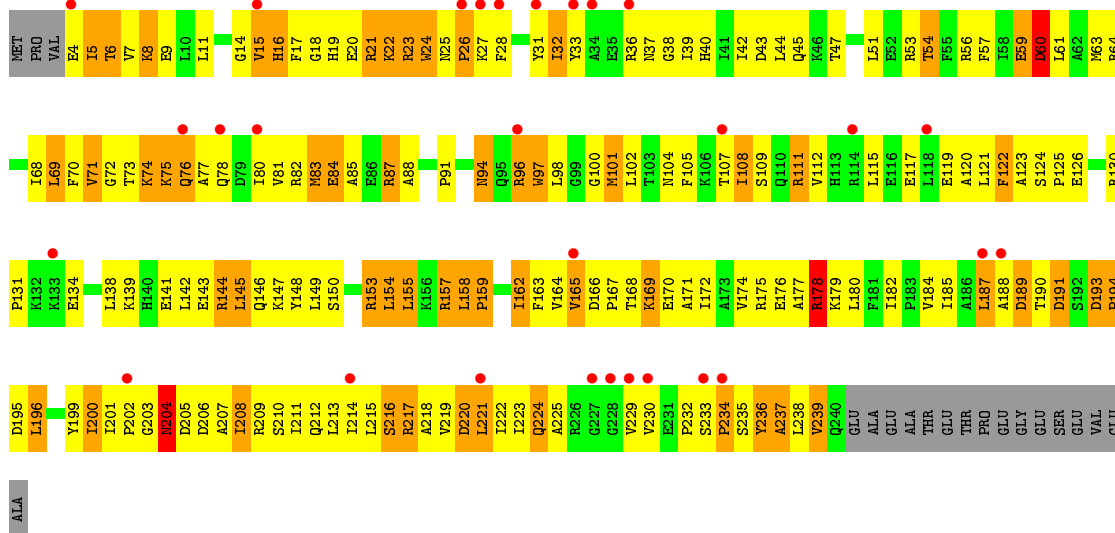
Chain CA:



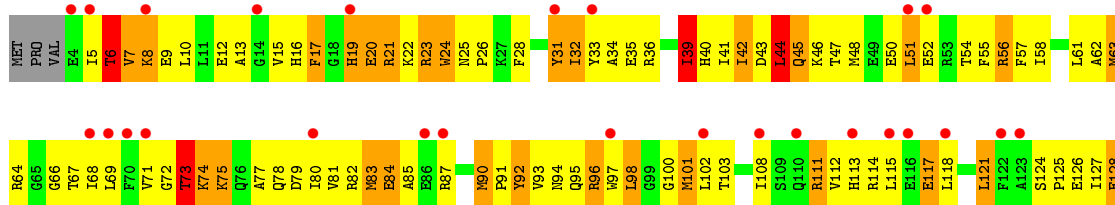
|       |       |        |      |      |      |      |      |      |      |      |      |      |      |       |
|-------|-------|--------|------|------|------|------|------|------|------|------|------|------|------|-------|
| A1102 | A1041 | A883   | G922 | G856 | A781 | C707 | G638 | U571 | C503 | G426 | A360 | G285 | U208 | A149  |
| C1103 | G1042 | C984   | A923 | C857 | A782 | C708 | G639 | A572 | C504 | U427 | G361 | G286 | U209 | C150  |
| A1105 | C1043 | G985   | G924 | G858 | C783 | G711 | A640 | A573 | G505 | G428 | A362 | G289 | U210 | A151  |
| C1106 | C1045 | A986   | G925 | A859 | C784 | G712 | G641 | A574 | A509 | U429 | A363 | C290 | G216 | A152  |
| G1107 | G1046 | G987   | G926 | A860 | G785 | G713 | C642 | G575 | A510 | A430 | C291 | C291 | C217 |       |
| C1108 | G1047 | G988   | G927 | A861 | G791 | G714 | G643 | G576 | G511 | A431 | U365 | G292 |      | G157  |
| A1109 | U1048 | C989   | C930 | C862 | A792 | G715 | C647 | G577 | U512 | A432 | C366 | G293 | G220 | G158  |
| C1110 | U1049 | A991   | C931 | U863 | A793 | A716 | A648 | C578 | U834 | U367 | U367 | G294 | C221 | G159  |
| A1111 | G1050 | U992   | C932 | A864 | A794 | A717 | A649 | G579 | U835 | U368 | A298 | U222 | U222 | A160  |
| C1112 | C1051 | A993   | C933 | A865 | G797 | C719 | G650 | G580 | U516 | C435 | C369 | U223 | U223 | A161  |
| C1113 | U1052 | A994   | G934 | C866 | G798 | C720 | G651 | G581 | C518 | C436 | C370 | U224 | U224 | C163  |
| G1116 | G1053 | A995   | C935 | G867 | G799 | G721 | U652 | U582 | C519 | U437 | G372 | G226 | G226 | U162  |
| C1117 | C1054 | A996   | C936 | C868 | G800 | A722 | A853 | A583 | A520 | G438 | C373 | G230 | G230 | C165  |
| G1118 | A1055 | U997   | A937 | U870 | U801 | U723 | G854 | G584 | G521 | A439 | A374 | G231 | G231 | G166  |
| C1119 | U1056 | U998   | A938 | U871 | A802 | U724 | A855 | G585 | C522 | A440 | U375 | G232 | G232 | G167  |
| G1120 | G1057 | G999   | G939 | A872 | G803 | A725 | G656 | G586 | G526 | C444 | G376 | C233 | C233 | G168  |
| U1121 | U1058 | G1001  | C940 | A873 | G804 | A726 | G657 | G587 | C527 | C445 | G377 | G234 | G234 | C169  |
| U1122 | C1059 | G1002  | G941 | G874 | U804 | A728 | G658 | U591 | C528 | G446 | G378 | G235 | G235 | U170  |
| A1123 | C1060 | A1003  | G942 | C875 | C806 | G731 | U659 | G592 | C529 | G447 | G379 | U239 | U239 | A171  |
| G1124 | U1061 | A1004  | U943 | G878 | A807 | C732 | G660 | G593 | G530 | U448 | G380 | G240 | G240 | A172  |
| C1125 | U1062 | A1005  | G944 | C879 | C808 | A733 | G661 | G594 | G531 | C449 | C381 | C241 | C241 | U173  |
| U1126 | U1063 | C1006  | G945 | A880 | C809 | G734 | G662 | G595 | U532 | C449 | A382 | C242 | C242 | C174  |
| G1127 | G1064 | C1007  | G946 | G881 | C812 | C735 | A663 | G596 | A533 | G450 | A383 | A243 | A243 | C175  |
| U1128 | U1065 | G1008  | A947 | G882 | U813 | C736 | G664 | C599 | A534 | A451 | A384 | U244 | U244 | C176  |
| C1129 | C1066 | G1009  | C948 | C883 | A814 | A737 | A665 | C600 | U534 | A452 | C386 | C245 | C245 | C177  |
| A1130 | A1067 | U1010  | U949 | U884 | A815 | C738 | G666 | C601 | A535 | A453 | U387 | G246 | G246 | A178  |
| U1131 | U1068 | U1011  | U950 | C885 | A816 | G741 | G667 | G604 | C536 | A454 | C320 | U247 | U247 | A179  |
| C1132 | C1069 | U1012  | G951 | G886 | U817 | G742 | G674 | G605 | C537 | C455 | A321 | A250 | A250 | U180  |
| G1133 | U1070 | C1013  | U952 | G887 | C818 | G743 | U677 | G606 | G538 | C456 | C322 | G258 | G258 | G181  |
| C1134 | U1071 | A1014  | G953 | G888 | G819 | G744 | U678 | G607 | A539 | C457 | C323 | G259 | G259 | U182  |
| U1135 | G1072 | U1015  | G954 | C889 | A820 | C745 | U679 | A608 | G540 | A458 | G392 | G260 | G260 | G183  |
| C1136 | U1073 | U1016  | U955 | U889 | G821 | C748 | U680 | A609 | G541 | A459 | C396 | U261 | U261 | A184  |
| U1137 | G1074 | C1017  | U956 | G890 | A822 | C749 | U681 | G612 | G542 | C466 | A465 | U262 | U262 | A185  |
| C1138 | U1075 | U1018  | U957 | U891 | C824 | C750 | C680 | C613 | C543 | G467 | C397 | G263 | G263 | C187  |
| G1139 | U1076 | U1019  | U958 | G892 | G825 | G751 | G681 | C614 | G544 | A468 | C398 | U264 | U264 | U189  |
| C1140 | U1077 | C1020  | U959 | C893 | C826 | U752 | A684 | C615 | C545 | G474 | C399 | G265 | G265 | G190  |
| U1141 | U1078 | U1021  | U960 | G894 | U827 | G753 | U685 | G616 | A547 | G475 | C403 | C267 | C267 | G191A |
| C1142 | G1079 | G1022  | U961 | G895 | A828 | A754 | U686 | G617 | G550 | G476 | G406 | G268 | G268 | G191B |
| U1143 | U1080 | U1023  | U962 | G896 | G829 | C755 | A687 | C618 | U551 | A478 | G407 | U269 | U269 | G191C |
| G1144 | U1081 | G1024  | C962 | C897 | G830 | G756 | G688 | U619 | U552 | A486 | A412 | C269 | C269 | U191D |
| C1145 | U1082 | U1025  | G963 | C898 | G831 | C757 | G689 | C620 | C553 | U486 | G413 | A270 | A270 | G191E |
| U1146 | U1083 | G1026  | A964 | G906 | U832 | U757 | G690 | A621 | C554 | U487 | A414 | G347 | G347 | U191F |
| C1147 | G1084 | C1027  | G965 | A907 | G833 | G758 | G691 | A622 | C555 | G491 | A415 | C271 | C271 | G191G |
| U1148 | U1085 | U1028  | C966 | U908 | U834 | A759 | G692 | G628 | U560 | G492 | A416 | A273 | A273 | U191H |
| C1149 | U1086 | C1028A | C967 | A909 | C842 | A768 | U697 | G629 | U561 | G493 | C417 | A274 | A274 | G191I |
| U1150 | U1087 | A968   | A968 | U905 | U843 | A769 | G698 | G630 | C562 | U494 | C418 | G278 | G278 | C194  |
| C1151 | G1088 | G1029  | U969 | U906 | C848 | U772 | C699 | G631 | C563 | U495 | C419 | A279 | A279 | U195  |
| U1152 | U1089 | C1030  | G970 | G907 | C849 | G773 | G700 | A632 | A564 | U496 | U420 | C280 | C280 | A196  |
| A1153 | C1090 | G1031  | G971 | A908 | U850 | G774 | G701 | A633 | U565 | U497 | U421 | G281 | G281 | A197  |
| C1154 | U1091 | A1032  | C972 | U908 | G851 | G775 | A702 | A634 | G566 | G498 | C422 | A282 | A282 | G198  |
| G1155 | U1092 | U1032A | G973 | A909 | G852 | A776 | G703 | C634 | G567 | G500 | G423 | G283 | G283 | U199  |
| C1156 | A1093 | G1032B | A974 | U910 | U843 | A780 | U705 | U635 | G570 | G501 | G424 | C284 | C284 | G200  |
| U1157 | G1094 | U1033  | A975 | C912 | C848 | U777 | U706 | U636 |      |      |      |      |      | G201  |
| C1158 | U1095 | G1034  | G976 | C913 | C849 | G778 | G704 | U637 |      |      |      |      |      |       |
| U1159 | C1096 | A1035  | A977 | A914 | U851 | G779 | A702 | A635 |      |      |      |      |      |       |
| C1160 | U1097 | G1036  | G978 | A915 | G853 | G776 | G705 | A636 |      |      |      |      |      |       |
| U1161 | C1098 | C1037  | C979 | A919 | G854 | A777 | U706 | U636 |      |      |      |      |      |       |
| C1162 | G1099 | U1038  | U980 | U921 | G855 | A780 | U705 | U636 |      |      |      |      |      |       |
|       | C1100 | U1039  | U981 |      | G855 |      |      |      |      |      |      |      |      |       |
|       | A1101 | U1040  | U982 |      | G855 |      |      |      |      |      |      |      |      |       |



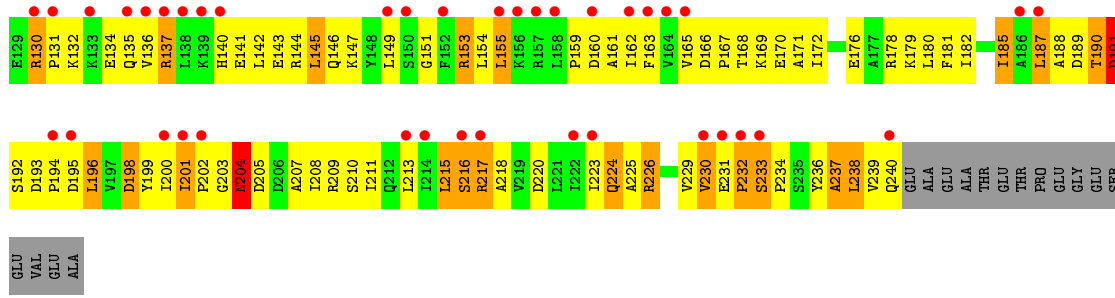
• Molecule 32: 30S RIBOSOMAL PROTEIN S2



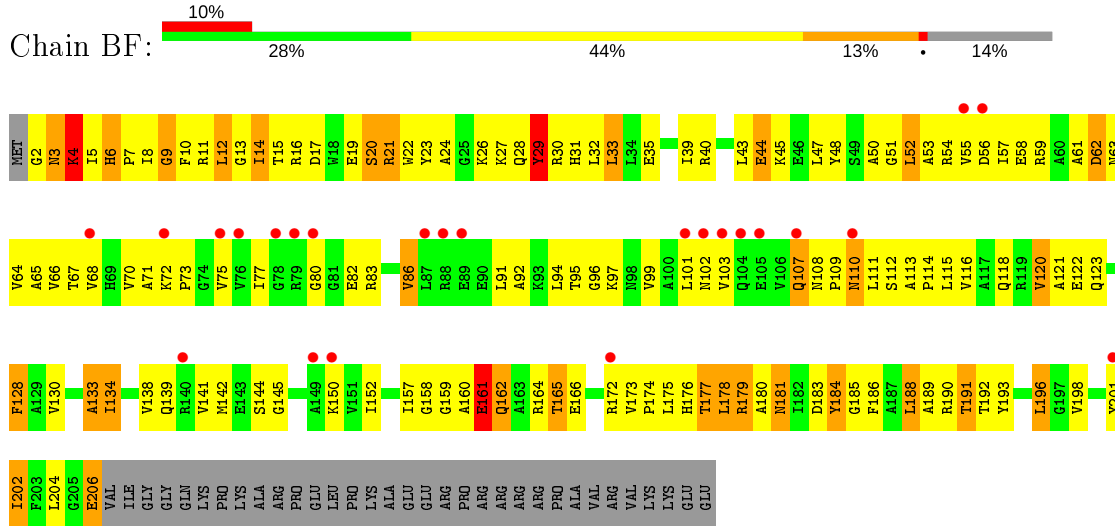
• Molecule 32: 30S RIBOSOMAL PROTEIN S2



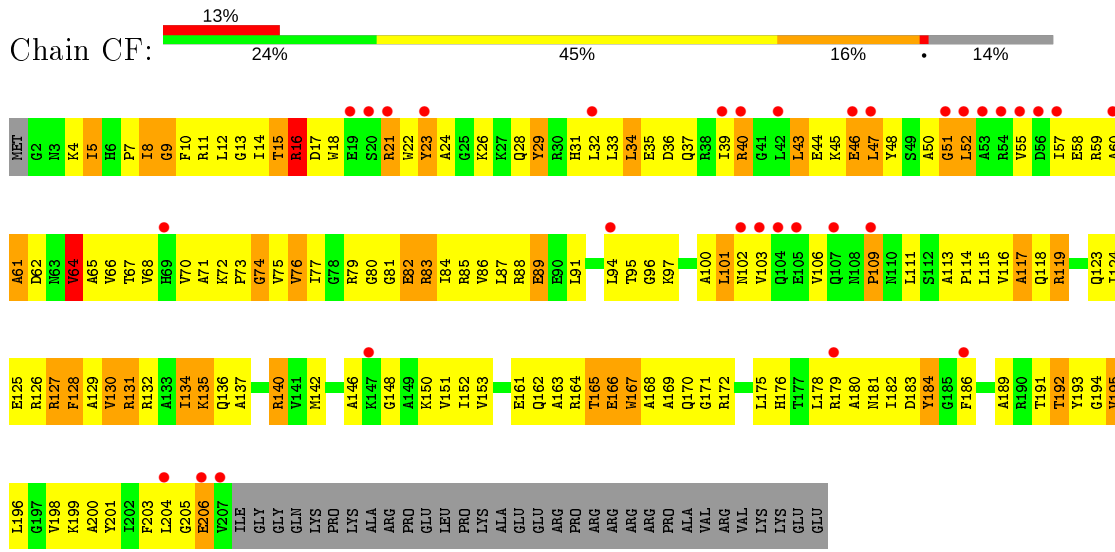




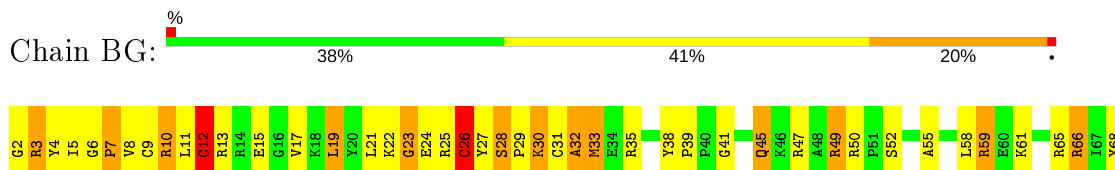
• Molecule 33: 30S RIBOSOMAL PROTEIN S3

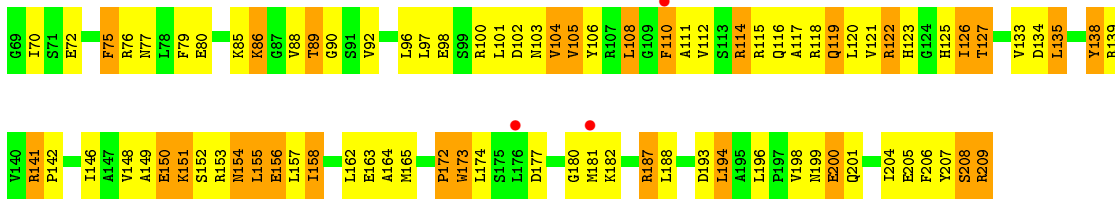


• Molecule 33: 30S RIBOSOMAL PROTEIN S3

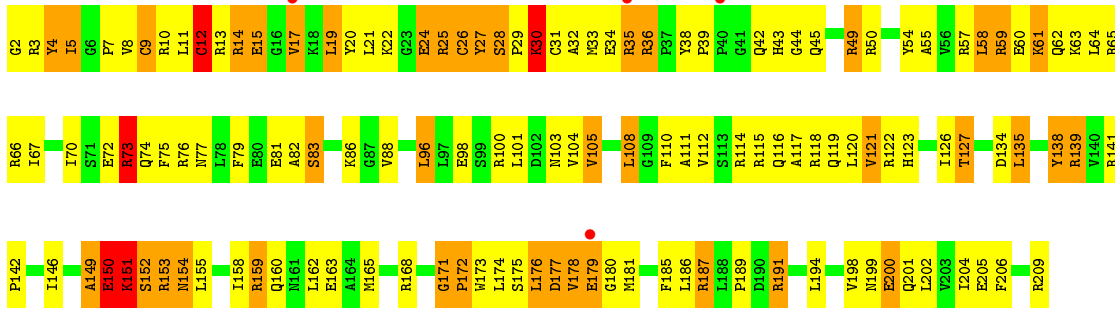


• Molecule 34: 30S RIBOSOMAL PROTEIN S4

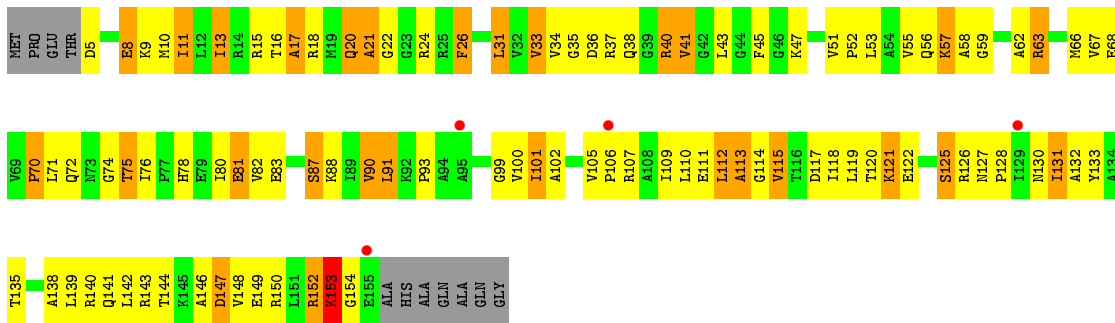




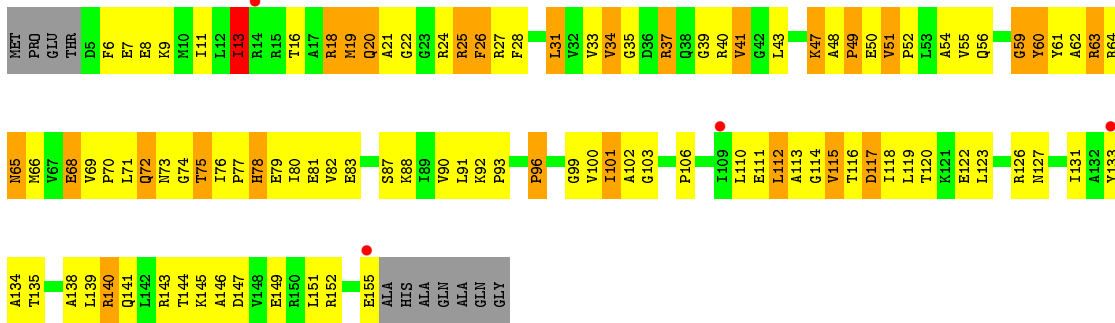
• Molecule 34: 30S RIBOSOMAL PROTEIN S4



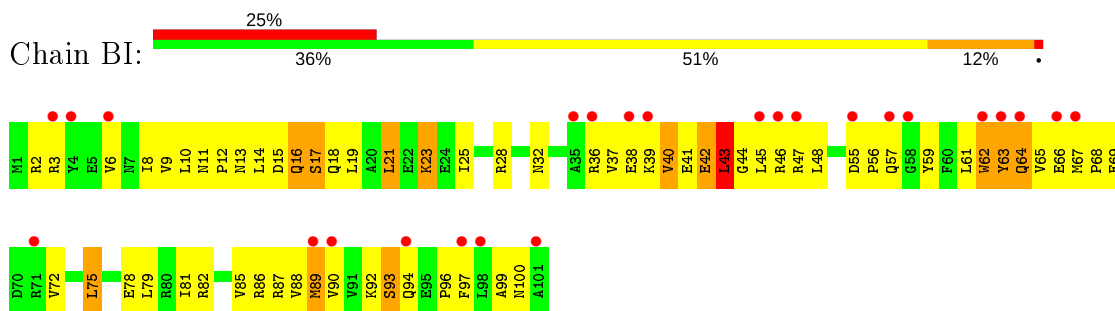
• Molecule 35: 30S RIBOSOMAL PROTEIN S5



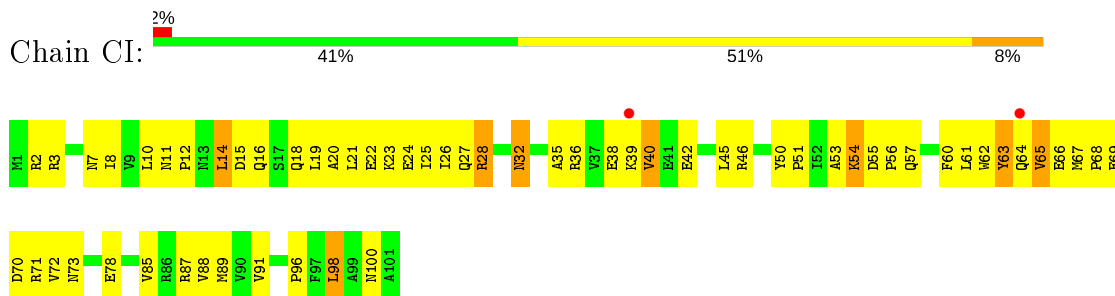
• Molecule 35: 30S RIBOSOMAL PROTEIN S5



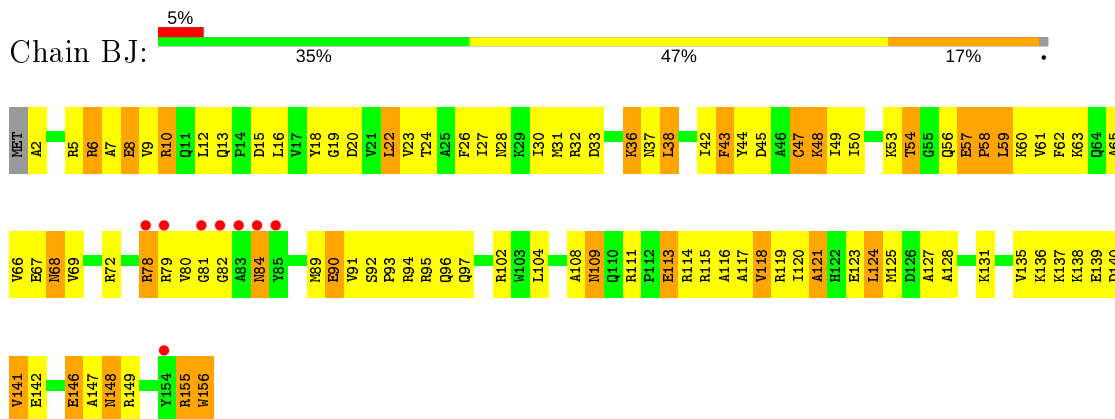
• Molecule 36: 30S RIBOSOMAL PROTEIN S6



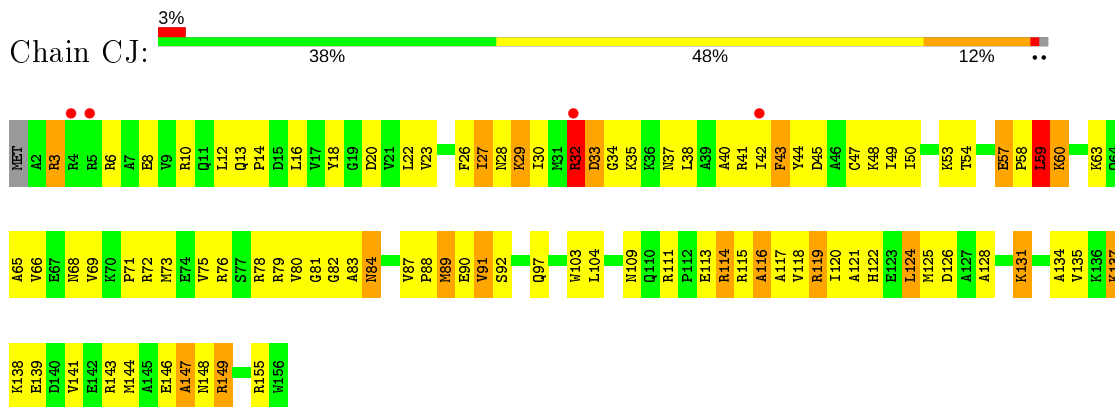
• Molecule 36: 30S RIBOSOMAL PROTEIN S6



• Molecule 37: 30S RIBOSOMAL PROTEIN S7

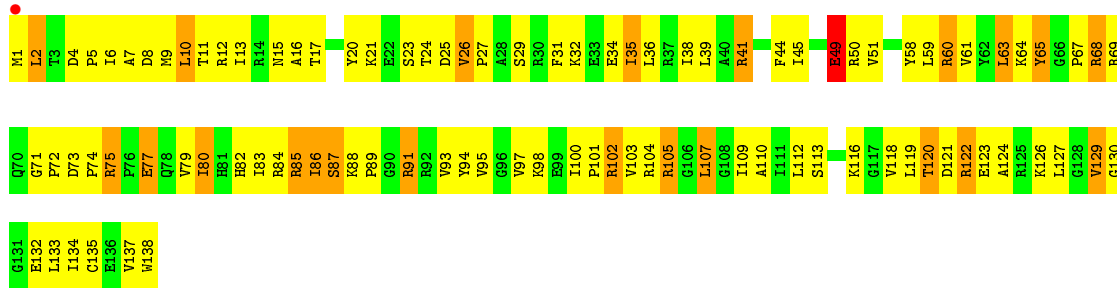


• Molecule 37: 30S RIBOSOMAL PROTEIN S7



• Molecule 38: 30S RIBOSOMAL PROTEIN S8

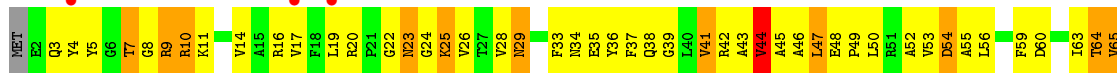




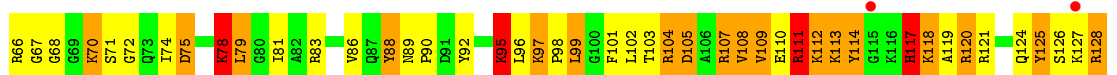
• Molecule 38: 30S RIBOSOMAL PROTEIN S8



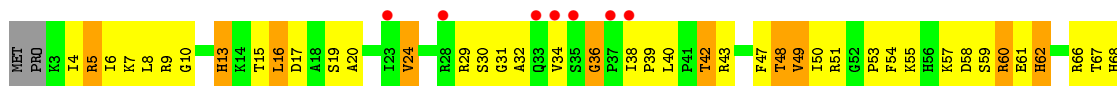
• Molecule 39: 30S RIBOSOMAL PROTEIN S9

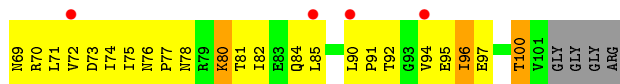


• Molecule 39: 30S RIBOSOMAL PROTEIN S9

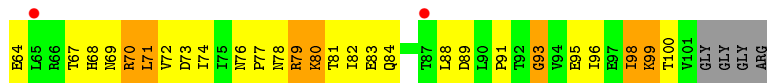


• Molecule 40: 30S RIBOSOMAL PROTEIN S10

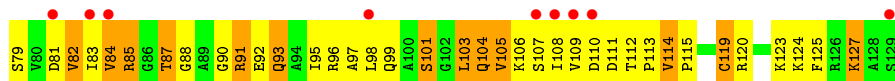
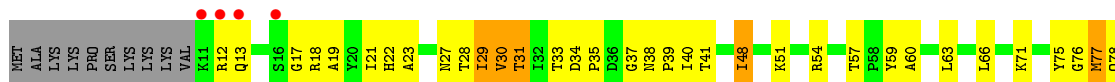
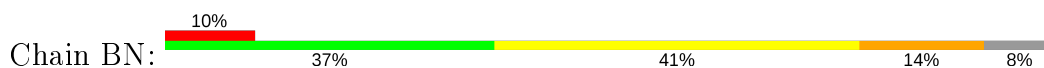




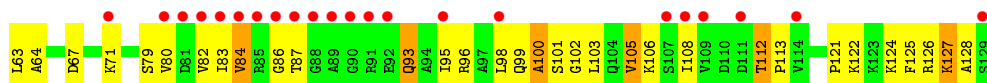
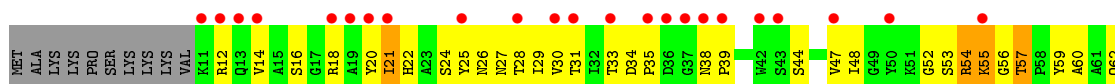
- Molecule 40: 30S RIBOSOMAL PROTEIN S10



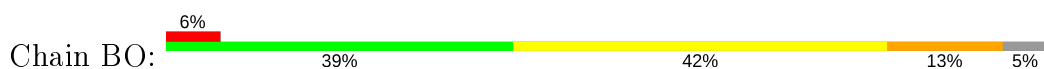
- Molecule 41: 30S RIBOSOMAL PROTEIN S11



- Molecule 41: 30S RIBOSOMAL PROTEIN S11

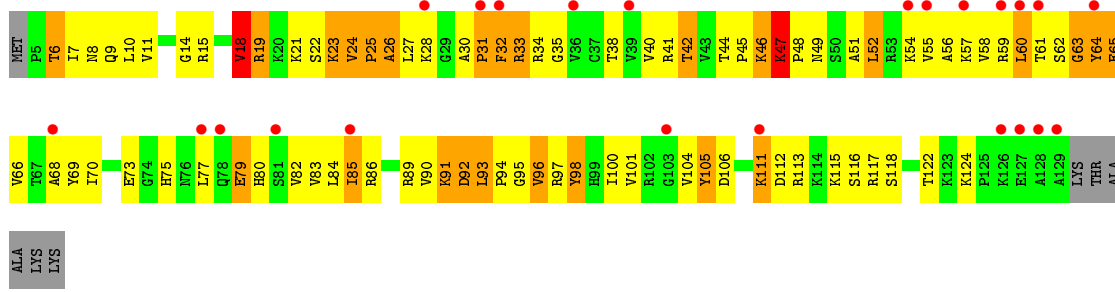


- Molecule 42: 30S RIBOSOMAL PROTEIN S12

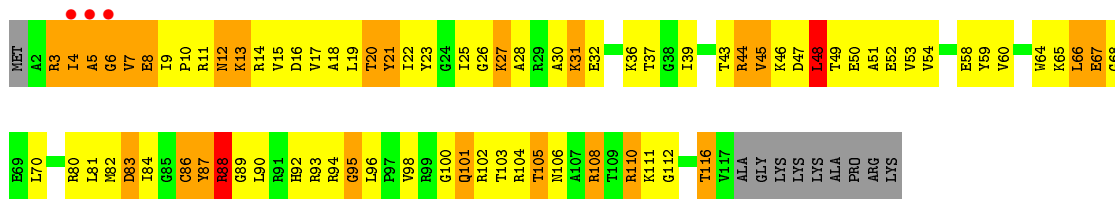


- Molecule 42: 30S RIBOSOMAL PROTEIN S12

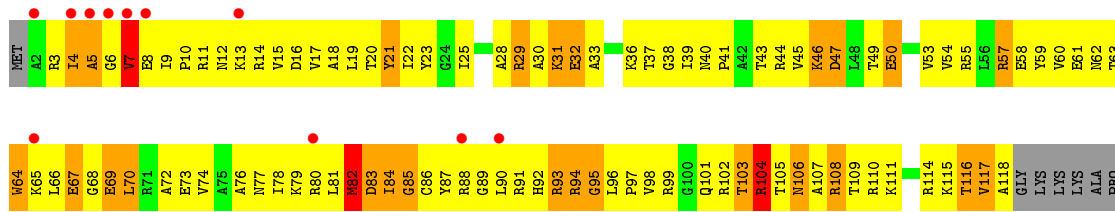
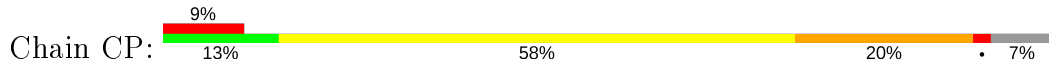




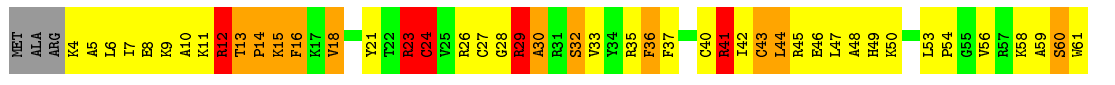
• Molecule 43: 30S RIBOSOMAL PROTEIN S13



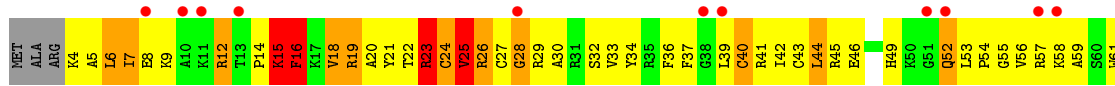
• Molecule 43: 30S RIBOSOMAL PROTEIN S13



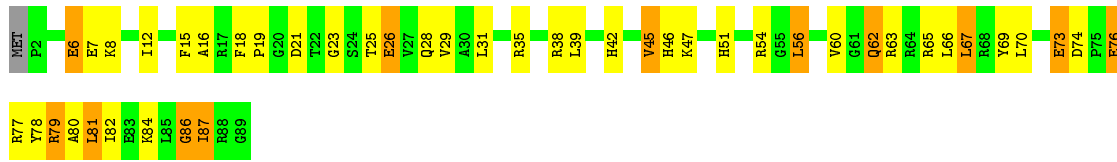
• Molecule 44: 30S RIBOSOMAL PROTEIN S14



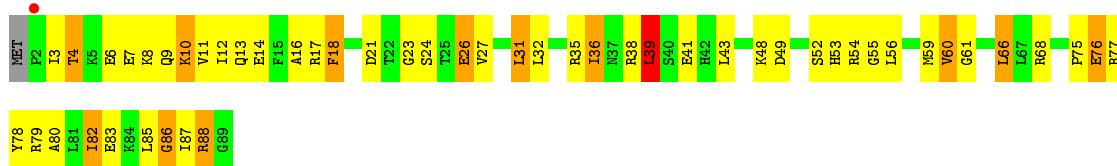
• Molecule 44: 30S RIBOSOMAL PROTEIN S14



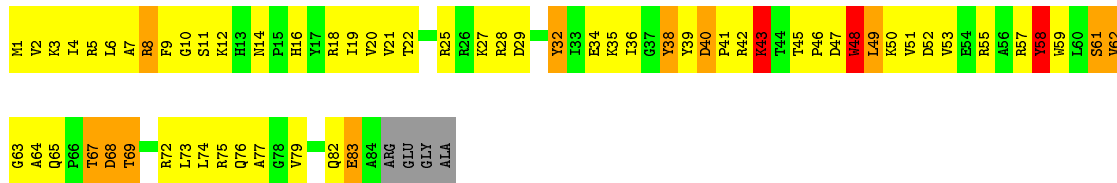
• Molecule 45: 30S RIBOSOMAL PROTEIN S15



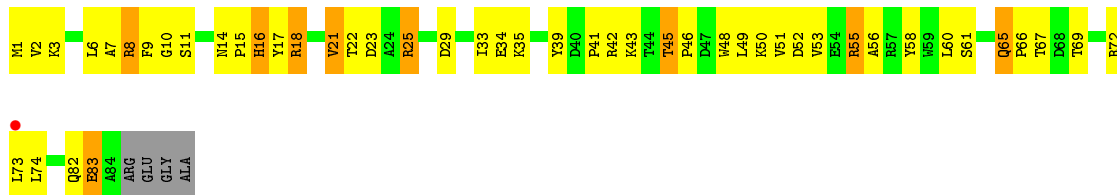
• Molecule 45: 30S RIBOSOMAL PROTEIN S15



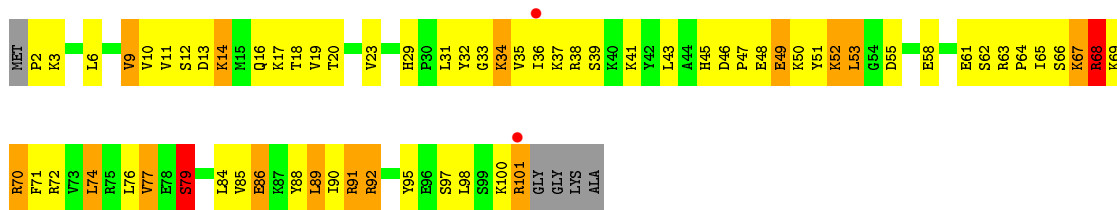
• Molecule 46: 30S RIBOSOMAL PROTEIN S16



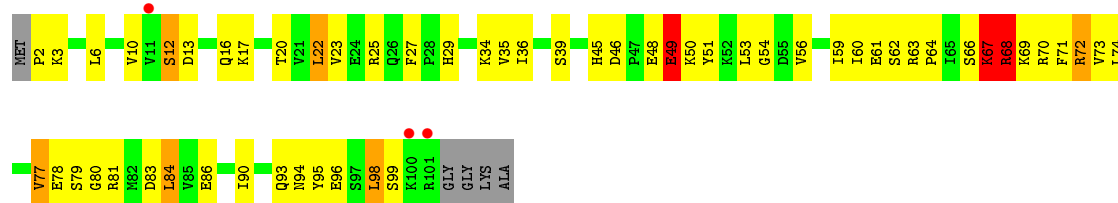
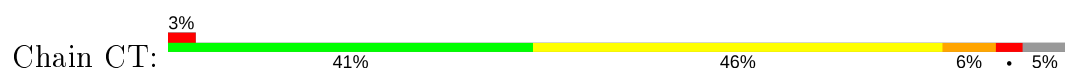
• Molecule 46: 30S RIBOSOMAL PROTEIN S16



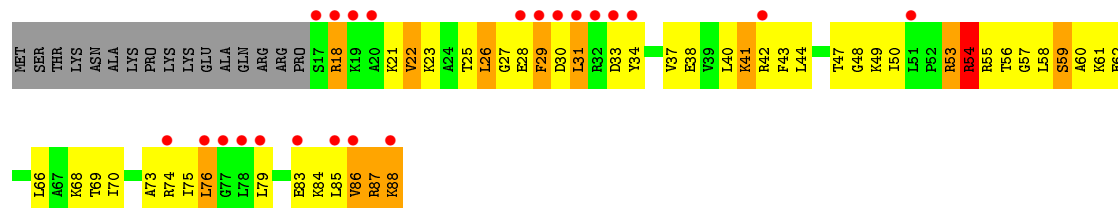
• Molecule 47: 30S RIBOSOMAL PROTEIN S17



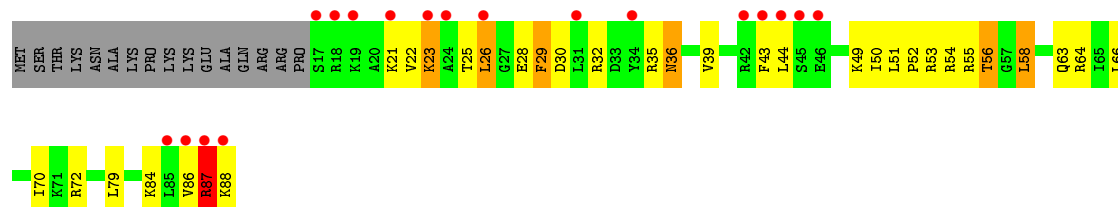
• Molecule 47: 30S RIBOSOMAL PROTEIN S17



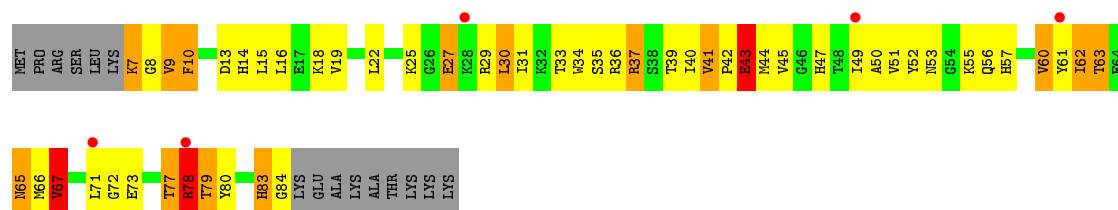
- Molecule 48: 30S RIBOSOMAL PROTEIN S18



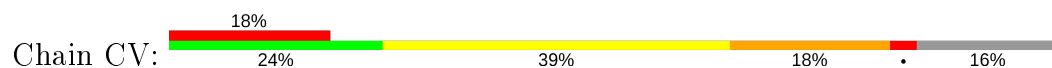
- Molecule 48: 30S RIBOSOMAL PROTEIN S18



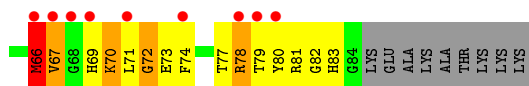
- Molecule 49: 30S RIBOSOMAL PROTEIN S19



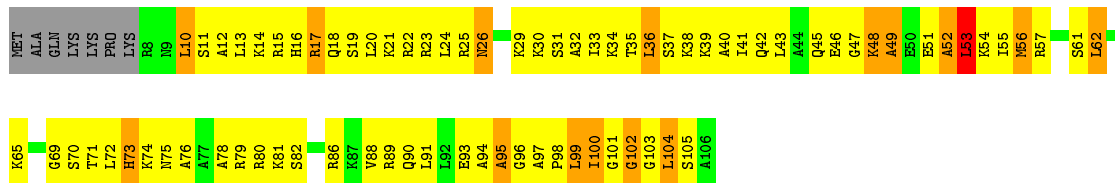
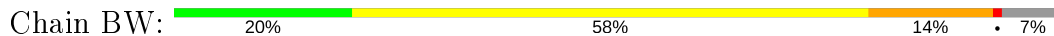
- Molecule 49: 30S RIBOSOMAL PROTEIN S19



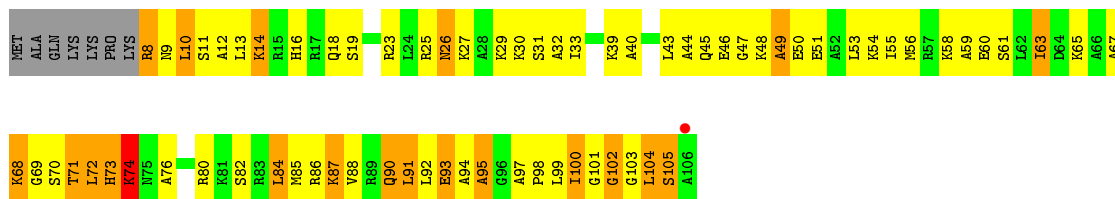




• Molecule 50: 30S RIBOSOMAL PROTEIN S20



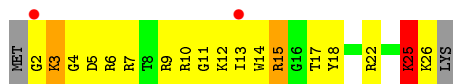
• Molecule 50: 30S RIBOSOMAL PROTEIN S20



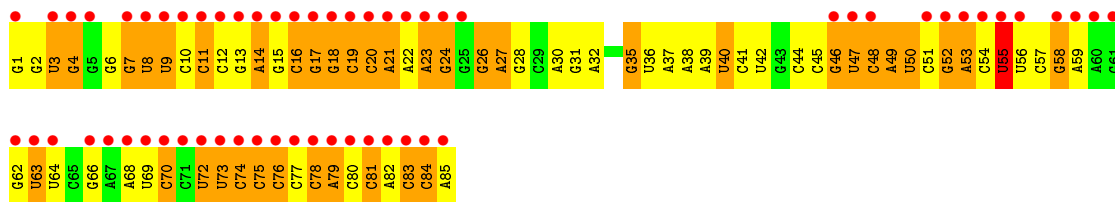
• Molecule 51: 30S RIBOSOMAL PROTEIN THX



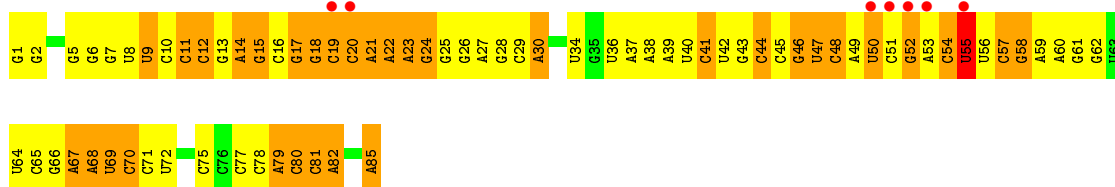
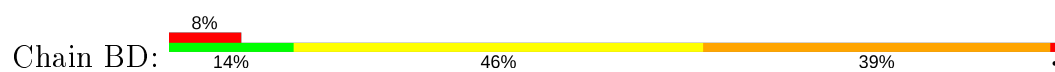
• Molecule 51: 30S RIBOSOMAL PROTEIN THX



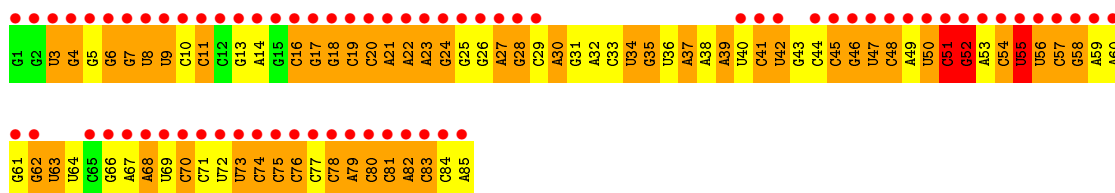
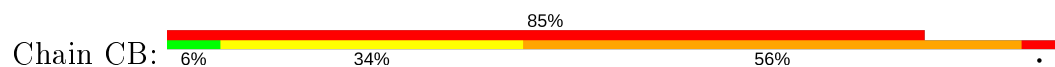
• Molecule 52: TRNA-TYR



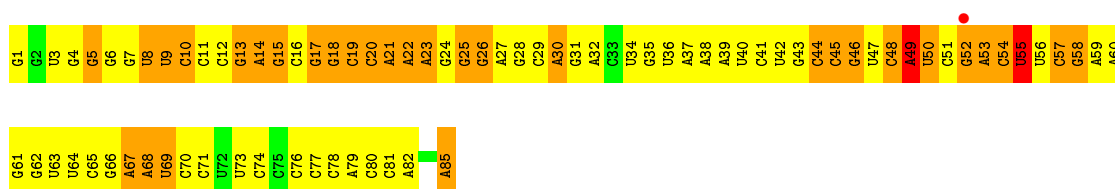
• Molecule 52: TRNA-TYR



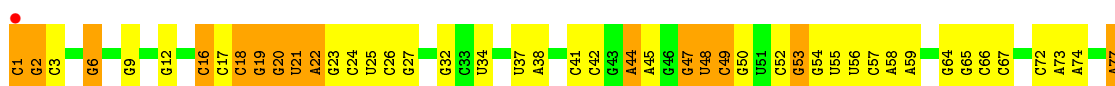
- Molecule 52: TRNA-TYR



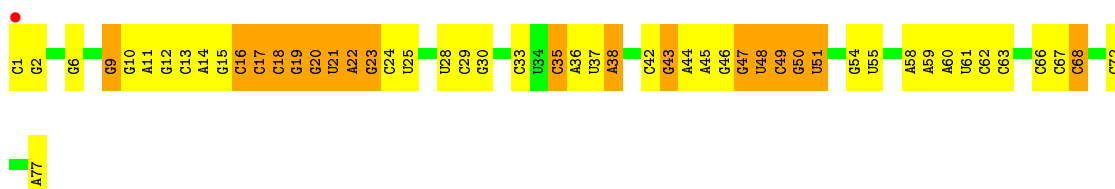
- Molecule 52: TRNA-TYR



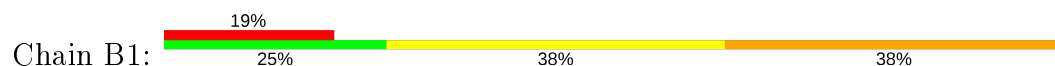
- Molecule 53: TRNA-FMET

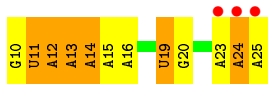


- Molecule 53: TRNA-FMET



- Molecule 54: MRNA





- Molecule 54: MRNA



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 210.00Å 450.33Å 622.86Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 152.64 – 3.30<br>152.64 – 3.00                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.8 (152.64-3.30)<br>89.2 (152.64-3.00)                    | Depositor<br>EDS |
| $R_{merge}$   | 0.41  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 0.57 (at 3.01Å)   | Xtrriage         |
| Refinement program  | PHENIX 1.7.1_743  | Depositor        |
| R, $R_{free}$   | 0.196 , 0.247<br>0.197 , 0.244                              | Depositor<br>DCC |
| $R_{free}$ test set   | 2000 reflections (0.17%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 76.1  | Xtrriage         |
| Anisotropy  | 0.204   | Xtrriage         |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.26 , 80.6   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$ | Xtrriage         |
| Estimated twinning fraction   | No twinning to report.                                      | Xtrriage         |
| $F_o, F_c$ correlation  | 0.94  | EDS              |
| Total number of atoms   | 304031  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 112.0   | wwPDB-VP         |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.35% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MIA, ZN, MG, OHX, PAR

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   | AA    | 0.73         | 18/70233 (0.0%) | 1.21        | 496/109643 (0.5%) |
| 1   | DA    | 0.64         | 9/70122 (0.0%)  | 1.10        | 332/109469 (0.3%) |
| 2   | AB    | 0.60         | 0/2928          | 1.24        | 32/4568 (0.7%)    |
| 2   | DB    | 0.50         | 0/2928          | 1.03        | 7/4568 (0.2%)     |
| 3   | AD    | 0.56         | 0/2165          | 0.81        | 1/2919 (0.0%)     |
| 3   | DD    | 0.52         | 0/2165          | 0.75        | 0/2919            |
| 4   | AE    | 0.47         | 0/1601          | 0.72        | 0/2160            |
| 4   | DE    | 0.45         | 0/1601          | 0.67        | 0/2160            |
| 5   | AF    | 0.51         | 0/1620          | 0.71        | 0/2194            |
| 5   | DF    | 0.38         | 0/1662          | 0.65        | 0/2249            |
| 6   | AG    | 0.36         | 0/1499          | 0.60        | 0/2016            |
| 6   | DG    | 0.28         | 0/1499          | 0.52        | 0/2016            |
| 7   | AH    | 0.43         | 0/1332          | 0.66        | 0/1802            |
| 7   | DH    | 0.29         | 0/1332          | 0.53        | 0/1802            |
| 8   | AK    | 0.36         | 0/1151          | 0.63        | 0/1558            |
| 8   | DK    | 0.36         | 0/1151          | 0.63        | 0/1558            |
| 9   | AM    | 0.43         | 0/1131          | 0.66        | 0/1525            |
| 9   | DM    | 0.34         | 0/1131          | 0.58        | 0/1525            |
| 10  | AN    | 0.46         | 0/943           | 0.65        | 0/1269            |
| 10  | DN    | 0.42         | 0/943           | 0.63        | 1/1269 (0.1%)     |
| 11  | AO    | 0.44         | 0/1162          | 0.81        | 1/1544 (0.1%)     |
| 11  | DO    | 0.32         | 0/1162          | 0.57        | 1/1544 (0.1%)     |
| 12  | AP    | 0.45         | 0/1143          | 0.63        | 0/1527            |
| 12  | DP    | 0.33         | 0/1143          | 0.54        | 0/1527            |
| 13  | A0    | 0.42         | 0/982           | 0.67        | 0/1312            |
| 13  | D0    | 0.40         | 0/974           | 0.66        | 0/1302            |
| 14  | AQ    | 0.45         | 0/892           | 0.72        | 0/1187            |
| 14  | DQ    | 0.33         | 0/892           | 0.60        | 0/1187            |
| 15  | AR    | 0.46         | 0/1155          | 0.66        | 0/1542            |
| 15  | DR    | 0.41         | 0/1155          | 0.61        | 0/1542            |
| 16  | A1    | 0.47         | 0/982           | 0.72        | 0/1306            |
| 16  | D1    | 0.37         | 0/982           | 0.57        | 0/1306            |

| Mol | Chain | Bond lengths |               | Bond angles |                 |
|-----|-------|--------------|---------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5         |
| 17  | A2    | 0.41         | 0/790         | 0.71        | 1/1057 (0.1%)   |
| 17  | D2    | 0.32         | 0/790         | 0.60        | 1/1057 (0.1%)   |
| 18  | AS    | 0.46         | 0/911         | 0.68        | 0/1220          |
| 18  | DS    | 0.44         | 0/911         | 0.62        | 0/1220          |
| 19  | AT    | 0.60         | 1/739 (0.1%)  | 0.69        | 0/993           |
| 19  | DT    | 0.48         | 0/739         | 0.63        | 0/993           |
| 20  | AU    | 0.50         | 0/798         | 0.69        | 0/1064          |
| 20  | DU    | 0.42         | 0/798         | 0.65        | 0/1064          |
| 21  | AV    | 0.37         | 0/1427        | 0.62        | 1/1935 (0.1%)   |
| 21  | DV    | 0.29         | 0/1460        | 0.53        | 0/1982          |
| 22  | A3    | 0.49         | 0/615         | 0.72        | 0/819           |
| 22  | D3    | 0.41         | 0/621         | 0.66        | 0/827           |
| 23  | AZ    | 0.46         | 0/770         | 0.70        | 0/1022          |
| 23  | DZ    | 0.44         | 0/770         | 0.69        | 0/1022          |
| 24  | AW    | 0.52         | 0/560         | 0.75        | 1/741 (0.1%)    |
| 24  | DW    | 0.40         | 0/560         | 0.59        | 0/741           |
| 25  | AX    | 0.41         | 0/474         | 0.57        | 0/635           |
| 25  | DX    | 0.33         | 0/474         | 0.55        | 0/635           |
| 26  | A4    | 0.39         | 0/545         | 0.61        | 1/733 (0.1%)    |
| 26  | D4    | 0.34         | 0/527         | 0.62        | 0/709           |
| 27  | A5    | 0.44         | 0/473         | 0.65        | 0/639           |
| 27  | D5    | 0.41         | 0/473         | 0.65        | 0/639           |
| 28  | A6    | 0.48         | 0/396         | 0.64        | 0/529           |
| 28  | D6    | 0.45         | 0/396         | 0.67        | 0/529           |
| 29  | A7    | 0.57         | 0/399         | 0.76        | 0/526           |
| 29  | D7    | 0.50         | 0/399         | 0.69        | 0/526           |
| 30  | A8    | 0.55         | 0/486         | 0.81        | 0/638           |
| 30  | D8    | 0.42         | 0/486         | 0.65        | 1/638 (0.2%)    |
| 31  | BA    | 0.54         | 0/36139       | 1.02        | 97/56406 (0.2%) |
| 31  | CA    | 0.50         | 0/36142       | 0.96        | 59/56410 (0.1%) |
| 32  | BE    | 0.30         | 0/1959        | 0.53        | 0/2642          |
| 32  | CE    | 0.28         | 0/1959        | 0.52        | 0/2642          |
| 33  | BF    | 0.34         | 0/1629        | 0.53        | 0/2195          |
| 33  | CF    | 0.29         | 0/1636        | 0.51        | 0/2205          |
| 34  | BG    | 0.44         | 2/1733 (0.1%) | 0.60        | 1/2318 (0.0%)   |
| 34  | CG    | 0.38         | 0/1733        | 0.59        | 1/2318 (0.0%)   |
| 35  | BH    | 0.39         | 0/1171        | 0.60        | 0/1576          |
| 35  | CH    | 0.36         | 0/1171        | 0.58        | 0/1576          |
| 36  | BI    | 0.37         | 0/856         | 0.56        | 0/1154          |
| 36  | CI    | 0.36         | 0/856         | 0.56        | 0/1154          |
| 37  | BJ    | 0.33         | 0/1276        | 0.52        | 0/1709          |
| 37  | CJ    | 0.30         | 0/1276        | 0.50        | 0/1709          |
| 38  | BK    | 0.35         | 0/1136        | 0.60        | 0/1527          |

| Mol | Chain | Bond lengths |                  | Bond angles |                    |
|-----|-------|--------------|------------------|-------------|--------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5            |
| 38  | CK    | 0.30         | 0/1136           | 0.54        | 0/1527             |
| 39  | BL    | 0.29         | 0/1029           | 0.52        | 0/1379             |
| 39  | CL    | 0.30         | 0/1029           | 0.53        | 0/1379             |
| 40  | BM    | 0.32         | 0/814            | 0.57        | 0/1095             |
| 40  | CM    | 0.30         | 0/814            | 0.55        | 0/1095             |
| 41  | BN    | 0.35         | 0/900            | 0.58        | 0/1213             |
| 41  | CN    | 0.35         | 0/900            | 0.56        | 0/1213             |
| 42  | BO    | 0.46         | 0/991            | 0.71        | 0/1327             |
| 42  | CO    | 0.38         | 0/991            | 0.65        | 0/1327             |
| 43  | BP    | 0.35         | 0/938            | 0.59        | 0/1258             |
| 43  | CP    | 0.28         | 0/943            | 0.52        | 0/1265             |
| 44  | BQ    | 0.44         | 1/485 (0.2%)     | 0.67        | 1/643 (0.2%)       |
| 44  | CQ    | 0.31         | 0/485            | 0.55        | 0/643              |
| 45  | BR    | 0.38         | 0/745            | 0.61        | 0/992              |
| 45  | CR    | 0.36         | 0/745            | 0.56        | 1/992 (0.1%)       |
| 46  | BS    | 0.31         | 0/721            | 0.56        | 0/970              |
| 46  | CS    | 0.34         | 0/721            | 0.58        | 0/970              |
| 47  | BT    | 0.38         | 0/847            | 0.57        | 0/1131             |
| 47  | CT    | 0.35         | 0/847            | 0.53        | 0/1131             |
| 48  | BU    | 0.36         | 0/596            | 0.63        | 0/790              |
| 48  | CU    | 0.36         | 0/596            | 0.57        | 0/790              |
| 49  | BV    | 0.32         | 0/638            | 0.56        | 0/860              |
| 49  | CV    | 0.31         | 0/638            | 0.56        | 0/860              |
| 50  | BW    | 0.30         | 0/765            | 0.57        | 0/1007             |
| 50  | CW    | 0.33         | 0/765            | 0.58        | 0/1007             |
| 51  | BX    | 0.32         | 0/221            | 0.52        | 0/288              |
| 51  | CX    | 0.33         | 0/221            | 0.53        | 0/288              |
| 52  | BB    | 0.76         | 0/1992           | 0.98        | 2/3099 (0.1%)      |
| 52  | BD    | 0.65         | 0/1992           | 0.90        | 3/3099 (0.1%)      |
| 52  | CB    | 0.85         | 0/1992           | 0.94        | 6/3099 (0.2%)      |
| 52  | CD    | 0.67         | 0/1992           | 0.88        | 6/3099 (0.2%)      |
| 53  | BC    | 0.50         | 0/1835           | 0.94        | 6/2859 (0.2%)      |
| 53  | CC    | 0.46         | 0/1835           | 0.91        | 1/2859 (0.0%)      |
| 54  | B1    | 0.72         | 0/390            | 0.91        | 1/606 (0.2%)       |
| 54  | C1    | 0.71         | 0/390            | 0.89        | 0/606              |
| All | All   | 0.58         | 31/324159 (0.0%) | 0.99        | 1062/485455 (0.2%) |

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 |
|-----|-------|---------------------|---------------------|
| 3   | AD    | 0                   | 3                   |
| 3   | DD    | 0                   | 1                   |
| 4   | AE    | 0                   | 1                   |
| 5   | AF    | 0                   | 1                   |
| 5   | DF    | 0                   | 1                   |
| 7   | AH    | 0                   | 1                   |
| 8   | AK    | 0                   | 1                   |
| 8   | DK    | 0                   | 1                   |
| 11  | AO    | 0                   | 1                   |
| 11  | DO    | 0                   | 1                   |
| 24  | AW    | 0                   | 1                   |
| 30  | A8    | 0                   | 1                   |
| 30  | D8    | 0                   | 1                   |
| 42  | BO    | 0                   | 1                   |
| All | All   | 0                   | 16                  |

The worst 5 of 31 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | AA    | 774  | A    | N9-C4 | -9.44 | 1.32        | 1.37     |
| 1   | DA    | 1342 | A    | N7-C5 | -8.92 | 1.33        | 1.39     |
| 1   | DA    | 783  | A    | N9-C4 | -8.89 | 1.32        | 1.37     |
| 1   | DA    | 2873 | A    | N7-C5 | -8.61 | 1.34        | 1.39     |
| 34  | BG    | 12   | CYS  | CB-SG | 7.57  | 1.95        | 1.82     |

The worst 5 of 1062 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1   | DA    | 1899 | G    | N3-C4-N9 | -16.88 | 115.87      | 126.00   |
| 1   | AA    | 1899 | G    | N3-C4-N9 | -14.54 | 117.28      | 126.00   |
| 1   | AA    | 774  | A    | C2-N3-C4 | -14.31 | 103.44      | 110.60   |
| 2   | AB    | 81   | G    | C6-C5-N7 | -14.19 | 121.89      | 130.40   |
| 1   | AA    | 783  | A    | C5-N7-C8 | -13.92 | 96.94       | 103.90   |

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 3   | AD    | 197 | GLY  | Peptide |
| 3   | AD    | 27  | THR  | Peptide |
| 3   | AD    | 47  | GLY  | Peptide |
| 4   | AE    | 20  | ALA  | Peptide |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 5   | AF    | 47  | GLY  | Peptide |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | AA    | 62707 | 0        | 31614    | 2894    | 0            |
| 1   | DA    | 62607 | 0        | 31564    | 2901    | 0            |
| 2   | AB    | 2617  | 0        | 1328     | 138     | 0            |
| 2   | DB    | 2617  | 0        | 1328     | 161     | 0            |
| 3   | AD    | 2115  | 0        | 2195     | 271     | 0            |
| 3   | DD    | 2115  | 0        | 2195     | 239     | 0            |
| 4   | AE    | 1568  | 0        | 1634     | 208     | 0            |
| 4   | DE    | 1568  | 0        | 1634     | 214     | 0            |
| 5   | AF    | 1585  | 0        | 1632     | 178     | 0            |
| 5   | DF    | 1627  | 0        | 1680     | 236     | 0            |
| 6   | AG    | 1474  | 0        | 1535     | 158     | 0            |
| 6   | DG    | 1474  | 0        | 1535     | 164     | 0            |
| 7   | AH    | 1307  | 0        | 1382     | 173     | 0            |
| 7   | DH    | 1307  | 0        | 1382     | 136     | 1            |
| 8   | AK    | 1136  | 0        | 1223     | 123     | 0            |
| 8   | DK    | 1136  | 0        | 1223     | 107     | 0            |
| 9   | AM    | 1104  | 0        | 1180     | 134     | 0            |
| 9   | DM    | 1104  | 0        | 1180     | 145     | 0            |
| 10  | AN    | 933   | 0        | 996      | 64      | 0            |
| 10  | DN    | 933   | 0        | 996      | 75      | 0            |
| 11  | AO    | 1145  | 0        | 1228     | 239     | 0            |
| 11  | DO    | 1145  | 0        | 1227     | 311     | 0            |
| 12  | AP    | 1122  | 0        | 1179     | 189     | 0            |
| 12  | DP    | 1122  | 0        | 1179     | 188     | 0            |
| 13  | A0    | 968   | 0        | 1033     | 129     | 0            |
| 13  | D0    | 960   | 0        | 1021     | 94      | 0            |
| 14  | AQ    | 882   | 0        | 943      | 123     | 0            |
| 14  | DQ    | 882   | 0        | 943      | 137     | 0            |
| 15  | AR    | 1141  | 0        | 1202     | 115     | 0            |
| 15  | DR    | 1141  | 0        | 1202     | 128     | 0            |
| 16  | A1    | 964   | 0        | 1022     | 120     | 0            |
| 16  | D1    | 964   | 0        | 1019     | 158     | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 17  | A2    | 779   | 0        | 852      | 101     | 0            |
| 17  | D2    | 779   | 0        | 852      | 135     | 0            |
| 18  | AS    | 900   | 0        | 964      | 95      | 0            |
| 18  | DS    | 900   | 0        | 964      | 72      | 0            |
| 19  | AT    | 725   | 0        | 778      | 65      | 0            |
| 19  | DT    | 725   | 0        | 778      | 99      | 0            |
| 20  | AU    | 785   | 0        | 878      | 101     | 0            |
| 20  | DU    | 785   | 0        | 878      | 133     | 0            |
| 21  | AV    | 1397  | 0        | 1430     | 168     | 0            |
| 21  | DV    | 1428  | 0        | 1454     | 184     | 0            |
| 22  | A3    | 607   | 0        | 628      | 63      | 0            |
| 22  | D3    | 613   | 0        | 633      | 68      | 0            |
| 23  | AZ    | 763   | 0        | 848      | 71      | 0            |
| 23  | DZ    | 763   | 0        | 848      | 53      | 0            |
| 24  | AW    | 558   | 0        | 610      | 39      | 0            |
| 24  | DW    | 558   | 0        | 610      | 55      | 0            |
| 25  | AX    | 469   | 0        | 518      | 37      | 0            |
| 25  | DX    | 469   | 0        | 518      | 39      | 0            |
| 26  | A4    | 533   | 0        | 522      | 88      | 0            |
| 26  | D4    | 515   | 0        | 510      | 90      | 0            |
| 27  | A5    | 459   | 0        | 480      | 87      | 0            |
| 27  | D5    | 459   | 0        | 478      | 52      | 0            |
| 28  | A6    | 389   | 0        | 404      | 56      | 0            |
| 28  | D6    | 389   | 0        | 404      | 64      | 0            |
| 29  | A7    | 391   | 0        | 432      | 41      | 0            |
| 29  | D7    | 391   | 0        | 432      | 37      | 0            |
| 30  | A8    | 480   | 0        | 549      | 131     | 0            |
| 30  | D8    | 480   | 0        | 549      | 130     | 0            |
| 31  | BA    | 32284 | 0        | 16296    | 1832    | 1            |
| 31  | CA    | 32287 | 0        | 16295    | 1769    | 0            |
| 32  | BE    | 1924  | 0        | 1975     | 195     | 0            |
| 32  | CE    | 1924  | 0        | 1975     | 225     | 0            |
| 33  | BF    | 1605  | 0        | 1668     | 134     | 0            |
| 33  | CF    | 1612  | 0        | 1677     | 179     | 0            |
| 34  | BG    | 1703  | 0        | 1763     | 175     | 0            |
| 34  | CG    | 1703  | 0        | 1763     | 186     | 0            |
| 35  | BH    | 1155  | 0        | 1213     | 115     | 0            |
| 35  | CH    | 1155  | 0        | 1213     | 116     | 0            |
| 36  | BI    | 843   | 0        | 857      | 70      | 0            |
| 36  | CI    | 843   | 0        | 857      | 53      | 0            |
| 37  | BJ    | 1257  | 0        | 1296     | 107     | 0            |
| 37  | CJ    | 1257  | 0        | 1296     | 106     | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 38  | BK    | 1116  | 0        | 1177     | 113     | 0            |
| 38  | CK    | 1116  | 0        | 1177     | 79      | 0            |
| 39  | BL    | 1010  | 0        | 1037     | 110     | 0            |
| 39  | CL    | 1010  | 0        | 1037     | 156     | 0            |
| 40  | BM    | 801   | 0        | 849      | 94      | 0            |
| 40  | CM    | 801   | 0        | 849      | 130     | 0            |
| 41  | BN    | 885   | 0        | 904      | 65      | 0            |
| 41  | CN    | 885   | 0        | 904      | 71      | 0            |
| 42  | BO    | 975   | 0        | 1062     | 65      | 0            |
| 42  | CO    | 975   | 0        | 1062     | 123     | 0            |
| 43  | BP    | 928   | 0        | 987      | 106     | 0            |
| 43  | CP    | 933   | 0        | 992      | 134     | 0            |
| 44  | BQ    | 476   | 0        | 511      | 58      | 0            |
| 44  | CQ    | 476   | 0        | 512      | 79      | 0            |
| 45  | BR    | 734   | 0        | 771      | 47      | 0            |
| 45  | CR    | 734   | 0        | 771      | 51      | 0            |
| 46  | BS    | 705   | 0        | 725      | 77      | 0            |
| 46  | CS    | 705   | 0        | 725      | 52      | 0            |
| 47  | BT    | 834   | 0        | 904      | 84      | 0            |
| 47  | CT    | 834   | 0        | 904      | 58      | 0            |
| 48  | BU    | 591   | 0        | 662      | 61      | 0            |
| 48  | CU    | 591   | 0        | 662      | 38      | 0            |
| 49  | BV    | 624   | 0        | 636      | 72      | 0            |
| 49  | CV    | 624   | 0        | 636      | 83      | 0            |
| 50  | BW    | 763   | 0        | 861      | 97      | 0            |
| 50  | CW    | 763   | 0        | 861      | 82      | 0            |
| 51  | BX    | 217   | 0        | 234      | 16      | 0            |
| 51  | CX    | 217   | 0        | 234      | 22      | 0            |
| 52  | BB    | 1814  | 0        | 931      | 140     | 0            |
| 52  | BD    | 1814  | 0        | 932      | 148     | 0            |
| 52  | CB    | 1814  | 0        | 931      | 149     | 0            |
| 52  | CD    | 1814  | 0        | 932      | 156     | 0            |
| 53  | BC    | 1643  | 0        | 837      | 55      | 0            |
| 53  | CC    | 1643  | 0        | 837      | 79      | 0            |
| 54  | B1    | 347   | 0        | 174      | 20      | 0            |
| 54  | C1    | 347   | 0        | 174      | 48      | 0            |
| 55  | A0    | 1     | 0        | 0        | 0       | 0            |
| 55  | A1    | 2     | 0        | 0        | 0       | 0            |
| 55  | A3    | 1     | 0        | 0        | 0       | 0            |
| 55  | A5    | 1     | 0        | 0        | 0       | 0            |
| 55  | A7    | 1     | 0        | 0        | 0       | 0            |
| 55  | AA    | 332   | 0        | 0        | 0       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 55  | AB    | 6     | 0        | 0        | 0       | 0            |
| 55  | AE    | 3     | 0        | 0        | 0       | 0            |
| 55  | AF    | 2     | 0        | 0        | 0       | 0            |
| 55  | AO    | 1     | 0        | 0        | 0       | 0            |
| 55  | B1    | 1     | 0        | 0        | 0       | 0            |
| 55  | BA    | 114   | 0        | 0        | 0       | 0            |
| 55  | BB    | 13    | 0        | 0        | 0       | 0            |
| 55  | BC    | 4     | 0        | 0        | 0       | 0            |
| 55  | BD    | 1     | 0        | 0        | 0       | 0            |
| 55  | BF    | 1     | 0        | 0        | 0       | 0            |
| 55  | BS    | 1     | 0        | 0        | 0       | 0            |
| 55  | BW    | 1     | 0        | 0        | 0       | 0            |
| 55  | C1    | 2     | 0        | 0        | 0       | 0            |
| 55  | CA    | 121   | 0        | 0        | 0       | 0            |
| 55  | CB    | 3     | 0        | 0        | 0       | 0            |
| 55  | CC    | 7     | 0        | 0        | 0       | 0            |
| 55  | CN    | 1     | 0        | 0        | 0       | 0            |
| 55  | D0    | 1     | 0        | 0        | 0       | 0            |
| 55  | D5    | 1     | 0        | 0        | 0       | 0            |
| 55  | D7    | 1     | 0        | 0        | 0       | 0            |
| 55  | DA    | 272   | 0        | 0        | 0       | 0            |
| 55  | DB    | 7     | 0        | 0        | 0       | 0            |
| 55  | DE    | 1     | 0        | 0        | 0       | 0            |
| 56  | A1    | 14    | 0        | 0        | 0       | 0            |
| 56  | A3    | 7     | 0        | 0        | 1       | 0            |
| 56  | A6    | 7     | 0        | 0        | 1       | 0            |
| 56  | AA    | 1659  | 0        | 0        | 140     | 0            |
| 56  | AB    | 91    | 0        | 0        | 6       | 0            |
| 56  | AE    | 7     | 0        | 0        | 0       | 0            |
| 56  | AF    | 7     | 0        | 0        | 3       | 0            |
| 56  | AO    | 14    | 0        | 0        | 2       | 0            |
| 56  | AW    | 7     | 0        | 0        | 0       | 0            |
| 56  | BA    | 693   | 0        | 0        | 66      | 0            |
| 56  | BB    | 14    | 0        | 0        | 0       | 0            |
| 56  | BC    | 21    | 0        | 0        | 2       | 0            |
| 56  | BD    | 21    | 0        | 0        | 1       | 0            |
| 56  | BG    | 7     | 0        | 0        | 2       | 0            |
| 56  | BL    | 7     | 0        | 0        | 0       | 0            |
| 56  | BR    | 7     | 0        | 0        | 0       | 0            |
| 56  | CA    | 651   | 0        | 0        | 83      | 0            |
| 56  | CB    | 21    | 0        | 0        | 2       | 0            |
| 56  | CC    | 21    | 0        | 0        | 7       | 0            |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 56  | CD    | 7      | 0        | 0        | 1       | 0            |
| 56  | CK    | 7      | 0        | 0        | 1       | 0            |
| 56  | CR    | 7      | 0        | 0        | 0       | 0            |
| 56  | CV    | 7      | 0        | 0        | 1       | 0            |
| 56  | D1    | 7      | 0        | 0        | 0       | 0            |
| 56  | D3    | 7      | 0        | 0        | 1       | 0            |
| 56  | D5    | 7      | 0        | 0        | 1       | 0            |
| 56  | D8    | 7      | 0        | 0        | 5       | 0            |
| 56  | DA    | 1533   | 0        | 0        | 128     | 0            |
| 56  | DB    | 91     | 0        | 0        | 6       | 0            |
| 56  | DF    | 7      | 0        | 0        | 1       | 0            |
| 56  | DO    | 7      | 0        | 0        | 0       | 0            |
| 57  | BA    | 42     | 0        | 45       | 3       | 0            |
| 57  | CA    | 42     | 0        | 45       | 1       | 0            |
| 58  | BG    | 1      | 0        | 0        | 0       | 0            |
| 58  | BQ    | 1      | 0        | 0        | 0       | 0            |
| 58  | CG    | 1      | 0        | 0        | 0       | 0            |
| 58  | CQ    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 304031 | 0        | 201063   | 19321   | 1            |

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 38.

The worst 5 of 19321 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) |
|------------------|------------------|--------------------------|-------------------|
| 11:DO:71:VAL:CG1 | 11:DO:72:PRO:HD3 | 1.34                     | 1.57              |
| 30:A8:34:TRP:CB  | 30:A8:35:GLN:HB2 | 1.34                     | 1.53              |
| 20:DU:89:PHE:CE1 | 20:DU:90:LEU:HG  | 1.40                     | 1.50              |
| 9:DM:17:ASP:HA   | 9:DM:55:VAL:CG2  | 1.36                     | 1.49              |
| 27:D5:4:HIS:HB3  | 27:D5:5:PRO:CD   | 1.40                     | 1.48              |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1         | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------------|--------------------------|-------------------|
| 31:BA:85:U:O2' | 7:DH:100:GLY:O[3_555] | 1.86                     | 0.34              |

## 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 X-ray entries followed by that with respect to entries of similar resolution.

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 |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 3   | AD    | 270/276 (98%) | 208 (77%) | 45 (17%) | 17 (6%)  | 1           | 9  |
| 3   | DD    | 270/276 (98%) | 226 (84%) | 31 (12%) | 13 (5%)  | 2           | 14 |
| 4   | AE    | 203/206 (98%) | 138 (68%) | 33 (16%) | 32 (16%) | 0           | 1  |
| 4   | DE    | 203/206 (98%) | 128 (63%) | 34 (17%) | 41 (20%) | 0           | 0  |
| 5   | AF    | 200/210 (95%) | 153 (76%) | 28 (14%) | 19 (10%) | 0           | 4  |
| 5   | DF    | 206/210 (98%) | 133 (65%) | 46 (22%) | 27 (13%) | 0           | 1  |
| 6   | AG    | 179/182 (98%) | 127 (71%) | 36 (20%) | 16 (9%)  | 1           | 4  |
| 6   | DG    | 179/182 (98%) | 128 (72%) | 30 (17%) | 21 (12%) | 0           | 2  |
| 7   | AH    | 168/180 (93%) | 111 (66%) | 25 (15%) | 32 (19%) | 0           | 1  |
| 7   | DH    | 168/180 (93%) | 92 (55%)  | 52 (31%) | 24 (14%) | 0           | 1  |
| 8   | AK    | 144/148 (97%) | 75 (52%)  | 44 (31%) | 25 (17%) | 0           | 1  |
| 8   | DK    | 144/148 (97%) | 98 (68%)  | 27 (19%) | 19 (13%) | 0           | 1  |
| 9   | AM    | 136/140 (97%) | 96 (71%)  | 21 (15%) | 19 (14%) | 0           | 1  |
| 9   | DM    | 136/140 (97%) | 98 (72%)  | 21 (15%) | 17 (12%) | 0           | 1  |
| 10  | AN    | 120/122 (98%) | 101 (84%) | 15 (12%) | 4 (3%)   | 4           | 22 |
| 10  | DN    | 120/122 (98%) | 97 (81%)  | 15 (12%) | 8 (7%)   | 1           | 8  |
| 11  | AO    | 148/150 (99%) | 91 (62%)  | 29 (20%) | 28 (19%) | 0           | 1  |
| 11  | DO    | 148/150 (99%) | 83 (56%)  | 21 (14%) | 44 (30%) | 0           | 0  |
| 12  | AP    | 139/141 (99%) | 93 (67%)  | 27 (19%) | 19 (14%) | 0           | 1  |
| 12  | DP    | 139/141 (99%) | 88 (63%)  | 29 (21%) | 22 (16%) | 0           | 1  |
| 13  | A0    | 116/118 (98%) | 86 (74%)  | 21 (18%) | 9 (8%)   | 1           | 6  |
| 13  | D0    | 115/118 (98%) | 83 (72%)  | 18 (16%) | 14 (12%) | 0           | 1  |
| 14  | AQ    | 109/112 (97%) | 74 (68%)  | 26 (24%) | 9 (8%)   | 1           | 5  |
| 14  | DQ    | 109/112 (97%) | 60 (55%)  | 32 (29%) | 17 (16%) | 0           | 1  |
| 15  | AR    | 135/146 (92%) | 101 (75%) | 19 (14%) | 15 (11%) | 0           | 2  |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 15  | DR    | 135/146 (92%) | 101 (75%) | 23 (17%) | 11 (8%)  | 1           | 6  |
| 16  | A1    | 115/118 (98%) | 82 (71%)  | 19 (16%) | 14 (12%) | 0           | 1  |
| 16  | D1    | 115/118 (98%) | 73 (64%)  | 29 (25%) | 13 (11%) | 0           | 2  |
| 17  | A2    | 99/101 (98%)  | 81 (82%)  | 10 (10%) | 8 (8%)   | 1           | 6  |
| 17  | D2    | 99/101 (98%)  | 64 (65%)  | 19 (19%) | 16 (16%) | 0           | 1  |
| 18  | AS    | 111/113 (98%) | 94 (85%)  | 13 (12%) | 4 (4%)   | 3           | 20 |
| 18  | DS    | 111/113 (98%) | 89 (80%)  | 13 (12%) | 9 (8%)   | 1           | 6  |
| 19  | AT    | 90/96 (94%)   | 78 (87%)  | 8 (9%)   | 4 (4%)   | 2           | 16 |
| 19  | DT    | 90/96 (94%)   | 67 (74%)  | 15 (17%) | 8 (9%)   | 1           | 4  |
| 20  | AU    | 100/110 (91%) | 65 (65%)  | 18 (18%) | 17 (17%) | 0           | 1  |
| 20  | DU    | 100/110 (91%) | 56 (56%)  | 18 (18%) | 26 (26%) | 0           | 0  |
| 21  | AV    | 173/206 (84%) | 105 (61%) | 42 (24%) | 26 (15%) | 0           | 1  |
| 21  | DV    | 177/206 (86%) | 100 (56%) | 35 (20%) | 42 (24%) | 0           | 0  |
| 22  | A3    | 74/85 (87%)   | 58 (78%)  | 11 (15%) | 5 (7%)   | 1           | 8  |
| 22  | D3    | 75/85 (88%)   | 54 (72%)  | 15 (20%) | 6 (8%)   | 1           | 6  |
| 23  | AZ    | 95/98 (97%)   | 75 (79%)  | 14 (15%) | 6 (6%)   | 1           | 9  |
| 23  | DZ    | 95/98 (97%)   | 72 (76%)  | 12 (13%) | 11 (12%) | 0           | 2  |
| 24  | AW    | 64/72 (89%)   | 55 (86%)  | 3 (5%)   | 6 (9%)   | 0           | 4  |
| 24  | DW    | 64/72 (89%)   | 46 (72%)  | 11 (17%) | 7 (11%)  | 0           | 2  |
| 25  | AX    | 57/60 (95%)   | 47 (82%)  | 8 (14%)  | 2 (4%)   | 3           | 21 |
| 25  | DX    | 57/60 (95%)   | 44 (77%)  | 9 (16%)  | 4 (7%)   | 1           | 7  |
| 26  | A4    | 64/71 (90%)   | 33 (52%)  | 14 (22%) | 17 (27%) | 0           | 0  |
| 26  | D4    | 61/71 (86%)   | 23 (38%)  | 12 (20%) | 26 (43%) | 0           | 0  |
| 27  | A5    | 57/60 (95%)   | 39 (68%)  | 10 (18%) | 8 (14%)  | 0           | 1  |
| 27  | D5    | 57/60 (95%)   | 44 (77%)  | 7 (12%)  | 6 (10%)  | 0           | 3  |
| 28  | A6    | 43/54 (80%)   | 21 (49%)  | 13 (30%) | 9 (21%)  | 0           | 0  |
| 28  | D6    | 43/54 (80%)   | 23 (54%)  | 9 (21%)  | 11 (26%) | 0           | 0  |
| 29  | A7    | 43/49 (88%)   | 41 (95%)  | 0        | 2 (5%)   | 2           | 14 |
| 29  | D7    | 43/49 (88%)   | 38 (88%)  | 3 (7%)   | 2 (5%)   | 2           | 14 |
| 30  | A8    | 58/65 (89%)   | 39 (67%)  | 11 (19%) | 8 (14%)  | 0           | 1  |
| 30  | D8    | 58/65 (89%)   | 40 (69%)  | 8 (14%)  | 10 (17%) | 0           | 1  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 32  | BE    | 235/256 (92%) | 155 (66%) | 44 (19%) | 36 (15%) | 0           | 1  |
| 32  | CE    | 235/256 (92%) | 152 (65%) | 49 (21%) | 34 (14%) | 0           | 1  |
| 33  | BF    | 203/239 (85%) | 137 (68%) | 47 (23%) | 19 (9%)  | 0           | 4  |
| 33  | CF    | 204/239 (85%) | 124 (61%) | 55 (27%) | 25 (12%) | 0           | 1  |
| 34  | BG    | 206/208 (99%) | 152 (74%) | 34 (16%) | 20 (10%) | 0           | 3  |
| 34  | CG    | 206/208 (99%) | 152 (74%) | 31 (15%) | 23 (11%) | 0           | 2  |
| 35  | BH    | 149/162 (92%) | 115 (77%) | 26 (17%) | 8 (5%)   | 2           | 12 |
| 35  | CH    | 149/162 (92%) | 115 (77%) | 25 (17%) | 9 (6%)   | 1           | 10 |
| 36  | BI    | 99/101 (98%)  | 71 (72%)  | 23 (23%) | 5 (5%)   | 2           | 13 |
| 36  | CI    | 99/101 (98%)  | 85 (86%)  | 12 (12%) | 2 (2%)   | 7           | 32 |
| 37  | BJ    | 153/156 (98%) | 111 (72%) | 32 (21%) | 10 (6%)  | 1           | 9  |
| 37  | CJ    | 153/156 (98%) | 118 (77%) | 22 (14%) | 13 (8%)  | 1           | 5  |
| 38  | BK    | 136/138 (99%) | 105 (77%) | 24 (18%) | 7 (5%)   | 2           | 13 |
| 38  | CK    | 136/138 (99%) | 100 (74%) | 24 (18%) | 12 (9%)  | 1           | 5  |
| 39  | BL    | 125/128 (98%) | 89 (71%)  | 25 (20%) | 11 (9%)  | 1           | 5  |
| 39  | CL    | 125/128 (98%) | 80 (64%)  | 29 (23%) | 16 (13%) | 0           | 1  |
| 40  | BM    | 97/105 (92%)  | 76 (78%)  | 20 (21%) | 1 (1%)   | 15          | 46 |
| 40  | CM    | 97/105 (92%)  | 73 (75%)  | 19 (20%) | 5 (5%)   | 2           | 13 |
| 41  | BN    | 117/129 (91%) | 85 (73%)  | 24 (20%) | 8 (7%)   | 1           | 8  |
| 41  | CN    | 117/129 (91%) | 93 (80%)  | 19 (16%) | 5 (4%)   | 2           | 16 |
| 42  | BO    | 123/132 (93%) | 93 (76%)  | 18 (15%) | 12 (10%) | 0           | 3  |
| 42  | CO    | 123/132 (93%) | 79 (64%)  | 27 (22%) | 17 (14%) | 0           | 1  |
| 43  | BP    | 114/126 (90%) | 69 (60%)  | 27 (24%) | 18 (16%) | 0           | 1  |
| 43  | CP    | 115/126 (91%) | 71 (62%)  | 24 (21%) | 20 (17%) | 0           | 1  |
| 44  | BQ    | 56/61 (92%)   | 38 (68%)  | 5 (9%)   | 13 (23%) | 0           | 0  |
| 44  | CQ    | 56/61 (92%)   | 32 (57%)  | 13 (23%) | 11 (20%) | 0           | 0  |
| 45  | BR    | 86/89 (97%)   | 62 (72%)  | 19 (22%) | 5 (6%)   | 1           | 11 |
| 45  | CR    | 86/89 (97%)   | 72 (84%)  | 11 (13%) | 3 (4%)   | 3           | 21 |
| 46  | BS    | 82/88 (93%)   | 57 (70%)  | 15 (18%) | 10 (12%) | 0           | 1  |
| 46  | CS    | 82/88 (93%)   | 55 (67%)  | 21 (26%) | 6 (7%)   | 1           | 7  |
| 47  | BT    | 98/105 (93%)  | 74 (76%)  | 17 (17%) | 7 (7%)   | 1           | 7  |

Continued on next page...



Continued from previous page...

| Mol | Chain | Analysed          | Favoured   | Allowed    | Outliers   | Percentiles |    |
|-----|-------|-------------------|------------|------------|------------|-------------|----|
| 47  | CT    | 98/105 (93%)      | 83 (85%)   | 9 (9%)     | 6 (6%)     | 1           | 10 |
| 48  | BU    | 70/88 (80%)       | 53 (76%)   | 11 (16%)   | 6 (9%)     | 1           | 5  |
| 48  | CU    | 70/88 (80%)       | 58 (83%)   | 10 (14%)   | 2 (3%)     | 4           | 24 |
| 49  | BV    | 76/93 (82%)       | 56 (74%)   | 13 (17%)   | 7 (9%)     | 1           | 4  |
| 49  | CV    | 76/93 (82%)       | 49 (64%)   | 18 (24%)   | 9 (12%)    | 0           | 2  |
| 50  | BW    | 97/106 (92%)      | 65 (67%)   | 21 (22%)   | 11 (11%)   | 0           | 2  |
| 50  | CW    | 97/106 (92%)      | 70 (72%)   | 13 (13%)   | 14 (14%)   | 0           | 1  |
| 51  | BX    | 23/27 (85%)       | 15 (65%)   | 5 (22%)    | 3 (13%)    | 0           | 1  |
| 51  | CX    | 23/27 (85%)       | 15 (65%)   | 6 (26%)    | 2 (9%)     | 1           | 5  |
| All | All   | 11319/12052 (94%) | 7969 (70%) | 2044 (18%) | 1306 (12%) | 0           | 2  |

5 of 1306 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | AD    | 3   | VAL  |
| 3   | AD    | 28  | GLU  |
| 3   | AD    | 29  | PRO  |
| 3   | AD    | 33  | LEU  |
| 3   | AD    | 37  | LEU  |

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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 |   |
|-----|-------|---------------|-----------|----------|-------------|---|
| 3   | AD    | 214/218 (98%) | 154 (72%) | 60 (28%) | 0           | 1 |
| 3   | DD    | 214/218 (98%) | 164 (77%) | 50 (23%) | 1           | 3 |
| 4   | AE    | 165/166 (99%) | 131 (79%) | 34 (21%) | 1           | 4 |
| 4   | DE    | 165/166 (99%) | 120 (73%) | 45 (27%) | 0           | 1 |
| 5   | AF    | 161/166 (97%) | 126 (78%) | 35 (22%) | 1           | 4 |
| 5   | DF    | 165/166 (99%) | 130 (79%) | 35 (21%) | 1           | 4 |
| 6   | AG    | 155/156 (99%) | 124 (80%) | 31 (20%) | 1           | 5 |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 6   | DG    | 155/156 (99%)  | 128 (83%) | 27 (17%) | 2           | 8  |
| 7   | AH    | 142/148 (96%)  | 112 (79%) | 30 (21%) | 1           | 4  |
| 7   | DH    | 142/148 (96%)  | 116 (82%) | 26 (18%) | 1           | 7  |
| 8   | AK    | 122/124 (98%)  | 97 (80%)  | 25 (20%) | 1           | 4  |
| 8   | DK    | 122/124 (98%)  | 100 (82%) | 22 (18%) | 1           | 7  |
| 9   | AM    | 117/119 (98%)  | 87 (74%)  | 30 (26%) | 0           | 2  |
| 9   | DM    | 117/119 (98%)  | 82 (70%)  | 35 (30%) | 0           | 1  |
| 10  | AN    | 100/100 (100%) | 81 (81%)  | 19 (19%) | 1           | 6  |
| 10  | DN    | 100/100 (100%) | 84 (84%)  | 16 (16%) | 2           | 11 |
| 11  | AO    | 116/116 (100%) | 81 (70%)  | 35 (30%) | 0           | 1  |
| 11  | DO    | 116/116 (100%) | 77 (66%)  | 39 (34%) | 0           | 1  |
| 12  | AP    | 111/111 (100%) | 88 (79%)  | 23 (21%) | 1           | 4  |
| 12  | DP    | 111/111 (100%) | 79 (71%)  | 32 (29%) | 0           | 1  |
| 13  | A0    | 101/101 (100%) | 77 (76%)  | 24 (24%) | 0           | 2  |
| 13  | D0    | 100/101 (99%)  | 80 (80%)  | 20 (20%) | 1           | 5  |
| 14  | AQ    | 87/88 (99%)    | 63 (72%)  | 24 (28%) | 0           | 1  |
| 14  | DQ    | 87/88 (99%)    | 66 (76%)  | 21 (24%) | 0           | 2  |
| 15  | AR    | 120/127 (94%)  | 97 (81%)  | 23 (19%) | 1           | 6  |
| 15  | DR    | 120/127 (94%)  | 90 (75%)  | 30 (25%) | 0           | 2  |
| 16  | A1    | 93/94 (99%)    | 71 (76%)  | 22 (24%) | 1           | 2  |
| 16  | D1    | 93/94 (99%)    | 77 (83%)  | 16 (17%) | 2           | 9  |
| 17  | A2    | 82/82 (100%)   | 58 (71%)  | 24 (29%) | 0           | 1  |
| 17  | D2    | 82/82 (100%)   | 53 (65%)  | 29 (35%) | 0           | 0  |
| 18  | AS    | 92/92 (100%)   | 69 (75%)  | 23 (25%) | 0           | 2  |
| 18  | DS    | 92/92 (100%)   | 72 (78%)  | 20 (22%) | 1           | 4  |
| 19  | AT    | 74/78 (95%)    | 58 (78%)  | 16 (22%) | 1           | 4  |
| 19  | DT    | 74/78 (95%)    | 56 (76%)  | 18 (24%) | 0           | 2  |
| 20  | AU    | 85/91 (93%)    | 65 (76%)  | 20 (24%) | 1           | 3  |
| 20  | DU    | 85/91 (93%)    | 57 (67%)  | 28 (33%) | 0           | 1  |
| 21  | AV    | 154/179 (86%)  | 126 (82%) | 28 (18%) | 1           | 7  |
| 21  | DV    | 158/179 (88%)  | 133 (84%) | 25 (16%) | 2           | 11 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 22  | A3    | 61/67 (91%)    | 48 (79%)  | 13 (21%) | 1           | 4  |
| 22  | D3    | 62/67 (92%)    | 55 (89%)  | 7 (11%)  | 6           | 22 |
| 23  | AZ    | 82/83 (99%)    | 64 (78%)  | 18 (22%) | 1           | 3  |
| 23  | DZ    | 82/83 (99%)    | 64 (78%)  | 18 (22%) | 1           | 3  |
| 24  | AW    | 62/67 (92%)    | 44 (71%)  | 18 (29%) | 0           | 1  |
| 24  | DW    | 62/67 (92%)    | 48 (77%)  | 14 (23%) | 1           | 3  |
| 25  | AX    | 51/52 (98%)    | 42 (82%)  | 9 (18%)  | 2           | 8  |
| 25  | DX    | 51/52 (98%)    | 41 (80%)  | 10 (20%) | 1           | 5  |
| 26  | A4    | 59/63 (94%)    | 49 (83%)  | 10 (17%) | 2           | 9  |
| 26  | D4    | 57/63 (90%)    | 45 (79%)  | 12 (21%) | 1           | 4  |
| 27  | A5    | 51/52 (98%)    | 39 (76%)  | 12 (24%) | 1           | 3  |
| 27  | D5    | 51/52 (98%)    | 43 (84%)  | 8 (16%)  | 2           | 12 |
| 28  | A6    | 44/52 (85%)    | 32 (73%)  | 12 (27%) | 0           | 1  |
| 28  | D6    | 44/52 (85%)    | 38 (86%)  | 6 (14%)  | 3           | 16 |
| 29  | A7    | 38/42 (90%)    | 32 (84%)  | 6 (16%)  | 2           | 11 |
| 29  | D7    | 38/42 (90%)    | 29 (76%)  | 9 (24%)  | 1           | 2  |
| 30  | A8    | 50/55 (91%)    | 36 (72%)  | 14 (28%) | 0           | 1  |
| 30  | D8    | 50/55 (91%)    | 35 (70%)  | 15 (30%) | 0           | 1  |
| 32  | BE    | 205/220 (93%)  | 167 (82%) | 38 (18%) | 1           | 7  |
| 32  | CE    | 205/220 (93%)  | 168 (82%) | 37 (18%) | 1           | 7  |
| 33  | BF    | 159/188 (85%)  | 127 (80%) | 32 (20%) | 1           | 5  |
| 33  | CF    | 160/188 (85%)  | 132 (82%) | 28 (18%) | 2           | 8  |
| 34  | BG    | 180/180 (100%) | 149 (83%) | 31 (17%) | 2           | 9  |
| 34  | CG    | 180/180 (100%) | 143 (79%) | 37 (21%) | 1           | 4  |
| 35  | BH    | 116/123 (94%)  | 89 (77%)  | 27 (23%) | 1           | 3  |
| 35  | CH    | 116/123 (94%)  | 89 (77%)  | 27 (23%) | 1           | 3  |
| 36  | BI    | 90/90 (100%)   | 80 (89%)  | 10 (11%) | 6           | 23 |
| 36  | CI    | 90/90 (100%)   | 78 (87%)  | 12 (13%) | 4           | 17 |
| 37  | BJ    | 126/127 (99%)  | 96 (76%)  | 30 (24%) | 0           | 2  |
| 37  | CJ    | 126/127 (99%)  | 103 (82%) | 23 (18%) | 1           | 7  |
| 38  | BK    | 119/119 (100%) | 95 (80%)  | 24 (20%) | 1           | 5  |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Analysed        | Rotameric  | Outliers   | Percentiles |     |
|-----|-------|-----------------|------------|------------|-------------|-----|
| 38  | CK    | 119/119 (100%)  | 101 (85%)  | 18 (15%)   | 3           | 13  |
| 39  | BL    | 98/99 (99%)     | 77 (79%)   | 21 (21%)   | 1           | 4   |
| 39  | CL    | 98/99 (99%)     | 73 (74%)   | 25 (26%)   | 0           | 2   |
| 40  | BM    | 89/92 (97%)     | 73 (82%)   | 16 (18%)   | 1           | 7   |
| 40  | CM    | 89/92 (97%)     | 72 (81%)   | 17 (19%)   | 1           | 6   |
| 41  | BN    | 90/99 (91%)     | 76 (84%)   | 14 (16%)   | 2           | 12  |
| 41  | CN    | 90/99 (91%)     | 79 (88%)   | 11 (12%)   | 5           | 20  |
| 42  | BO    | 104/109 (95%)   | 84 (81%)   | 20 (19%)   | 1           | 6   |
| 42  | CO    | 104/109 (95%)   | 80 (77%)   | 24 (23%)   | 1           | 3   |
| 43  | BP    | 94/101 (93%)    | 77 (82%)   | 17 (18%)   | 1           | 7   |
| 43  | CP    | 94/101 (93%)    | 76 (81%)   | 18 (19%)   | 1           | 6   |
| 44  | BQ    | 48/50 (96%)     | 35 (73%)   | 13 (27%)   | 0           | 1   |
| 44  | CQ    | 48/50 (96%)     | 38 (79%)   | 10 (21%)   | 1           | 4   |
| 45  | BR    | 79/80 (99%)     | 69 (87%)   | 10 (13%)   | 4           | 19  |
| 45  | CR    | 79/80 (99%)     | 65 (82%)   | 14 (18%)   | 2           | 8   |
| 46  | BS    | 72/74 (97%)     | 58 (81%)   | 14 (19%)   | 1           | 5   |
| 46  | CS    | 72/74 (97%)     | 60 (83%)   | 12 (17%)   | 2           | 10  |
| 47  | BT    | 95/97 (98%)     | 78 (82%)   | 17 (18%)   | 2           | 8   |
| 47  | CT    | 95/97 (98%)     | 82 (86%)   | 13 (14%)   | 3           | 16  |
| 48  | BU    | 63/77 (82%)     | 53 (84%)   | 10 (16%)   | 2           | 11  |
| 48  | CU    | 63/77 (82%)     | 53 (84%)   | 10 (16%)   | 2           | 11  |
| 49  | BV    | 67/80 (84%)     | 50 (75%)   | 17 (25%)   | 0           | 2   |
| 49  | CV    | 67/80 (84%)     | 47 (70%)   | 20 (30%)   | 0           | 1   |
| 50  | BW    | 76/82 (93%)     | 64 (84%)   | 12 (16%)   | 2           | 11  |
| 50  | CW    | 76/82 (93%)     | 63 (83%)   | 13 (17%)   | 2           | 9   |
| 51  | BX    | 20/22 (91%)     | 20 (100%)  | 0          | 100         | 100 |
| 51  | CX    | 20/22 (91%)     | 18 (90%)   | 2 (10%)    | 7           | 27  |
| All | All   | 9565/9996 (96%) | 7550 (79%) | 2015 (21%) | 1           | 4   |

5 of 2015 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43  | BP    | 86  | CYS  |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | CH    | 65  | ASN  |
| 19  | DT    | 80  | ILE  |
| 45  | BR    | 67  | LEU  |
| 32  | CE    | 73  | THR  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 288 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47  | BT    | 16  | GLN  |
| 38  | CK    | 82  | HIS  |
| 21  | DV    | 132 | ASN  |
| 50  | BW    | 26  | ASN  |
| 34  | CG    | 43  | HIS  |

### 5.3.3 RNA [i](#)

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | AA    | 2911/2912 (99%) | 694 (23%)         | 62 (2%)         |
| 1   | DA    | 2905/2912 (99%) | 731 (25%)         | 60 (2%)         |
| 2   | AB    | 121/122 (99%)   | 23 (19%)          | 0               |
| 2   | DB    | 121/122 (99%)   | 28 (23%)          | 1 (0%)          |
| 31  | BA    | 1501/1506 (99%) | 351 (23%)         | 39 (2%)         |
| 31  | CA    | 1501/1506 (99%) | 351 (23%)         | 49 (3%)         |
| 52  | BB    | 83/85 (97%)     | 45 (54%)          | 5 (6%)          |
| 52  | BD    | 83/85 (97%)     | 38 (45%)          | 5 (6%)          |
| 52  | CB    | 83/85 (97%)     | 49 (59%)          | 8 (9%)          |
| 52  | CD    | 83/85 (97%)     | 35 (42%)          | 6 (7%)          |
| 53  | BC    | 76/77 (98%)     | 17 (22%)          | 3 (3%)          |
| 53  | CC    | 76/77 (98%)     | 20 (26%)          | 3 (3%)          |
| 54  | B1    | 15/16 (93%)     | 7 (46%)           | 2 (13%)         |
| 54  | C1    | 15/16 (93%)     | 8 (53%)           | 3 (20%)         |
| All | All   | 9574/9606 (99%) | 2397 (25%)        | 246 (2%)        |

5 of 2397 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 9   | U    |
| 1   | AA    | 17  | G    |
| 1   | AA    | 23  | G    |
| 1   | AA    | 34  | C    |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 35  | G    |

5 of 246 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 52  | BD    | 21   | A    |
| 31  | CA    | 686  | U    |
| 1   | DA    | 2225 | A    |
| 54  | B1    | 11   | U    |
| 31  | CA    | 243  | A    |

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

4 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$ |
| 52  | MIA  | BD    | 38  | 52   | 24,31,32     | 1.88 | 2 (8%)      | 26,44,47    | 2.95 | 9 (34%)     |
| 52  | MIA  | CB    | 38  | 52   | 24,31,32     | 2.15 | 4 (16%)     | 26,44,47    | 2.61 | 7 (26%)     |
| 52  | MIA  | BB    | 38  | 52   | 24,31,32     | 1.95 | 2 (8%)      | 26,44,47    | 2.13 | 8 (30%)     |
| 52  | MIA  | CD    | 38  | 52   | 24,31,32     | 1.87 | 2 (8%)      | 26,44,47    | 2.89 | 10 (38%)    |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 52  | MIA  | BD    | 38  | 52   | -       | 6/11/33/34 | 0/3/3/3 |
| 52  | MIA  | CB    | 38  | 52   | -       | 2/11/33/34 | 0/3/3/3 |
| 52  | MIA  | BB    | 38  | 52   | -       | 2/11/33/34 | 0/3/3/3 |
| 52  | MIA  | CD    | 38  | 52   | -       | 7/11/33/34 | 0/3/3/3 |

The worst 5 of 10 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 52  | CB    | 38  | MIA  | C6-N6   | 6.99 | 1.47        | 1.34     |
| 52  | CB    | 38  | MIA  | C13-C14 | 6.59 | 1.51        | 1.32     |
| 52  | BB    | 38  | MIA  | C13-C14 | 6.46 | 1.50        | 1.32     |
| 52  | BB    | 38  | MIA  | C6-N6   | 6.34 | 1.46        | 1.34     |
| 52  | BD    | 38  | MIA  | C6-N6   | 6.29 | 1.46        | 1.34     |

The worst 5 of 34 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 52  | BD    | 38  | MIA  | C11-S10-C2  | 11.91 | 111.16      | 102.27   |
| 52  | CD    | 38  | MIA  | C11-S10-C2  | 10.71 | 110.27      | 102.27   |
| 52  | CB    | 38  | MIA  | C11-S10-C2  | 10.02 | 109.75      | 102.27   |
| 52  | BB    | 38  | MIA  | C11-S10-C2  | 5.31  | 106.23      | 102.27   |
| 52  | CD    | 38  | MIA  | C12-C13-C14 | -4.71 | 117.97      | 127.14   |

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 52  | BD    | 38  | MIA  | O4'-C4'-C5'-O5' |
| 52  | BD    | 38  | MIA  | C3'-C4'-C5'-O5' |
| 52  | BD    | 38  | MIA  | N1-C2-S10-C11   |
| 52  | BD    | 38  | MIA  | N3-C2-S10-C11   |
| 52  | BD    | 38  | MIA  | C12-C13-C14-C15 |

There are no ring outliers.

4 monomers are involved in 16 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 52  | BD    | 38  | MIA  | 7       | 0            |
| 52  | CB    | 38  | MIA  | 5       | 0            |
| 52  | BB    | 38  | MIA  | 2       | 0            |
| 52  | CD    | 38  | MIA  | 2       | 0            |

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1619 ligands modelled in this entry, 907 are monoatomic - leaving 712 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 |
| 56  | OHX  | AO    | 203  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1785 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3453 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3483 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1791 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3433 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3372 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | A1    | 204  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3456 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3395 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3480 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3386 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3420 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1791 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3407 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3387 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3535 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1729 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3416 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1766 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3527 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3349 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3347 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3342 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3160 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1718 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3353 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1795 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3396 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3469 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3388 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3503 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 56  | OHX  | DA    | 3127 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DB    | 211  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3378 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3466 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1768 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3553 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3411 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1740 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3474 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3487 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1733 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1725 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1742 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3377 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | D8    | 101  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3464 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3442 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3367 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1783 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3366 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BC    | 106  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1774 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3406 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3389 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1781 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3170 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3359 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3477 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3451 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3516 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3365 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3360 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1789 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1796 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1732 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3335 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3476 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1772 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1788 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1726 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3397 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1763 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AB    | 214  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 56  | OHX  | CA    | 1774 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3459 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1766 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3442 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3421 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1764 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3423 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3168 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3546 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DO    | 201  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1725 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1754 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3212 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1787 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1802 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BD    | 104  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3352 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3439 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3368 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1807 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3486 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1748 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3478 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3332 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3514 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3343 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3418 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1746 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DB    | 219  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3245 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3409 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3555 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3358 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DB    | 217  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3361 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3492 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1745 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3339 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3368 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1794 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3449 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3509 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1775 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 56  | OHX  | DA    | 3409 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3333 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3548 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3377 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3392 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AB    | 207  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1776 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3258 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3387 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3065 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1765 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1796 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1778 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3466 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3393 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3473 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1797 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | A6    | 101  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3398 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3552 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3374 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3453 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3345 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1785 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3484 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3354 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3369 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3363 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3132 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3506 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3446 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1730 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3348 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DB    | 215  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1769 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3124 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3374 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3347 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3543 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3562 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1738 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3568 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3489 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 56  | OHX  | AA    | 3410 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3563 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1722 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3522 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3491 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3490 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1736 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3373 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3500 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3136 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1812 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3359 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3215 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3538 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1727 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3393 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3248 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3469 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3395 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3551 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3481 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CC    | 109  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3432 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3226 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1779 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DB    | 220  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3413 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1809 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3346 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3071 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3109 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3468 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3430 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1728 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CR    | 101  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3176 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1772 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3091 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1811 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3431 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3544 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3541 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1716 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 56  | OHX  | DA    | 3463 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | DA    | 3375 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | BA    | 1792 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | DB    | 214  | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | AA    | 3549 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | DA    | 3444 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | CK    | 201  | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | DA    | 3452 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | DA    | 3439 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | BA    | 1768 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | AA    | 3559 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | DA    | 3443 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | DA    | 3378 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | BA    | 1759 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | BA    | 1813 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | DA    | 3383 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | AA    | 3566 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | AA    | 3422 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | AA    | 3557 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | BA    | 1758 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | AA    | 3369 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | CA    | 1778 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | AA    | 3353 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | DB    | 218  | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | DA    | 3366 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | AA    | 3531 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | AA    | 3360 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | CA    | 1740 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | BA    | 1784 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | AA    | 3430 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | AA    | 3345 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | DA    | 3174 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 57  | PAR  | CA    | 1722 | -    | 45,45,45     | 0.70 | 0        | 64,67,67    | 1.83 | 15 (23%) |
| 56  | OHX  | AA    | 3330 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | CA    | 1786 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | DA    | 3338 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | AA    | 3460 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | BA    | 1779 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | CA    | 1731 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 57  | PAR  | BA    | 1715 | -    | 45,45,45     | 0.73 | 2 (4%)   | 64,67,67    | 1.72 | 13 (20%) |
| 56  | OHX  | AA    | 3528 | -    | 0,6,6        | 0.00 | -        | -           |      |          |
| 56  | OHX  | AA    | 3338 | -    | 0,6,6        | 0.00 | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 56  | OHX  | AA    | 3375 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3536 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1737 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3405 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3340 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3404 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3423 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1764 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3462 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AF    | 303  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3422 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1769 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3414 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1754 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3429 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CB    | 106  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1730 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3507 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3436 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3425 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3118 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3246 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3249 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1793 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3454 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1745 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1803 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3376 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3471 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3520 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AW    | 101  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3329 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3392 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3364 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3477 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1780 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3479 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3513 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3105 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3352 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3434 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3358 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1743 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 56  | OHX  | CA    | 1777 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3471 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1813 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3451 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3558 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1803 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1723 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3459 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3565 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1790 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3351 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1756 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1798 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3391 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3502 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3462 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3433 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1783 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3351 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | D3    | 101  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3427 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1753 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3472 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AB    | 209  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | A1    | 203  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3505 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1742 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3243 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3489 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3441 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DF    | 301  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3539 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AB    | 213  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3485 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3380 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BL    | 201  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3449 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3521 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3083 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3103 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1809 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3412 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1727 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 56  | OHX  | AA    | 3495 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3498 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3554 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AE    | 304  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3480 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3406 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3403 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3381 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3371 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3455 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1747 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3379 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3496 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3337 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3331 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3493 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3470 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1770 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3470 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1770 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3404 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3416 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3062 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3397 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3561 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3402 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3427 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3163 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1812 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3386 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AB    | 208  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1788 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3424 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3460 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3341 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3440 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1731 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3165 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3463 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AB    | 211  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3474 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3485 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3335 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 56  | OHX  | AA    | 3475 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3257 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3508 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BB    | 115  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1724 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3534 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1732 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3435 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1805 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3518 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3390 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1717 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1750 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AB    | 212  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AB    | 210  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3255 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1761 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3173 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3421 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3327 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3537 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3545 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3171 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3408 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3526 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1739 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1793 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | D1    | 201  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1723 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3547 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3426 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3445 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3064 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3214 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3488 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3391 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1795 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3370 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3510 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3426 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3068 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3380 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1758 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 56  | OHX  | DB    | 209  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3419 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3418 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1748 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3458 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1757 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3556 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1720 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3487 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1807 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3354 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1797 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3340 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3361 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1760 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1765 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3482 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1719 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3407 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3448 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3384 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3389 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3569 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1729 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1787 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3461 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3479 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1777 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3529 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3476 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1767 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3448 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3367 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3370 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1762 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1749 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1810 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3482 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1784 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1752 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1749 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3224 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3438 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 56  | OHX  | BA    | 1743 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3223 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3384 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1755 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1726 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CB    | 104  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3438 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DB    | 216  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3512 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3363 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3456 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3511 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1741 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3134 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3400 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3415 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3431 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3515 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3357 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1733 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3217 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3425 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3344 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3420 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3450 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3564 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AB    | 219  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1815 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1806 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3390 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1811 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1744 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BC    | 105  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3350 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AB    | 216  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3530 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3445 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3464 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3356 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | D5    | 102  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3483 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3475 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1805 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 56  | OHX  | DA    | 3428 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1771 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3401 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3465 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3381 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1747 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3419 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3365 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1763 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3501 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1752 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BD    | 102  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1738 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1790 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3437 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3450 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3166 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3408 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BD    | 103  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1724 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3413 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3401 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3457 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3364 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3403 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3382 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1761 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3525 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3437 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3446 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3435 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3348 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3172 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1746 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1771 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DB    | 208  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1782 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3326 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1737 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1814 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3523 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3441 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3399 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 56  | OHX  | DA    | 3398 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3169 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3221 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3410 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1786 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3465 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3388 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1798 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1759 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3550 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3481 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3412 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3533 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3484 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DB    | 210  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BG    | 302  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3490 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1808 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3434 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3499 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1808 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1751 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3342 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1789 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3494 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3111 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3519 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CC    | 110  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1760 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3379 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3157 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3468 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1810 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DB    | 213  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1741 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1744 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1799 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1792 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1739 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1782 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3447 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AB    | 217  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3504 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 56  | OHX  | DA    | 3417 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3428 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3087 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3376 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3497 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1773 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3061 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1776 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3486 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3415 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3560 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CV    | 101  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3371 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1734 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3220 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3429 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CD    | 101  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AB    | 218  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3094 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3458 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3517 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1767 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DB    | 212  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1751 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3218 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BB    | 114  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3491 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3402 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3385 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3467 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3362 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3396 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3524 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3447 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1762 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3075 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1814 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1728 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3336 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3417 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3394 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3440 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3411 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 56  | OHX  | AA    | 3328 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3532 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1800 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3344 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | A3    | 102  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3455 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3454 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1756 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3540 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CB    | 105  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3444 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1806 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3383 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1735 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1757 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3432 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1781 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1780 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3355 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3400 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AB    | 215  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3385 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1721 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1804 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3567 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3346 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3082 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AO    | 202  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3084 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3473 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3081 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3461 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1794 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1799 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3467 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3394 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3341 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3488 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3424 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3350 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3162 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1775 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1801 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 56  | OHX  | BA    | 1736 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3373 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1773 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3362 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3472 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3414 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3452 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1734 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1753 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1802 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1804 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CC    | 108  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3099 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3251 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3457 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3254 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1801 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3436 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3349 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3443 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1800 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3542 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BA    | 1735 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3405 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BC    | 107  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3159 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3382 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3478 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3253 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3336 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | BR    | 101  | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | AA    | 3355 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3073 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | DA    | 3399 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1755 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |
| 56  | OHX  | CA    | 1750 | -    | 0,6,6        | 0.00 | -        | -           | -    | -        |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 57  | PAR  | CA    | 1722 | -    | -       | 5/18/94/94 | 0/4/4/4 |
| 57  | PAR  | BA    | 1715 | -    | -       | 6/18/94/94 | 0/4/4/4 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 57  | BA    | 1715 | PAR  | C21-N21 | -2.29 | 1.43        | 1.47     |
| 57  | BA    | 1715 | PAR  | C31-C21 | -2.16 | 1.50        | 1.53     |

The worst 5 of 28 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 57  | CA    | 1722 | PAR  | C11-O51-C51 | 5.04  | 123.58      | 113.69   |
| 57  | CA    | 1722 | PAR  | C13-O52-C52 | -4.44 | 106.98      | 117.96   |
| 57  | BA    | 1715 | PAR  | C44-C34-C24 | 4.32  | 118.49      | 111.07   |
| 57  | BA    | 1715 | PAR  | C11-O51-C51 | 4.28  | 122.08      | 113.69   |
| 57  | CA    | 1722 | PAR  | C62-C12-N12 | -4.23 | 102.59      | 110.97   |

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 57  | CA    | 1722 | PAR  | O43-C43-C53-O53 |
| 57  | CA    | 1722 | PAR  | C33-C43-C53-O53 |
| 57  | CA    | 1722 | PAR  | C41-C51-C61-O61 |
| 57  | BA    | 1715 | PAR  | C41-C51-C61-O61 |
| 57  | BA    | 1715 | PAR  | O43-C43-C53-O53 |

There are no ring outliers.

332 monomers are involved in 465 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 56  | AO    | 203  | OHX  | 1       | 0            |
| 56  | CA    | 1785 | OHX  | 3       | 0            |
| 56  | DA    | 3483 | OHX  | 1       | 0            |
| 56  | AA    | 3433 | OHX  | 3       | 0            |
| 56  | BA    | 1791 | OHX  | 3       | 0            |
| 56  | AA    | 3407 | OHX  | 1       | 0            |
| 56  | AA    | 3535 | OHX  | 1       | 0            |
| 56  | AA    | 3416 | OHX  | 3       | 0            |
| 56  | CA    | 1766 | OHX  | 1       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 56  | AA    | 3527 | OHX  | 1       | 0            |
| 56  | AA    | 3347 | OHX  | 1       | 0            |
| 56  | AA    | 3342 | OHX  | 2       | 0            |
| 56  | DA    | 3388 | OHX  | 2       | 0            |
| 56  | DA    | 3127 | OHX  | 1       | 0            |
| 56  | AA    | 3466 | OHX  | 1       | 0            |
| 56  | CA    | 1768 | OHX  | 1       | 0            |
| 56  | AA    | 3553 | OHX  | 1       | 0            |
| 56  | AA    | 3487 | OHX  | 1       | 0            |
| 56  | CA    | 1733 | OHX  | 1       | 0            |
| 56  | CA    | 1725 | OHX  | 2       | 0            |
| 56  | DA    | 3377 | OHX  | 2       | 0            |
| 56  | D8    | 101  | OHX  | 5       | 0            |
| 56  | AA    | 3367 | OHX  | 3       | 0            |
| 56  | BC    | 106  | OHX  | 1       | 0            |
| 56  | DA    | 3389 | OHX  | 3       | 0            |
| 56  | AA    | 3516 | OHX  | 1       | 0            |
| 56  | BA    | 1789 | OHX  | 1       | 0            |
| 56  | BA    | 1732 | OHX  | 1       | 0            |
| 56  | CA    | 1788 | OHX  | 2       | 0            |
| 56  | CA    | 1774 | OHX  | 1       | 0            |
| 56  | DA    | 3459 | OHX  | 1       | 0            |
| 56  | BA    | 1766 | OHX  | 1       | 0            |
| 56  | CA    | 1764 | OHX  | 1       | 0            |
| 56  | AA    | 3546 | OHX  | 1       | 0            |
| 56  | DA    | 3212 | OHX  | 1       | 0            |
| 56  | DA    | 3368 | OHX  | 1       | 0            |
| 56  | BA    | 1807 | OHX  | 1       | 0            |
| 56  | AA    | 3514 | OHX  | 1       | 0            |
| 56  | DA    | 3343 | OHX  | 3       | 0            |
| 56  | DA    | 3418 | OHX  | 1       | 0            |
| 56  | CA    | 1746 | OHX  | 1       | 0            |
| 56  | DB    | 219  | OHX  | 1       | 0            |
| 56  | AA    | 3409 | OHX  | 2       | 0            |
| 56  | AA    | 3555 | OHX  | 1       | 0            |
| 56  | AA    | 3509 | OHX  | 1       | 0            |
| 56  | BA    | 1775 | OHX  | 1       | 0            |
| 56  | AA    | 3333 | OHX  | 1       | 0            |
| 56  | AA    | 3377 | OHX  | 1       | 0            |
| 56  | AA    | 3392 | OHX  | 1       | 0            |
| 56  | DA    | 3258 | OHX  | 1       | 0            |
| 56  | BA    | 1796 | OHX  | 1       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 56  | AA    | 3473 | OHX  | 2       | 0            |
| 56  | CA    | 1797 | OHX  | 2       | 0            |
| 56  | A6    | 101  | OHX  | 1       | 0            |
| 56  | DA    | 3374 | OHX  | 3       | 0            |
| 56  | AA    | 3453 | OHX  | 2       | 0            |
| 56  | BA    | 1785 | OHX  | 5       | 0            |
| 56  | DA    | 3484 | OHX  | 1       | 0            |
| 56  | DA    | 3132 | OHX  | 1       | 0            |
| 56  | AA    | 3506 | OHX  | 1       | 0            |
| 56  | CA    | 1730 | OHX  | 1       | 0            |
| 56  | AA    | 3374 | OHX  | 2       | 0            |
| 56  | CA    | 1738 | OHX  | 2       | 0            |
| 56  | AA    | 3568 | OHX  | 1       | 0            |
| 56  | DA    | 3489 | OHX  | 2       | 0            |
| 56  | AA    | 3373 | OHX  | 1       | 0            |
| 56  | BA    | 1812 | OHX  | 1       | 0            |
| 56  | DA    | 3215 | OHX  | 1       | 0            |
| 56  | AA    | 3538 | OHX  | 2       | 0            |
| 56  | CA    | 1727 | OHX  | 1       | 0            |
| 56  | DA    | 3248 | OHX  | 1       | 0            |
| 56  | DA    | 3395 | OHX  | 1       | 0            |
| 56  | AA    | 3551 | OHX  | 2       | 0            |
| 56  | AA    | 3432 | OHX  | 1       | 0            |
| 56  | CA    | 1779 | OHX  | 3       | 0            |
| 56  | DB    | 220  | OHX  | 1       | 0            |
| 56  | CA    | 1809 | OHX  | 1       | 0            |
| 56  | AA    | 3346 | OHX  | 1       | 0            |
| 56  | AA    | 3468 | OHX  | 1       | 0            |
| 56  | DA    | 3430 | OHX  | 1       | 0            |
| 56  | BA    | 1728 | OHX  | 1       | 0            |
| 56  | DA    | 3176 | OHX  | 1       | 0            |
| 56  | BA    | 1772 | OHX  | 2       | 0            |
| 56  | CA    | 1811 | OHX  | 1       | 0            |
| 56  | BA    | 1716 | OHX  | 1       | 0            |
| 56  | BA    | 1792 | OHX  | 1       | 0            |
| 56  | DA    | 3444 | OHX  | 2       | 0            |
| 56  | CK    | 201  | OHX  | 1       | 0            |
| 56  | DA    | 3439 | OHX  | 1       | 0            |
| 56  | DA    | 3443 | OHX  | 1       | 0            |
| 56  | BA    | 1813 | OHX  | 2       | 0            |
| 56  | AA    | 3566 | OHX  | 1       | 0            |
| 56  | AA    | 3422 | OHX  | 1       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 56  | AA    | 3557 | OHX  | 2       | 0            |
| 56  | CA    | 1778 | OHX  | 1       | 0            |
| 56  | AA    | 3531 | OHX  | 1       | 0            |
| 56  | CA    | 1740 | OHX  | 1       | 0            |
| 56  | BA    | 1784 | OHX  | 2       | 0            |
| 57  | CA    | 1722 | PAR  | 1       | 0            |
| 56  | AA    | 3330 | OHX  | 5       | 0            |
| 56  | CA    | 1786 | OHX  | 1       | 0            |
| 56  | CA    | 1731 | OHX  | 1       | 0            |
| 57  | BA    | 1715 | PAR  | 3       | 0            |
| 56  | AA    | 3375 | OHX  | 1       | 0            |
| 56  | AA    | 3536 | OHX  | 2       | 0            |
| 56  | AA    | 3405 | OHX  | 1       | 0            |
| 56  | DA    | 3340 | OHX  | 1       | 0            |
| 56  | AA    | 3423 | OHX  | 1       | 0            |
| 56  | AF    | 303  | OHX  | 3       | 0            |
| 56  | DA    | 3422 | OHX  | 1       | 0            |
| 56  | CA    | 1769 | OHX  | 1       | 0            |
| 56  | AA    | 3507 | OHX  | 2       | 0            |
| 56  | DA    | 3118 | OHX  | 1       | 0            |
| 56  | DA    | 3246 | OHX  | 1       | 0            |
| 56  | CA    | 1793 | OHX  | 1       | 0            |
| 56  | BA    | 1745 | OHX  | 2       | 0            |
| 56  | CA    | 1803 | OHX  | 1       | 0            |
| 56  | AA    | 3376 | OHX  | 1       | 0            |
| 56  | AA    | 3329 | OHX  | 1       | 0            |
| 56  | AA    | 3364 | OHX  | 1       | 0            |
| 56  | AA    | 3479 | OHX  | 1       | 0            |
| 56  | CA    | 1777 | OHX  | 1       | 0            |
| 56  | DA    | 3471 | OHX  | 2       | 0            |
| 56  | AA    | 3558 | OHX  | 2       | 0            |
| 56  | AA    | 3565 | OHX  | 1       | 0            |
| 56  | CA    | 1790 | OHX  | 2       | 0            |
| 56  | BA    | 1756 | OHX  | 1       | 0            |
| 56  | AA    | 3391 | OHX  | 2       | 0            |
| 56  | AA    | 3502 | OHX  | 2       | 0            |
| 56  | AA    | 3462 | OHX  | 1       | 0            |
| 56  | AA    | 3351 | OHX  | 1       | 0            |
| 56  | D3    | 101  | OHX  | 1       | 0            |
| 56  | CA    | 1753 | OHX  | 1       | 0            |
| 56  | AB    | 209  | OHX  | 1       | 0            |
| 56  | AA    | 3505 | OHX  | 1       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 56  | CA    | 1742 | OHX  | 1       | 0            |
| 56  | DA    | 3441 | OHX  | 1       | 0            |
| 56  | DF    | 301  | OHX  | 1       | 0            |
| 56  | AB    | 213  | OHX  | 1       | 0            |
| 56  | DA    | 3083 | OHX  | 1       | 0            |
| 56  | DA    | 3103 | OHX  | 3       | 0            |
| 56  | AA    | 3412 | OHX  | 2       | 0            |
| 56  | AA    | 3554 | OHX  | 1       | 0            |
| 56  | DA    | 3406 | OHX  | 1       | 0            |
| 56  | DA    | 3403 | OHX  | 2       | 0            |
| 56  | AA    | 3371 | OHX  | 1       | 0            |
| 56  | BA    | 1747 | OHX  | 1       | 0            |
| 56  | DA    | 3379 | OHX  | 2       | 0            |
| 56  | AA    | 3496 | OHX  | 1       | 0            |
| 56  | DA    | 3337 | OHX  | 1       | 0            |
| 56  | AA    | 3331 | OHX  | 1       | 0            |
| 56  | CA    | 1770 | OHX  | 1       | 0            |
| 56  | DA    | 3470 | OHX  | 2       | 0            |
| 56  | BA    | 1770 | OHX  | 1       | 0            |
| 56  | DA    | 3416 | OHX  | 1       | 0            |
| 56  | DA    | 3062 | OHX  | 1       | 0            |
| 56  | AA    | 3561 | OHX  | 2       | 0            |
| 56  | DA    | 3427 | OHX  | 3       | 0            |
| 56  | BA    | 1788 | OHX  | 1       | 0            |
| 56  | AA    | 3463 | OHX  | 1       | 0            |
| 56  | AA    | 3335 | OHX  | 1       | 0            |
| 56  | AA    | 3475 | OHX  | 1       | 0            |
| 56  | DA    | 3257 | OHX  | 1       | 0            |
| 56  | BA    | 1724 | OHX  | 1       | 0            |
| 56  | BA    | 1805 | OHX  | 1       | 0            |
| 56  | DA    | 3390 | OHX  | 1       | 0            |
| 56  | BA    | 1717 | OHX  | 1       | 0            |
| 56  | DA    | 3255 | OHX  | 1       | 0            |
| 56  | BA    | 1761 | OHX  | 1       | 0            |
| 56  | DA    | 3173 | OHX  | 2       | 0            |
| 56  | AA    | 3545 | OHX  | 1       | 0            |
| 56  | CA    | 1739 | OHX  | 1       | 0            |
| 56  | BA    | 1793 | OHX  | 2       | 0            |
| 56  | CA    | 1723 | OHX  | 2       | 0            |
| 56  | AA    | 3547 | OHX  | 6       | 0            |
| 56  | DA    | 3445 | OHX  | 1       | 0            |
| 56  | DA    | 3064 | OHX  | 3       | 0            |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Clashes</b> | <b>Symm-Clashes</b> |
|------------|--------------|------------|-------------|----------------|---------------------|
| 56         | DA           | 3214       | OHX         | 2              | 0                   |
| 56         | DA           | 3391       | OHX         | 1              | 0                   |
| 56         | AA           | 3370       | OHX         | 1              | 0                   |
| 56         | DA           | 3426       | OHX         | 1              | 0                   |
| 56         | DA           | 3068       | OHX         | 1              | 0                   |
| 56         | CA           | 1758       | OHX         | 1              | 0                   |
| 56         | DB           | 209        | OHX         | 1              | 0                   |
| 56         | AA           | 3419       | OHX         | 1              | 0                   |
| 56         | AA           | 3418       | OHX         | 1              | 0                   |
| 56         | AA           | 3458       | OHX         | 1              | 0                   |
| 56         | BA           | 1757       | OHX         | 1              | 0                   |
| 56         | AA           | 3556       | OHX         | 1              | 0                   |
| 56         | BA           | 1720       | OHX         | 1              | 0                   |
| 56         | DA           | 3487       | OHX         | 1              | 0                   |
| 56         | AA           | 3361       | OHX         | 1              | 0                   |
| 56         | CA           | 1760       | OHX         | 1              | 0                   |
| 56         | DA           | 3407       | OHX         | 1              | 0                   |
| 56         | AA           | 3384       | OHX         | 1              | 0                   |
| 56         | AA           | 3569       | OHX         | 3              | 0                   |
| 56         | AA           | 3529       | OHX         | 1              | 0                   |
| 56         | CA           | 1762       | OHX         | 7              | 0                   |
| 56         | CA           | 1749       | OHX         | 1              | 0                   |
| 56         | CA           | 1784       | OHX         | 1              | 0                   |
| 56         | DA           | 3438       | OHX         | 1              | 0                   |
| 56         | DA           | 3223       | OHX         | 1              | 0                   |
| 56         | DA           | 3384       | OHX         | 1              | 0                   |
| 56         | BA           | 1755       | OHX         | 1              | 0                   |
| 56         | CA           | 1726       | OHX         | 1              | 0                   |
| 56         | CB           | 104        | OHX         | 1              | 0                   |
| 56         | AA           | 3438       | OHX         | 1              | 0                   |
| 56         | AA           | 3512       | OHX         | 1              | 0                   |
| 56         | CA           | 1741       | OHX         | 2              | 0                   |
| 56         | DA           | 3415       | OHX         | 1              | 0                   |
| 56         | BA           | 1733       | OHX         | 3              | 0                   |
| 56         | DA           | 3344       | OHX         | 3              | 0                   |
| 56         | AB           | 219        | OHX         | 2              | 0                   |
| 56         | CA           | 1815       | OHX         | 1              | 0                   |
| 56         | BA           | 1806       | OHX         | 2              | 0                   |
| 56         | BA           | 1811       | OHX         | 2              | 0                   |
| 56         | BC           | 105        | OHX         | 1              | 0                   |
| 56         | AA           | 3350       | OHX         | 1              | 0                   |
| 56         | AA           | 3530       | OHX         | 1              | 0                   |

*Continued on next page...*

*Continued from previous page...*

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Clashes</b> | <b>Symm-Clashes</b> |
|------------|--------------|------------|-------------|----------------|---------------------|
| 56         | AA           | 3445       | OHX         | 1              | 0                   |
| 56         | AA           | 3464       | OHX         | 1              | 0                   |
| 56         | D5           | 102        | OHX         | 1              | 0                   |
| 56         | CA           | 1805       | OHX         | 1              | 0                   |
| 56         | DA           | 3428       | OHX         | 2              | 0                   |
| 56         | DA           | 3465       | OHX         | 1              | 0                   |
| 56         | DA           | 3419       | OHX         | 2              | 0                   |
| 56         | AA           | 3365       | OHX         | 4              | 0                   |
| 56         | BA           | 1763       | OHX         | 1              | 0                   |
| 56         | BD           | 102        | OHX         | 1              | 0                   |
| 56         | BA           | 1790       | OHX         | 1              | 0                   |
| 56         | DA           | 3437       | OHX         | 1              | 0                   |
| 56         | CA           | 1724       | OHX         | 1              | 0                   |
| 56         | DA           | 3401       | OHX         | 1              | 0                   |
| 56         | DA           | 3457       | OHX         | 1              | 0                   |
| 56         | DA           | 3364       | OHX         | 1              | 0                   |
| 56         | DA           | 3382       | OHX         | 1              | 0                   |
| 56         | AA           | 3525       | OHX         | 1              | 0                   |
| 56         | DA           | 3348       | OHX         | 1              | 0                   |
| 56         | DA           | 3172       | OHX         | 2              | 0                   |
| 56         | BA           | 1746       | OHX         | 1              | 0                   |
| 56         | CA           | 1771       | OHX         | 1              | 0                   |
| 56         | CA           | 1737       | OHX         | 2              | 0                   |
| 56         | AA           | 3523       | OHX         | 1              | 0                   |
| 56         | AA           | 3441       | OHX         | 1              | 0                   |
| 56         | AA           | 3399       | OHX         | 2              | 0                   |
| 56         | DA           | 3398       | OHX         | 1              | 0                   |
| 56         | DA           | 3169       | OHX         | 1              | 0                   |
| 56         | DA           | 3221       | OHX         | 2              | 0                   |
| 56         | DA           | 3410       | OHX         | 2              | 0                   |
| 56         | AA           | 3388       | OHX         | 2              | 0                   |
| 56         | CA           | 1798       | OHX         | 4              | 0                   |
| 56         | CA           | 1759       | OHX         | 1              | 0                   |
| 56         | AA           | 3550       | OHX         | 1              | 0                   |
| 56         | AA           | 3481       | OHX         | 1              | 0                   |
| 56         | DA           | 3412       | OHX         | 1              | 0                   |
| 56         | DB           | 210        | OHX         | 1              | 0                   |
| 56         | BG           | 302        | OHX         | 2              | 0                   |
| 56         | CA           | 1751       | OHX         | 1              | 0                   |
| 56         | AA           | 3494       | OHX         | 1              | 0                   |
| 56         | DA           | 3111       | OHX         | 2              | 0                   |
| 56         | CC           | 110        | OHX         | 1              | 0                   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 56  | BA    | 1760 | OHX  | 1       | 0            |
| 56  | DA    | 3468 | OHX  | 1       | 0            |
| 56  | CA    | 1810 | OHX  | 2       | 0            |
| 56  | DB    | 213  | OHX  | 1       | 0            |
| 56  | CA    | 1792 | OHX  | 2       | 0            |
| 56  | CA    | 1782 | OHX  | 1       | 0            |
| 56  | AA    | 3504 | OHX  | 4       | 0            |
| 56  | DA    | 3087 | OHX  | 1       | 0            |
| 56  | DA    | 3376 | OHX  | 1       | 0            |
| 56  | AA    | 3497 | OHX  | 2       | 0            |
| 56  | BA    | 1773 | OHX  | 2       | 0            |
| 56  | DA    | 3061 | OHX  | 1       | 0            |
| 56  | CA    | 1776 | OHX  | 1       | 0            |
| 56  | DA    | 3486 | OHX  | 1       | 0            |
| 56  | AA    | 3415 | OHX  | 3       | 0            |
| 56  | AA    | 3560 | OHX  | 1       | 0            |
| 56  | CV    | 101  | OHX  | 1       | 0            |
| 56  | BA    | 1734 | OHX  | 1       | 0            |
| 56  | CD    | 101  | OHX  | 1       | 0            |
| 56  | AB    | 218  | OHX  | 1       | 0            |
| 56  | DB    | 212  | OHX  | 1       | 0            |
| 56  | DA    | 3385 | OHX  | 2       | 0            |
| 56  | DA    | 3362 | OHX  | 1       | 0            |
| 56  | AA    | 3524 | OHX  | 1       | 0            |
| 56  | AA    | 3447 | OHX  | 1       | 0            |
| 56  | BA    | 1762 | OHX  | 1       | 0            |
| 56  | CA    | 1728 | OHX  | 1       | 0            |
| 56  | AA    | 3417 | OHX  | 1       | 0            |
| 56  | DA    | 3411 | OHX  | 1       | 0            |
| 56  | A3    | 102  | OHX  | 1       | 0            |
| 56  | DA    | 3454 | OHX  | 1       | 0            |
| 56  | CA    | 1756 | OHX  | 2       | 0            |
| 56  | AA    | 3540 | OHX  | 1       | 0            |
| 56  | CB    | 105  | OHX  | 1       | 0            |
| 56  | AA    | 3383 | OHX  | 1       | 0            |
| 56  | CA    | 1735 | OHX  | 1       | 0            |
| 56  | CA    | 1757 | OHX  | 1       | 0            |
| 56  | BA    | 1780 | OHX  | 1       | 0            |
| 56  | DA    | 3400 | OHX  | 2       | 0            |
| 56  | AB    | 215  | OHX  | 1       | 0            |
| 56  | BA    | 1721 | OHX  | 3       | 0            |
| 56  | AA    | 3567 | OHX  | 1       | 0            |

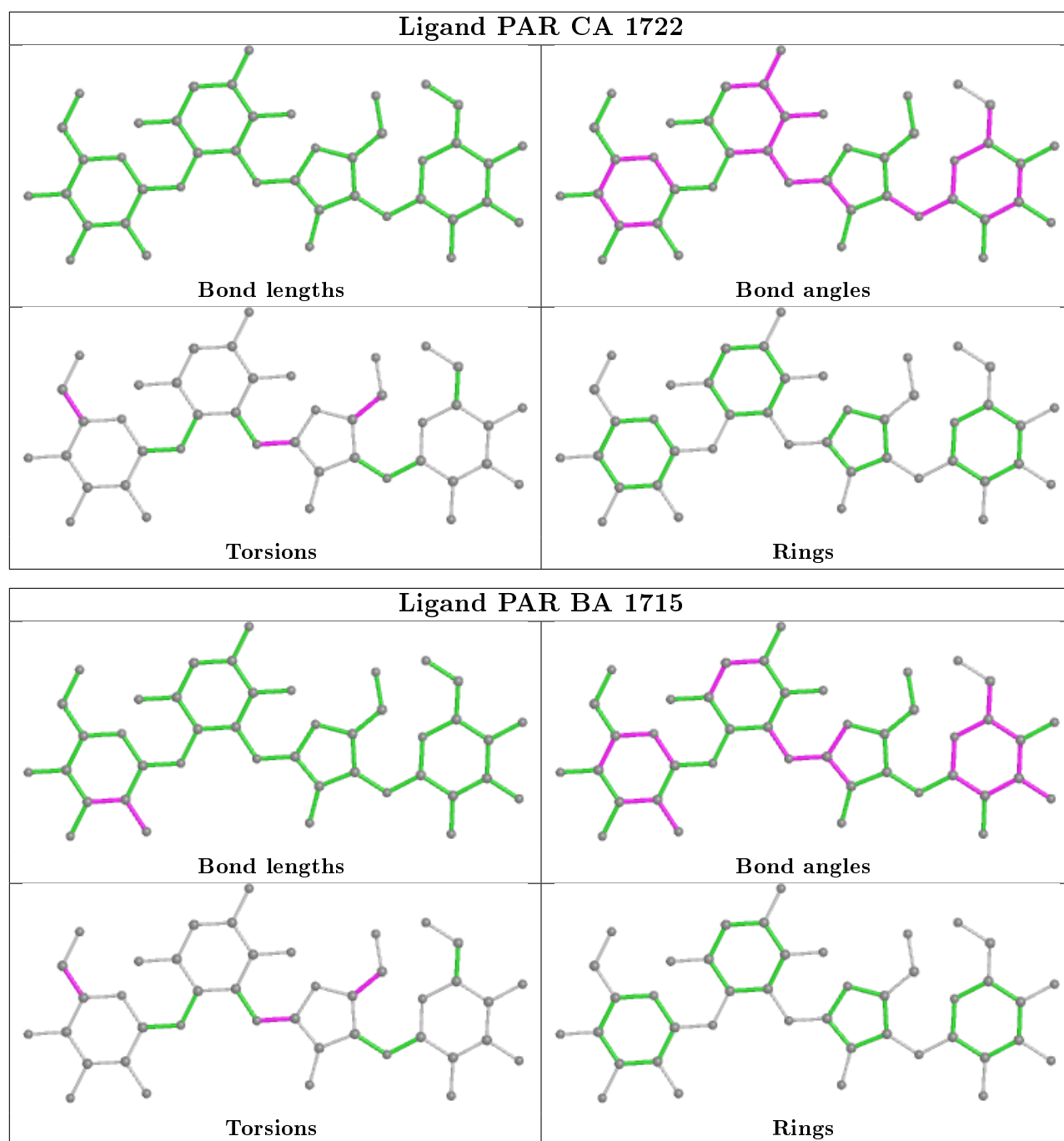
*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 56  | DA    | 3346 | OHX  | 1       | 0            |
| 56  | AO    | 202  | OHX  | 1       | 0            |
| 56  | DA    | 3473 | OHX  | 1       | 0            |
| 56  | DA    | 3081 | OHX  | 1       | 0            |
| 56  | DA    | 3461 | OHX  | 1       | 0            |
| 56  | BA    | 1794 | OHX  | 1       | 0            |
| 56  | BA    | 1799 | OHX  | 1       | 0            |
| 56  | AA    | 3467 | OHX  | 1       | 0            |
| 56  | DA    | 3341 | OHX  | 1       | 0            |
| 56  | DA    | 3488 | OHX  | 3       | 0            |
| 56  | DA    | 3162 | OHX  | 1       | 0            |
| 56  | CA    | 1775 | OHX  | 1       | 0            |
| 56  | BA    | 1801 | OHX  | 1       | 0            |
| 56  | CA    | 1773 | OHX  | 1       | 0            |
| 56  | AA    | 3362 | OHX  | 2       | 0            |
| 56  | AA    | 3414 | OHX  | 1       | 0            |
| 56  | CA    | 1734 | OHX  | 2       | 0            |
| 56  | BA    | 1802 | OHX  | 4       | 0            |
| 56  | CC    | 108  | OHX  | 6       | 0            |
| 56  | DA    | 3099 | OHX  | 1       | 0            |
| 56  | DA    | 3251 | OHX  | 1       | 0            |
| 56  | BA    | 1735 | OHX  | 1       | 0            |
| 56  | DA    | 3159 | OHX  | 1       | 0            |
| 56  | DA    | 3478 | OHX  | 2       | 0            |
| 56  | DA    | 3253 | OHX  | 1       | 0            |
| 56  | DA    | 3336 | OHX  | 1       | 0            |
| 56  | DA    | 3399 | OHX  | 1       | 0            |
| 56  | CA    | 1755 | OHX  | 1       | 0            |
| 56  | CA    | 1750 | OHX  | 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.



## 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 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed         | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|------------------|--------|---------------|-----------------------|-------|
| 1   | AA    | 2912/2912 (100%) | -0.31  | 41 (1%) 75 75 | 44, 79, 216, 250      | 0     |
| 1   | DA    | 2907/2912 (99%)  | -0.24  | 47 (1%) 72 70 | 56, 94, 236, 252      | 0     |
| 2   | AB    | 122/122 (100%)   | -0.46  | 1 (0%) 86 86  | 77, 99, 118, 184      | 0     |
| 2   | DB    | 122/122 (100%)   | -0.33  | 1 (0%) 86 86  | 98, 129, 153, 204     | 0     |
| 3   | AD    | 272/276 (98%)    | 0.09   | 2 (0%) 87 88  | 42, 67, 88, 106       | 0     |
| 3   | DD    | 272/276 (98%)    | 0.42   | 11 (4%) 38 36 | 52, 78, 98, 130       | 0     |
| 4   | AE    | 205/206 (99%)    | 0.24   | 10 (4%) 29 27 | 54, 90, 135, 147      | 0     |
| 4   | DE    | 205/206 (99%)    | 0.19   | 9 (4%) 34 33  | 61, 102, 153, 167     | 0     |
| 5   | AF    | 202/210 (96%)    | -0.16  | 3 (1%) 73 72  | 49, 84, 121, 136      | 0     |
| 5   | DF    | 208/210 (99%)    | 0.35   | 17 (8%) 11 11 | 63, 108, 164, 189     | 0     |
| 6   | AG    | 181/182 (99%)    | 0.79   | 28 (15%) 2 2  | 90, 112, 143, 155     | 0     |
| 6   | DG    | 181/182 (99%)    | 0.99   | 33 (18%) 1 1  | 122, 146, 169, 175    | 0     |
| 7   | AH    | 170/180 (94%)    | 0.08   | 6 (3%) 44 42  | 89, 116, 133, 162     | 0     |
| 7   | DH    | 170/180 (94%)    | 0.57   | 21 (12%) 4 3  | 162, 204, 226, 236    | 0     |
| 8   | AK    | 146/148 (98%)    | 0.21   | 7 (4%) 30 28  | 79, 134, 153, 155     | 0     |
| 8   | DK    | 146/148 (98%)    | 0.17   | 6 (4%) 37 35  | 88, 135, 157, 163     | 0     |
| 9   | AM    | 138/140 (98%)    | 0.16   | 6 (4%) 35 34  | 68, 92, 129, 141      | 0     |
| 9   | DM    | 138/140 (98%)    | 0.18   | 2 (1%) 75 75  | 83, 117, 146, 159     | 0     |
| 10  | AN    | 122/122 (100%)   | 0.25   | 2 (1%) 72 70  | 61, 79, 96, 107       | 0     |
| 10  | DN    | 122/122 (100%)   | 0.37   | 7 (5%) 23 23  | 75, 97, 114, 124      | 0     |
| 11  | AO    | 150/150 (100%)   | -0.06  | 7 (4%) 31 29  | 46, 93, 120, 166      | 0     |
| 11  | DO    | 150/150 (100%)   | 1.11   | 39 (26%) 0 0  | 45, 106, 147, 183     | 0     |
| 12  | AP    | 141/141 (100%)   | 0.36   | 13 (9%) 9 9   | 58, 86, 108, 136      | 0     |
| 12  | DP    | 141/141 (100%)   | 0.87   | 25 (17%) 1 1  | 58, 111, 143, 164     | 0     |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 13  | A0    | 118/118 (100%) | 0.02   | 1 (0%) 86 86  | 57, 86, 110, 118      | 0     |
| 13  | D0    | 117/118 (99%)  | -0.15  | 0 100 100     | 68, 89, 109, 124      | 0     |
| 14  | AQ    | 111/112 (99%)  | -0.06  | 2 (1%) 68 67  | 67, 97, 120, 133      | 0     |
| 14  | DQ    | 111/112 (99%)  | -0.04  | 3 (2%) 54 52  | 85, 126, 150, 162     | 0     |
| 15  | AR    | 137/146 (93%)  | 0.18   | 3 (2%) 62 60  | 75, 96, 149, 175      | 0     |
| 15  | DR    | 137/146 (93%)  | 0.48   | 11 (8%) 12 11 | 81, 106, 168, 189     | 0     |
| 16  | A1    | 117/118 (99%)  | -0.21  | 2 (1%) 70 68  | 58, 81, 110, 142      | 0     |
| 16  | D1    | 117/118 (99%)  | 0.60   | 9 (7%) 13 12  | 71, 109, 145, 167     | 0     |
| 17  | A2    | 101/101 (100%) | 0.14   | 5 (4%) 28 27  | 51, 104, 126, 143     | 0     |
| 17  | D2    | 101/101 (100%) | 1.28   | 24 (23%) 0 0  | 65, 134, 147, 155     | 0     |
| 18  | AS    | 113/113 (100%) | 0.16   | 2 (1%) 68 67  | 61, 77, 108, 161      | 0     |
| 18  | DS    | 113/113 (100%) | 0.06   | 3 (2%) 54 52  | 66, 82, 116, 162      | 0     |
| 19  | AT    | 92/96 (95%)    | -0.02  | 1 (1%) 80 81  | 59, 73, 99, 111       | 0     |
| 19  | DT    | 92/96 (95%)    | 0.15   | 5 (5%) 25 24  | 74, 92, 117, 133      | 0     |
| 20  | AU    | 102/110 (92%)  | 0.36   | 8 (7%) 13 12  | 79, 105, 156, 168     | 0     |
| 20  | DU    | 102/110 (92%)  | 0.76   | 18 (17%) 1 1  | 97, 122, 169, 185     | 0     |
| 21  | AV    | 175/206 (84%)  | 1.95   | 82 (46%) 0 0  | 90, 131, 195, 198     | 0     |
| 21  | DV    | 179/206 (86%)  | 2.70   | 85 (47%) 0 0  | 127, 165, 214, 226    | 0     |
| 22  | A3    | 76/85 (89%)    | 0.04   | 2 (2%) 56 53  | 65, 78, 95, 130       | 0     |
| 22  | D3    | 77/85 (90%)    | 0.14   | 3 (3%) 39 37  | 78, 97, 119, 152      | 0     |
| 23  | AZ    | 97/98 (98%)    | -0.12  | 1 (1%) 82 82  | 59, 79, 131, 161      | 0     |
| 23  | DZ    | 97/98 (98%)    | -0.05  | 2 (2%) 63 62  | 69, 89, 136, 157      | 0     |
| 24  | AW    | 66/72 (91%)    | 0.04   | 1 (1%) 73 72  | 63, 87, 103, 128      | 0     |
| 24  | DW    | 66/72 (91%)    | 0.53   | 2 (3%) 50 49  | 88, 112, 132, 142     | 0     |
| 25  | AX    | 59/60 (98%)    | -0.25  | 0 100 100     | 66, 86, 119, 134      | 0     |
| 25  | DX    | 59/60 (98%)    | 0.97   | 11 (18%) 1 1  | 87, 113, 146, 167     | 0     |
| 26  | A4    | 66/71 (92%)    | 2.25   | 32 (48%) 0 0  | 130, 162, 180, 188    | 0     |
| 26  | D4    | 63/71 (88%)    | 4.06   | 48 (76%) 0 0  | 149, 192, 200, 204    | 0     |
| 27  | A5    | 59/60 (98%)    | 0.59   | 7 (11%) 4 4   | 54, 95, 172, 174      | 0     |
| 27  | D5    | 59/60 (98%)    | 0.43   | 6 (10%) 6 6   | 61, 96, 179, 195      | 0     |
| 28  | A6    | 45/54 (83%)    | 9.35   | 45 (100%) 0 0 | 129, 159, 174, 182    | 0     |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|--------------|-----------------------|-------|
| 28  | D6    | 45/54 (83%)     | 6.57   | 39 (86%) 0 0 | 146, 174, 190, 192    | 0     |
| 29  | A7    | 45/49 (91%)     | -0.13  | 0 100 100    | 46, 55, 72, 78        | 0     |
| 29  | D7    | 45/49 (91%)     | 0.06   | 0 100 100    | 56, 66, 79, 96        | 0     |
| 30  | A8    | 60/65 (92%)     | 0.26   | 3 (5%) 28 27 | 56, 74, 97, 120       | 0     |
| 30  | D8    | 60/65 (92%)     | 0.55   | 5 (8%) 11 11 | 75, 91, 113, 138      | 0     |
| 31  | BA    | 1502/1506 (99%) | -0.54  | 4 (0%) 94 94 | 58, 111, 193, 251     | 0     |
| 31  | CA    | 1502/1506 (99%) | -0.54  | 3 (0%) 95 96 | 69, 122, 195, 251     | 0     |
| 32  | BE    | 237/256 (92%)   | 0.56   | 29 (12%) 4 3 | 117, 150, 188, 200    | 0     |
| 32  | CE    | 237/256 (92%)   | 1.33   | 65 (27%) 0 0 | 128, 166, 201, 216    | 0     |
| 33  | BF    | 205/239 (85%)   | 0.59   | 24 (11%) 4 4 | 95, 124, 157, 167     | 0     |
| 33  | CF    | 206/239 (86%)   | 0.84   | 32 (15%) 2 2 | 130, 151, 179, 185    | 0     |
| 34  | BG    | 208/208 (100%)  | -0.05  | 3 (1%) 75 75 | 95, 119, 141, 152     | 0     |
| 34  | CG    | 208/208 (100%)  | 0.15   | 4 (1%) 66 65 | 94, 114, 136, 151     | 0     |
| 35  | BH    | 151/162 (93%)   | 0.32   | 4 (2%) 56 53 | 81, 109, 130, 166     | 0     |
| 35  | CH    | 151/162 (93%)   | 0.17   | 4 (2%) 56 53 | 106, 124, 148, 171    | 0     |
| 36  | BI    | 101/101 (100%)  | 1.31   | 25 (24%) 0 0 | 86, 111, 127, 152     | 0     |
| 36  | CI    | 101/101 (100%)  | 0.47   | 2 (1%) 65 64 | 83, 108, 131, 149     | 0     |
| 37  | BJ    | 155/156 (99%)   | -0.10  | 8 (5%) 27 25 | 109, 127, 154, 167    | 0     |
| 37  | CJ    | 155/156 (99%)   | -0.08  | 4 (2%) 56 53 | 120, 136, 159, 167    | 0     |
| 38  | BK    | 138/138 (100%)  | -0.31  | 1 (0%) 87 88 | 90, 115, 128, 133     | 0     |
| 38  | CK    | 138/138 (100%)  | 0.02   | 2 (1%) 75 75 | 105, 129, 141, 151    | 0     |
| 39  | BL    | 127/128 (99%)   | -0.19  | 4 (3%) 49 48 | 98, 148, 166, 173     | 0     |
| 39  | CL    | 127/128 (99%)   | -0.36  | 2 (1%) 72 70 | 118, 160, 175, 179    | 0     |
| 40  | BM    | 99/105 (94%)    | 0.46   | 11 (11%) 5 5 | 93, 149, 177, 178     | 0     |
| 40  | CM    | 99/105 (94%)    | 0.26   | 4 (4%) 38 36 | 128, 165, 180, 184    | 0     |
| 41  | BN    | 119/129 (92%)   | 0.68   | 13 (10%) 5 5 | 81, 109, 138, 167     | 0     |
| 41  | CN    | 119/129 (92%)   | 1.67   | 45 (37%) 0 0 | 89, 116, 144, 172     | 0     |
| 42  | BO    | 125/132 (94%)   | 0.33   | 8 (6%) 19 19 | 73, 86, 118, 162      | 0     |
| 42  | CO    | 125/132 (94%)   | 1.02   | 23 (18%) 1 1 | 91, 113, 138, 172     | 0     |
| 43  | BP    | 116/126 (92%)   | -0.12  | 3 (2%) 56 53 | 97, 135, 151, 157     | 0     |
| 43  | CP    | 117/126 (92%)   | 0.33   | 11 (9%) 8 9  | 108, 162, 175, 177    | 0     |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2         | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 44  | BQ    | 58/61 (95%)       | -0.24  | 0 100 100       | 96, 113, 128, 134     | 0     |
| 44  | CQ    | 58/61 (95%)       | 0.97   | 11 (18%) 1 1    | 132, 145, 162, 167    | 0     |
| 45  | BR    | 88/89 (98%)       | 0.23   | 0 100 100       | 81, 103, 125, 130     | 0     |
| 45  | CR    | 88/89 (98%)       | 0.09   | 1 (1%) 80 81    | 88, 116, 138, 145     | 0     |
| 46  | BS    | 84/88 (95%)       | -0.10  | 0 100 100       | 105, 122, 147, 180    | 0     |
| 46  | CS    | 84/88 (95%)       | -0.06  | 1 (1%) 79 78    | 96, 108, 131, 164     | 0     |
| 47  | BT    | 100/105 (95%)     | -0.11  | 2 (2%) 65 64    | 95, 114, 128, 135     | 0     |
| 47  | CT    | 100/105 (95%)     | -0.12  | 3 (3%) 50 49    | 96, 117, 138, 149     | 0     |
| 48  | BU    | 72/88 (81%)       | 1.54   | 22 (30%) 0 0    | 94, 111, 147, 169     | 0     |
| 48  | CU    | 72/88 (81%)       | 1.66   | 18 (25%) 0 0    | 98, 120, 160, 178     | 0     |
| 49  | BV    | 78/93 (83%)       | 0.10   | 5 (6%) 19 19    | 113, 135, 155, 159    | 0     |
| 49  | CV    | 78/93 (83%)       | 0.79   | 17 (21%) 0 1    | 146, 170, 187, 192    | 0     |
| 50  | BW    | 99/106 (93%)      | -0.61  | 0 100 100       | 113, 129, 159, 167    | 0     |
| 50  | CW    | 99/106 (93%)      | -0.16  | 1 (1%) 82 82    | 100, 122, 157, 170    | 0     |
| 51  | BX    | 25/27 (92%)       | -0.55  | 0 100 100       | 110, 123, 139, 157    | 0     |
| 51  | CX    | 25/27 (92%)       | 0.04   | 2 (8%) 12 11    | 126, 148, 165, 175    | 0     |
| 52  | BB    | 84/85 (98%)       | 3.42   | 59 (70%) 0 0    | 98, 138, 163, 176     | 0     |
| 52  | BD    | 84/85 (98%)       | 0.27   | 7 (8%) 11 11    | 78, 144, 223, 233     | 0     |
| 52  | CB    | 84/85 (98%)       | 5.75   | 72 (85%) 0 0    | 113, 143, 166, 176    | 0     |
| 52  | CD    | 84/85 (98%)       | -0.13  | 1 (1%) 79 78    | 86, 144, 222, 230     | 0     |
| 53  | BC    | 77/77 (100%)      | -0.27  | 1 (1%) 77 77    | 82, 117, 146, 159     | 0     |
| 53  | CC    | 77/77 (100%)      | -0.19  | 1 (1%) 77 77    | 92, 127, 156, 164     | 0     |
| 54  | B1    | 16/16 (100%)      | 0.78   | 3 (18%) 1 1     | 81, 117, 161, 169     | 0     |
| 54  | C1    | 16/16 (100%)      | 0.88   | 2 (12%) 3 3     | 90, 122, 168, 176     | 0     |
| All | All   | 21100/21658 (97%) | 0.14   | 1382 (6%) 18 18 | 42, 108, 188, 252     | 0     |

The worst 5 of 1382 RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 28  | A6    | 29   | ASN  | 16.7 |
| 52  | CB    | 52   | G    | 16.0 |
| 52  | CB    | 16   | C    | 15.1 |
| 28  | A6    | 18   | ARG  | 14.8 |
| 1   | AA    | 2901 | C    | 14.4 |

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 52  | MIA  | CB    | 38  | 29/30 | 0.89 | 0.38 | 99,111,127,136             | 0     |
| 52  | MIA  | BD    | 38  | 29/30 | 0.90 | 0.24 | 126,140,181,195            | 0     |
| 52  | MIA  | CD    | 38  | 29/30 | 0.91 | 0.23 | 127,140,183,200            | 0     |
| 52  | MIA  | BB    | 38  | 29/30 | 0.95 | 0.19 | 92,99,110,128              | 0     |

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 55  | MG   | AA    | 3291 | 1/1   | 0.11 | 0.43 | 99,99,99,99                | 0     |
| 55  | MG   | CA    | 1685 | 1/1   | 0.13 | 0.48 | 104,104,104,104            | 0     |
| 55  | MG   | CA    | 1672 | 1/1   | 0.22 | 0.76 | 125,125,125,125            | 0     |
| 55  | MG   | DA    | 3320 | 1/1   | 0.26 | 0.44 | 132,132,132,132            | 0     |
| 55  | MG   | AA    | 3222 | 1/1   | 0.29 | 0.42 | 85,85,85,85                | 0     |
| 55  | MG   | AA    | 3078 | 1/1   | 0.30 | 0.27 | 97,97,97,97                | 0     |
| 55  | MG   | CA    | 1629 | 1/1   | 0.33 | 0.50 | 166,166,166,166            | 0     |
| 55  | MG   | BB    | 104  | 1/1   | 0.37 | 0.77 | 100,100,100,100            | 0     |
| 55  | MG   | CA    | 1686 | 1/1   | 0.39 | 0.61 | 110,110,110,110            | 0     |
| 55  | MG   | BB    | 108  | 1/1   | 0.40 | 0.27 | 80,80,80,80                | 0     |
| 55  | MG   | DA    | 3053 | 1/1   | 0.41 | 0.43 | 116,116,116,116            | 0     |
| 55  | MG   | AA    | 3343 | 1/1   | 0.42 | 0.27 | 92,92,92,92                | 0     |
| 55  | MG   | DA    | 3307 | 1/1   | 0.42 | 0.49 | 119,119,119,119            | 0     |
| 55  | MG   | AA    | 3306 | 1/1   | 0.42 | 0.40 | 100,100,100,100            | 0     |
| 55  | MG   | BA    | 1639 | 1/1   | 0.45 | 0.20 | 101,101,101,101            | 0     |
| 55  | MG   | DA    | 3049 | 1/1   | 0.45 | 0.36 | 104,104,104,104            | 0     |
| 55  | MG   | BB    | 113  | 1/1   | 0.47 | 0.25 | 80,80,80,80                | 0     |
| 55  | MG   | AA    | 3089 | 1/1   | 0.49 | 0.23 | 130,130,130,130            | 0     |

*Continued on next page...*

Continued from previous page...

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 55  | MG   | CA    | 1681 | 1/1   | 0.50 | 0.28 | 111,111,111,111            | 0     |
| 55  | MG   | CA    | 1628 | 1/1   | 0.51 | 0.20 | 137,137,137,137            | 0     |
| 55  | MG   | BA    | 1685 | 1/1   | 0.53 | 0.22 | 93,93,93,93                | 0     |
| 55  | MG   | BW    | 201  | 1/1   | 0.55 | 0.19 | 92,92,92,92                | 0     |
| 55  | MG   | BA    | 1695 | 1/1   | 0.55 | 0.23 | 132,132,132,132            | 0     |
| 55  | MG   | DA    | 3322 | 1/1   | 0.56 | 0.18 | 152,152,152,152            | 0     |
| 55  | MG   | BA    | 1602 | 1/1   | 0.56 | 0.23 | 66,66,66,66                | 0     |
| 55  | MG   | DA    | 3203 | 1/1   | 0.58 | 0.59 | 69,69,69,69                | 0     |
| 55  | MG   | BB    | 106  | 1/1   | 0.59 | 0.56 | 102,102,102,102            | 0     |
| 55  | MG   | CA    | 1692 | 1/1   | 0.59 | 0.22 | 104,104,104,104            | 0     |
| 55  | MG   | AA    | 3084 | 1/1   | 0.60 | 0.27 | 104,104,104,104            | 0     |
| 55  | MG   | CA    | 1683 | 1/1   | 0.60 | 0.39 | 79,79,79,79                | 0     |
| 55  | MG   | CA    | 1665 | 1/1   | 0.60 | 0.28 | 114,114,114,114            | 0     |
| 55  | MG   | BA    | 1657 | 1/1   | 0.61 | 0.33 | 87,87,87,87                | 0     |
| 55  | MG   | BA    | 1706 | 1/1   | 0.63 | 0.34 | 111,111,111,111            | 0     |
| 55  | MG   | BA    | 1625 | 1/1   | 0.63 | 0.32 | 66,66,66,66                | 0     |
| 55  | MG   | BA    | 1670 | 1/1   | 0.63 | 0.30 | 100,100,100,100            | 0     |
| 55  | MG   | DA    | 3252 | 1/1   | 0.64 | 0.61 | 81,81,81,81                | 0     |
| 55  | MG   | DA    | 3330 | 1/1   | 0.65 | 0.68 | 81,81,81,81                | 0     |
| 55  | MG   | BS    | 101  | 1/1   | 0.65 | 0.19 | 81,81,81,81                | 0     |
| 55  | MG   | CA    | 1720 | 1/1   | 0.65 | 0.90 | 110,110,110,110            | 0     |
| 55  | MG   | AA    | 3096 | 1/1   | 0.66 | 0.59 | 76,76,76,76                | 0     |
| 55  | MG   | BA    | 1714 | 1/1   | 0.66 | 0.63 | 83,83,83,83                | 0     |
| 56  | OHX  | BD    | 104  | 7/7   | 0.66 | 0.35 | 94,101,103,107             | 3     |
| 55  | MG   | AA    | 3300 | 1/1   | 0.66 | 0.27 | 81,81,81,81                | 0     |
| 55  | MG   | AA    | 3337 | 1/1   | 0.66 | 0.64 | 73,73,73,73                | 0     |
| 55  | MG   | BB    | 105  | 1/1   | 0.67 | 0.17 | 94,94,94,94                | 0     |
| 55  | MG   | DA    | 3311 | 1/1   | 0.67 | 0.41 | 63,63,63,63                | 0     |
| 55  | MG   | CA    | 1699 | 1/1   | 0.67 | 0.44 | 86,86,86,86                | 0     |
| 55  | MG   | BA    | 1704 | 1/1   | 0.67 | 0.09 | 127,127,127,127            | 0     |
| 55  | MG   | DA    | 3048 | 1/1   | 0.67 | 0.49 | 93,93,93,93                | 0     |
| 55  | MG   | CA    | 1641 | 1/1   | 0.68 | 0.48 | 85,85,85,85                | 0     |
| 55  | MG   | DA    | 3303 | 1/1   | 0.68 | 0.20 | 97,97,97,97                | 0     |
| 55  | MG   | A3    | 101  | 1/1   | 0.68 | 0.43 | 71,71,71,71                | 0     |
| 55  | MG   | AA    | 3305 | 1/1   | 0.68 | 0.56 | 66,66,66,66                | 0     |
| 55  | MG   | DB    | 206  | 1/1   | 0.68 | 0.51 | 81,81,81,81                | 0     |
| 55  | MG   | CA    | 1623 | 1/1   | 0.68 | 0.26 | 96,96,96,96                | 0     |
| 55  | MG   | CA    | 1646 | 1/1   | 0.68 | 0.29 | 79,79,79,79                | 0     |
| 55  | MG   | DA    | 3145 | 1/1   | 0.69 | 1.00 | 82,82,82,82                | 0     |
| 55  | MG   | CA    | 1609 | 1/1   | 0.69 | 0.37 | 112,112,112,112            | 0     |
| 55  | MG   | BB    | 102  | 1/1   | 0.69 | 0.29 | 92,92,92,92                | 0     |
| 55  | MG   | DA    | 3100 | 1/1   | 0.70 | 0.31 | 87,87,87,87                | 0     |

Continued on next page...



*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | BB    | 111  | 1/1   | 0.70 | 0.34 | 80,80,80,80                 | 0     |
| 55  | MG   | BA    | 1630 | 1/1   | 0.70 | 0.24 | 109,109,109,109             | 0     |
| 55  | MG   | CA    | 1719 | 1/1   | 0.70 | 0.35 | 94,94,94,94                 | 0     |
| 55  | MG   | DA    | 3181 | 1/1   | 0.70 | 0.31 | 98,98,98,98                 | 0     |
| 55  | MG   | CA    | 1708 | 1/1   | 0.70 | 0.11 | 95,95,95,95                 | 0     |
| 55  | MG   | DA    | 3327 | 1/1   | 0.70 | 0.25 | 73,73,73,73                 | 0     |
| 55  | MG   | BA    | 1624 | 1/1   | 0.71 | 0.65 | 79,79,79,79                 | 0     |
| 55  | MG   | AA    | 3091 | 1/1   | 0.71 | 0.28 | 85,85,85,85                 | 0     |
| 55  | MG   | CA    | 1704 | 1/1   | 0.71 | 0.12 | 135,135,135,135             | 0     |
| 56  | OHX  | AA    | 3508 | 7/7   | 0.72 | 0.12 | 192,206,214,236             | 1     |
| 55  | MG   | BA    | 1677 | 1/1   | 0.72 | 0.38 | 101,101,101,101             | 0     |
| 55  | MG   | CA    | 1614 | 1/1   | 0.72 | 0.18 | 118,118,118,118             | 0     |
| 55  | MG   | BA    | 1675 | 1/1   | 0.72 | 0.43 | 87,87,87,87                 | 0     |
| 55  | MG   | AA    | 3215 | 1/1   | 0.72 | 0.42 | 69,69,69,69                 | 0     |
| 55  | MG   | AA    | 3301 | 1/1   | 0.72 | 0.18 | 97,97,97,97                 | 0     |
| 55  | MG   | AA    | 3322 | 1/1   | 0.73 | 0.27 | 81,81,81,81                 | 0     |
| 55  | MG   | AA    | 3278 | 1/1   | 0.73 | 0.39 | 73,73,73,73                 | 0     |
| 55  | MG   | AA    | 3281 | 1/1   | 0.73 | 0.17 | 93,93,93,93                 | 0     |
| 55  | MG   | DA    | 3233 | 1/1   | 0.73 | 0.32 | 65,65,65,65                 | 0     |
| 55  | MG   | BA    | 1615 | 1/1   | 0.73 | 0.41 | 78,78,78,78                 | 0     |
| 55  | MG   | DA    | 3302 | 1/1   | 0.73 | 0.34 | 98,98,98,98                 | 0     |
| 55  | MG   | AA    | 3209 | 1/1   | 0.73 | 0.33 | 86,86,86,86                 | 0     |
| 55  | MG   | DA    | 3158 | 1/1   | 0.73 | 0.64 | 88,88,88,88                 | 0     |
| 55  | MG   | C1    | 101  | 1/1   | 0.73 | 0.29 | 102,102,102,102             | 0     |
| 55  | MG   | BA    | 1613 | 1/1   | 0.73 | 0.13 | 116,116,116,116             | 0     |
| 55  | MG   | CA    | 1716 | 1/1   | 0.73 | 0.34 | 79,79,79,79                 | 0     |
| 55  | MG   | AA    | 3245 | 1/1   | 0.73 | 0.68 | 70,70,70,70                 | 0     |
| 55  | MG   | CA    | 1651 | 1/1   | 0.74 | 0.18 | 73,73,73,73                 | 0     |
| 55  | MG   | AA    | 3277 | 1/1   | 0.74 | 0.46 | 94,94,94,94                 | 0     |
| 55  | MG   | BA    | 1674 | 1/1   | 0.74 | 0.22 | 67,67,67,67                 | 0     |
| 55  | MG   | CA    | 1653 | 1/1   | 0.74 | 0.23 | 75,75,75,75                 | 0     |
| 55  | MG   | DB    | 201  | 1/1   | 0.74 | 0.12 | 95,95,95,95                 | 0     |
| 55  | MG   | DA    | 3259 | 1/1   | 0.74 | 0.34 | 114,114,114,114             | 0     |
| 55  | MG   | BA    | 1703 | 1/1   | 0.74 | 0.22 | 90,90,90,90                 | 0     |
| 55  | MG   | DA    | 3201 | 1/1   | 0.74 | 0.46 | 86,86,86,86                 | 0     |
| 55  | MG   | DA    | 3112 | 1/1   | 0.74 | 0.55 | 85,85,85,85                 | 0     |
| 55  | MG   | AA    | 3269 | 1/1   | 0.74 | 0.36 | 59,59,59,59                 | 0     |
| 55  | MG   | CA    | 1718 | 1/1   | 0.75 | 0.28 | 84,84,84,84                 | 0     |
| 55  | MG   | AA    | 3323 | 1/1   | 0.75 | 0.26 | 58,58,58,58                 | 0     |
| 55  | MG   | DA    | 3328 | 1/1   | 0.75 | 0.21 | 99,99,99,99                 | 0     |
| 55  | MG   | BA    | 1621 | 1/1   | 0.75 | 0.27 | 77,77,77,77                 | 0     |
| 55  | MG   | BA    | 1683 | 1/1   | 0.75 | 0.33 | 85,85,85,85                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 56  | OHX  | CB    | 105  | 7/7   | 0.75 | 0.33 | 139,142,156,183            | 2     |
| 56  | OHX  | AA    | 3497 | 7/7   | 0.75 | 0.23 | 105,127,139,145            | 1     |
| 56  | OHX  | BA    | 1804 | 7/7   | 0.75 | 0.17 | 147,154,164,208            | 1     |
| 55  | MG   | AA    | 3141 | 1/1   | 0.75 | 0.34 | 80,80,80,80                | 0     |
| 55  | MG   | DA    | 3264 | 1/1   | 0.75 | 0.15 | 78,78,78,78                | 0     |
| 55  | MG   | CC    | 103  | 1/1   | 0.76 | 0.72 | 97,97,97,97                | 0     |
| 55  | MG   | AA    | 3324 | 1/1   | 0.76 | 0.18 | 84,84,84,84                | 0     |
| 55  | MG   | CC    | 104  | 1/1   | 0.76 | 0.49 | 89,89,89,89                | 0     |
| 55  | MG   | DA    | 3304 | 1/1   | 0.76 | 0.16 | 89,89,89,89                | 0     |
| 55  | MG   | DA    | 3039 | 1/1   | 0.77 | 0.20 | 102,102,102,102            | 0     |
| 55  | MG   | BA    | 1705 | 1/1   | 0.77 | 0.08 | 109,109,109,109            | 0     |
| 55  | MG   | BB    | 110  | 1/1   | 0.77 | 0.27 | 80,80,80,80                | 0     |
| 55  | MG   | CA    | 1617 | 1/1   | 0.77 | 0.13 | 126,126,126,126            | 0     |
| 55  | MG   | CA    | 1662 | 1/1   | 0.77 | 0.40 | 92,92,92,92                | 0     |
| 55  | MG   | CA    | 1668 | 1/1   | 0.77 | 0.43 | 80,80,80,80                | 0     |
| 55  | MG   | AA    | 3154 | 1/1   | 0.77 | 0.23 | 52,52,52,52                | 0     |
| 55  | MG   | CB    | 101  | 1/1   | 0.77 | 0.43 | 105,105,105,105            | 0     |
| 55  | MG   | AA    | 3083 | 1/1   | 0.77 | 0.34 | 94,94,94,94                | 0     |
| 55  | MG   | DA    | 3256 | 1/1   | 0.77 | 0.30 | 89,89,89,89                | 0     |
| 55  | MG   | CA    | 1674 | 1/1   | 0.77 | 0.60 | 97,97,97,97                | 0     |
| 55  | MG   | DA    | 3298 | 1/1   | 0.77 | 0.20 | 102,102,102,102            | 0     |
| 55  | MG   | DA    | 3288 | 1/1   | 0.77 | 0.27 | 82,82,82,82                | 0     |
| 55  | MG   | CA    | 1721 | 1/1   | 0.77 | 0.17 | 80,80,80,80                | 0     |
| 55  | MG   | DA    | 3331 | 1/1   | 0.78 | 0.45 | 69,69,69,69                | 0     |
| 55  | MG   | AA    | 3061 | 1/1   | 0.78 | 0.30 | 59,59,59,59                | 0     |
| 55  | MG   | C1    | 102  | 1/1   | 0.78 | 0.39 | 104,104,104,104            | 0     |
| 55  | MG   | DA    | 3092 | 1/1   | 0.78 | 0.27 | 74,74,74,74                | 0     |
| 55  | MG   | CA    | 1622 | 1/1   | 0.78 | 0.34 | 89,89,89,89                | 0     |
| 56  | OHX  | BA    | 1776 | 7/7   | 0.78 | 0.31 | 119,138,152,176            | 2     |
| 55  | MG   | AA    | 3279 | 1/1   | 0.78 | 0.52 | 90,90,90,90                | 0     |
| 55  | MG   | DA    | 3096 | 1/1   | 0.78 | 0.23 | 85,85,85,85                | 0     |
| 55  | MG   | AA    | 3236 | 1/1   | 0.78 | 0.49 | 66,66,66,66                | 0     |
| 55  | MG   | BA    | 1699 | 1/1   | 0.78 | 0.53 | 84,84,84,84                | 0     |
| 56  | OHX  | DB    | 219  | 7/7   | 0.78 | 0.17 | 147,161,178,209            | 1     |
| 55  | MG   | DA    | 3295 | 1/1   | 0.78 | 0.49 | 77,77,77,77                | 0     |
| 55  | MG   | CA    | 1689 | 1/1   | 0.78 | 0.18 | 80,80,80,80                | 0     |
| 55  | MG   | CA    | 1712 | 1/1   | 0.78 | 0.16 | 83,83,83,83                | 0     |
| 55  | MG   | BA    | 1708 | 1/1   | 0.79 | 0.19 | 80,80,80,80                | 0     |
| 55  | MG   | AB    | 201  | 1/1   | 0.79 | 0.28 | 85,85,85,85                | 0     |
| 55  | MG   | AA    | 3229 | 1/1   | 0.79 | 0.26 | 65,65,65,65                | 0     |
| 55  | MG   | AA    | 3062 | 1/1   | 0.79 | 0.25 | 97,97,97,97                | 0     |
| 55  | MG   | AA    | 3372 | 1/1   | 0.79 | 0.30 | 80,80,80,80                | 0     |

*Continued on next page...*

Continued from previous page...

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 55  | MG   | BA    | 1640 | 1/1   | 0.79 | 0.20 | 71,71,71,71                | 0     |
| 55  | MG   | DA    | 3196 | 1/1   | 0.79 | 0.41 | 54,54,54,54                | 0     |
| 55  | MG   | AA    | 3048 | 1/1   | 0.79 | 0.20 | 91,91,91,91                | 0     |
| 55  | MG   | AA    | 3111 | 1/1   | 0.79 | 0.37 | 69,69,69,69                | 0     |
| 55  | MG   | CA    | 1621 | 1/1   | 0.79 | 0.28 | 110,110,110,110            | 0     |
| 56  | OHX  | DA    | 3124 | 7/7   | 0.79 | 0.15 | 144,164,170,220            | 1     |
| 56  | OHX  | CA    | 1804 | 7/7   | 0.79 | 0.27 | 145,149,162,192            | 1     |
| 55  | MG   | CA    | 1624 | 1/1   | 0.79 | 0.11 | 114,114,114,114            | 0     |
| 55  | MG   | DA    | 3287 | 1/1   | 0.80 | 0.22 | 102,102,102,102            | 0     |
| 56  | OHX  | AA    | 3531 | 7/7   | 0.80 | 0.18 | 225,229,234,256            | 1     |
| 55  | MG   | AA    | 3043 | 1/1   | 0.80 | 0.35 | 75,75,75,75                | 0     |
| 56  | OHX  | BA    | 1813 | 7/7   | 0.80 | 0.19 | 151,161,170,205            | 1     |
| 55  | MG   | AA    | 3156 | 1/1   | 0.80 | 0.31 | 80,80,80,80                | 0     |
| 55  | MG   | AA    | 3235 | 1/1   | 0.80 | 0.11 | 57,57,57,57                | 0     |
| 55  | MG   | AA    | 3142 | 1/1   | 0.80 | 0.46 | 75,75,75,75                | 0     |
| 55  | MG   | DA    | 3325 | 1/1   | 0.80 | 0.31 | 91,91,91,91                | 0     |
| 55  | MG   | AA    | 3092 | 1/1   | 0.80 | 0.12 | 92,92,92,92                | 0     |
| 55  | MG   | BA    | 1612 | 1/1   | 0.80 | 0.33 | 100,100,100,100            | 0     |
| 55  | MG   | BA    | 1680 | 1/1   | 0.80 | 0.22 | 64,64,64,64                | 0     |
| 55  | MG   | BA    | 1687 | 1/1   | 0.81 | 0.24 | 96,96,96,96                | 0     |
| 55  | MG   | AA    | 3284 | 1/1   | 0.81 | 0.31 | 68,68,68,68                | 0     |
| 55  | MG   | DA    | 3042 | 1/1   | 0.81 | 0.23 | 74,74,74,74                | 0     |
| 55  | MG   | BA    | 1650 | 1/1   | 0.81 | 0.23 | 85,85,85,85                | 0     |
| 55  | MG   | AA    | 3076 | 1/1   | 0.81 | 0.24 | 81,81,81,81                | 0     |
| 55  | MG   | AA    | 3257 | 1/1   | 0.81 | 0.32 | 64,64,64,64                | 0     |
| 55  | MG   | BC    | 104  | 1/1   | 0.81 | 0.38 | 88,88,88,88                | 0     |
| 55  | MG   | BA    | 1636 | 1/1   | 0.81 | 0.14 | 111,111,111,111            | 0     |
| 55  | MG   | AF    | 302  | 1/1   | 0.81 | 0.20 | 83,83,83,83                | 0     |
| 55  | MG   | D7    | 101  | 1/1   | 0.81 | 0.49 | 69,69,69,69                | 0     |
| 55  | MG   | DA    | 3313 | 1/1   | 0.81 | 0.34 | 88,88,88,88                | 0     |
| 55  | MG   | DA    | 3242 | 1/1   | 0.81 | 0.57 | 99,99,99,99                | 0     |
| 55  | MG   | DA    | 3318 | 1/1   | 0.81 | 0.19 | 110,110,110,110            | 0     |
| 55  | MG   | B1    | 101  | 1/1   | 0.81 | 0.14 | 96,96,96,96                | 0     |
| 55  | MG   | AA    | 3295 | 1/1   | 0.81 | 0.45 | 89,89,89,89                | 0     |
| 55  | MG   | DA    | 3046 | 1/1   | 0.81 | 0.38 | 78,78,78,78                | 0     |
| 55  | MG   | BA    | 1637 | 1/1   | 0.81 | 0.21 | 99,99,99,99                | 0     |
| 55  | MG   | AA    | 3157 | 1/1   | 0.81 | 0.41 | 86,86,86,86                | 0     |
| 55  | MG   | AA    | 3105 | 1/1   | 0.81 | 0.46 | 65,65,65,65                | 0     |
| 55  | MG   | CA    | 1696 | 1/1   | 0.81 | 0.59 | 74,74,74,74                | 0     |
| 55  | MG   | AA    | 3259 | 1/1   | 0.81 | 0.13 | 60,60,60,60                | 0     |
| 55  | MG   | BB    | 103  | 1/1   | 0.81 | 0.21 | 105,105,105,105            | 0     |
| 55  | MG   | AA    | 3308 | 1/1   | 0.81 | 0.40 | 63,63,63,63                | 0     |

Continued on next page...

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 56  | OHX  | CA    | 1797 | 7/7   | 0.82 | 0.36 | 129,132,139,171            | 1     |
| 55  | MG   | DA    | 3333 | 1/1   | 0.82 | 0.31 | 84,84,84,84                | 0     |
| 55  | MG   | BA    | 1709 | 1/1   | 0.82 | 0.15 | 68,68,68,68                | 0     |
| 55  | MG   | DA    | 3069 | 1/1   | 0.82 | 0.13 | 63,63,63,63                | 0     |
| 55  | MG   | CA    | 1687 | 1/1   | 0.82 | 0.29 | 104,104,104,104            | 0     |
| 55  | MG   | DA    | 3310 | 1/1   | 0.82 | 0.22 | 73,73,73,73                | 0     |
| 55  | MG   | AA    | 3316 | 1/1   | 0.82 | 0.18 | 79,79,79,79                | 0     |
| 55  | MG   | DA    | 3054 | 1/1   | 0.82 | 0.15 | 56,56,56,56                | 0     |
| 55  | MG   | CA    | 1657 | 1/1   | 0.82 | 0.21 | 81,81,81,81                | 0     |
| 55  | MG   | AA    | 3193 | 1/1   | 0.82 | 0.39 | 86,86,86,86                | 0     |
| 55  | MG   | DA    | 3296 | 1/1   | 0.82 | 0.35 | 103,103,103,103            | 0     |
| 55  | MG   | A1    | 201  | 1/1   | 0.82 | 0.34 | 62,62,62,62                | 0     |
| 55  | MG   | AA    | 3143 | 1/1   | 0.82 | 0.49 | 87,87,87,87                | 0     |
| 55  | MG   | CA    | 1652 | 1/1   | 0.82 | 0.10 | 69,69,69,69                | 0     |
| 56  | OHX  | AA    | 3538 | 7/7   | 0.82 | 0.17 | 95,101,128,162             | 1     |
| 55  | MG   | AA    | 3334 | 1/1   | 0.82 | 0.15 | 90,90,90,90                | 0     |
| 55  | MG   | AA    | 3122 | 1/1   | 0.83 | 0.25 | 57,57,57,57                | 0     |
| 55  | MG   | DA    | 3270 | 1/1   | 0.83 | 0.68 | 73,73,73,73                | 0     |
| 55  | MG   | CA    | 1715 | 1/1   | 0.83 | 0.38 | 80,80,80,80                | 0     |
| 55  | MG   | CB    | 103  | 1/1   | 0.83 | 0.18 | 80,80,80,80                | 0     |
| 55  | MG   | CA    | 1643 | 1/1   | 0.83 | 0.50 | 68,68,68,68                | 0     |
| 56  | OHX  | AA    | 3520 | 7/7   | 0.83 | 0.25 | 88,95,98,151               | 2     |
| 55  | MG   | CA    | 1620 | 1/1   | 0.83 | 0.27 | 63,63,63,63                | 0     |
| 55  | MG   | AA    | 3120 | 1/1   | 0.83 | 0.50 | 74,74,74,74                | 0     |
| 56  | OHX  | AA    | 3507 | 7/7   | 0.83 | 0.48 | 120,135,161,172            | 2     |
| 55  | MG   | AA    | 3173 | 1/1   | 0.83 | 0.45 | 65,65,65,65                | 0     |
| 55  | MG   | CA    | 1703 | 1/1   | 0.83 | 0.48 | 84,84,84,84                | 0     |
| 55  | MG   | BA    | 1689 | 1/1   | 0.83 | 0.13 | 80,80,80,80                | 0     |
| 55  | MG   | DA    | 3284 | 1/1   | 0.83 | 0.24 | 89,89,89,89                | 0     |
| 55  | MG   | CA    | 1710 | 1/1   | 0.83 | 0.16 | 78,78,78,78                | 0     |
| 55  | MG   | CA    | 1677 | 1/1   | 0.83 | 0.44 | 73,73,73,73                | 0     |
| 55  | MG   | DA    | 3117 | 1/1   | 0.83 | 0.29 | 82,82,82,82                | 0     |
| 55  | MG   | DA    | 3332 | 1/1   | 0.83 | 0.18 | 78,78,78,78                | 0     |
| 55  | MG   | DA    | 3237 | 1/1   | 0.83 | 0.31 | 85,85,85,85                | 0     |
| 55  | MG   | AA    | 3138 | 1/1   | 0.83 | 0.21 | 78,78,78,78                | 0     |
| 55  | MG   | BA    | 1653 | 1/1   | 0.83 | 0.29 | 64,64,64,64                | 0     |
| 55  | MG   | CB    | 102  | 1/1   | 0.83 | 0.34 | 80,80,80,80                | 0     |
| 56  | OHX  | DA    | 3251 | 7/7   | 0.83 | 0.26 | 102,112,141,176            | 3     |
| 55  | MG   | CA    | 1676 | 1/1   | 0.84 | 0.34 | 78,78,78,78                | 0     |
| 55  | MG   | BA    | 1628 | 1/1   | 0.84 | 0.30 | 95,95,95,95                | 0     |
| 55  | MG   | AA    | 3290 | 1/1   | 0.84 | 0.35 | 66,66,66,66                | 0     |
| 55  | MG   | DA    | 3324 | 1/1   | 0.84 | 0.53 | 66,66,66,66                | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 56  | OHX  | CA    | 1774 | 7/7   | 0.84 | 0.18 | 137,150,161,190            | 1     |
| 55  | MG   | DA    | 3244 | 1/1   | 0.84 | 0.29 | 82,82,82,82                | 0     |
| 55  | MG   | DA    | 3278 | 1/1   | 0.84 | 0.38 | 84,84,84,84                | 0     |
| 55  | MG   | BA    | 1696 | 1/1   | 0.84 | 0.27 | 94,94,94,94                | 0     |
| 56  | OHX  | BA    | 1772 | 7/7   | 0.84 | 0.10 | 165,176,177,219            | 1     |
| 55  | MG   | CA    | 1626 | 1/1   | 0.84 | 0.31 | 124,124,124,124            | 0     |
| 55  | MG   | CA    | 1693 | 1/1   | 0.84 | 0.15 | 55,55,55,55                | 0     |
| 55  | MG   | AA    | 3217 | 1/1   | 0.84 | 0.20 | 66,66,66,66                | 0     |
| 55  | MG   | DA    | 3199 | 1/1   | 0.84 | 0.56 | 77,77,77,77                | 0     |
| 55  | MG   | CA    | 1667 | 1/1   | 0.84 | 0.43 | 78,78,78,78                | 0     |
| 55  | MG   | DA    | 3319 | 1/1   | 0.84 | 0.48 | 69,69,69,69                | 0     |
| 55  | MG   | CA    | 1605 | 1/1   | 0.84 | 0.26 | 75,75,75,75                | 0     |
| 55  | MG   | DA    | 3202 | 1/1   | 0.84 | 0.45 | 65,65,65,65                | 0     |
| 55  | MG   | BA    | 1635 | 1/1   | 0.84 | 0.06 | 86,86,86,86                | 0     |
| 55  | MG   | CC    | 107  | 1/1   | 0.85 | 0.27 | 80,80,80,80                | 0     |
| 55  | MG   | CA    | 1627 | 1/1   | 0.85 | 0.27 | 126,126,126,126            | 0     |
| 55  | MG   | DA    | 3306 | 1/1   | 0.85 | 0.51 | 86,86,86,86                | 0     |
| 55  | MG   | BA    | 1643 | 1/1   | 0.85 | 0.21 | 67,67,67,67                | 0     |
| 55  | MG   | AA    | 3060 | 1/1   | 0.85 | 0.24 | 89,89,89,89                | 0     |
| 56  | OHX  | AA    | 3546 | 7/7   | 0.85 | 0.19 | 101,114,120,164            | 2     |
| 55  | MG   | AA    | 3181 | 1/1   | 0.85 | 0.50 | 71,71,71,71                | 0     |
| 55  | MG   | A7    | 101  | 1/1   | 0.85 | 0.41 | 56,56,56,56                | 0     |
| 55  | MG   | AA    | 3107 | 1/1   | 0.85 | 0.42 | 51,51,51,51                | 0     |
| 55  | MG   | BA    | 1622 | 1/1   | 0.85 | 0.18 | 92,92,92,92                | 0     |
| 56  | OHX  | AA    | 3506 | 7/7   | 0.85 | 0.14 | 104,115,126,178            | 1     |
| 56  | OHX  | CC    | 108  | 7/7   | 0.85 | 0.16 | 130,137,148,169            | 1     |
| 55  | MG   | DB    | 207  | 1/1   | 0.85 | 0.18 | 70,70,70,70                | 0     |
| 55  | MG   | DA    | 3183 | 1/1   | 0.85 | 0.25 | 99,99,99,99                | 0     |
| 55  | MG   | DA    | 3110 | 1/1   | 0.85 | 0.53 | 60,60,60,60                | 0     |
| 55  | MG   | AA    | 3038 | 1/1   | 0.85 | 0.48 | 68,68,68,68                | 0     |
| 55  | MG   | AA    | 3311 | 1/1   | 0.85 | 0.31 | 90,90,90,90                | 0     |
| 55  | MG   | AA    | 3189 | 1/1   | 0.85 | 0.34 | 63,63,63,63                | 0     |
| 55  | MG   | DA    | 3300 | 1/1   | 0.85 | 0.33 | 63,63,63,63                | 0     |
| 55  | MG   | AA    | 3088 | 1/1   | 0.85 | 0.31 | 66,66,66,66                | 0     |
| 55  | MG   | BA    | 1666 | 1/1   | 0.85 | 0.44 | 81,81,81,81                | 0     |
| 55  | MG   | DA    | 3294 | 1/1   | 0.85 | 0.16 | 74,74,74,74                | 0     |
| 55  | MG   | AA    | 3247 | 1/1   | 0.85 | 0.51 | 66,66,66,66                | 0     |
| 55  | MG   | AA    | 3270 | 1/1   | 0.85 | 0.64 | 90,90,90,90                | 0     |
| 56  | OHX  | BA    | 1788 | 7/7   | 0.85 | 0.23 | 123,136,147,176            | 1     |
| 56  | OHX  | AA    | 3392 | 7/7   | 0.85 | 0.18 | 81,92,124,181              | 2     |
| 55  | MG   | AA    | 3183 | 1/1   | 0.85 | 0.32 | 59,59,59,59                | 0     |
| 56  | OHX  | CA    | 1815 | 7/7   | 0.85 | 0.11 | 158,163,177,221            | 1     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 56  | OHX  | DA    | 3488 | 7/7   | 0.85 | 0.23 | 87,112,131,159             | 1     |
| 55  | MG   | DA    | 3027 | 1/1   | 0.85 | 0.14 | 78,78,78,78                | 0     |
| 55  | MG   | BA    | 1664 | 1/1   | 0.85 | 0.29 | 54,54,54,54                | 0     |
| 55  | MG   | AA    | 3052 | 1/1   | 0.86 | 0.29 | 71,71,71,71                | 0     |
| 55  | MG   | BA    | 1644 | 1/1   | 0.86 | 0.35 | 62,62,62,62                | 0     |
| 55  | MG   | BA    | 1711 | 1/1   | 0.86 | 0.31 | 90,90,90,90                | 0     |
| 56  | OHX  | CA    | 1767 | 7/7   | 0.86 | 0.30 | 110,139,162,203            | 1     |
| 55  | MG   | AA    | 3310 | 1/1   | 0.86 | 0.22 | 71,71,71,71                | 0     |
| 56  | OHX  | DB    | 216  | 7/7   | 0.86 | 0.13 | 123,138,155,204            | 1     |
| 55  | MG   | AB    | 203  | 1/1   | 0.86 | 0.23 | 58,58,58,58                | 0     |
| 56  | OHX  | AA    | 3567 | 7/7   | 0.86 | 0.16 | 125,135,148,181            | 2     |
| 56  | OHX  | AA    | 3455 | 7/7   | 0.86 | 0.15 | 173,192,201,215            | 1     |
| 55  | MG   | AA    | 3282 | 1/1   | 0.86 | 0.10 | 103,103,103,103            | 0     |
| 55  | MG   | BA    | 1608 | 1/1   | 0.86 | 0.13 | 89,89,89,89                | 0     |
| 56  | OHX  | AA    | 3519 | 7/7   | 0.86 | 0.20 | 103,114,126,154            | 1     |
| 55  | MG   | DA    | 3279 | 1/1   | 0.86 | 0.29 | 68,68,68,68                | 0     |
| 55  | MG   | DB    | 205  | 1/1   | 0.86 | 0.18 | 64,64,64,64                | 0     |
| 55  | MG   | DA    | 3289 | 1/1   | 0.86 | 0.17 | 84,84,84,84                | 0     |
| 55  | MG   | CA    | 1671 | 1/1   | 0.86 | 0.28 | 78,78,78,78                | 0     |
| 55  | MG   | DA    | 3180 | 1/1   | 0.86 | 0.43 | 45,45,45,45                | 0     |
| 55  | MG   | CA    | 1618 | 1/1   | 0.86 | 0.09 | 82,82,82,82                | 0     |
| 56  | OHX  | DA    | 3454 | 7/7   | 0.86 | 0.20 | 136,143,163,191            | 1     |
| 56  | OHX  | BA    | 1778 | 7/7   | 0.86 | 0.22 | 125,131,152,191            | 1     |
| 56  | OHX  | DA    | 3474 | 7/7   | 0.86 | 0.21 | 120,126,143,173            | 1     |
| 56  | OHX  | DB    | 220  | 7/7   | 0.86 | 0.20 | 159,162,171,208            | 1     |
| 55  | MG   | AA    | 3289 | 1/1   | 0.86 | 0.47 | 61,61,61,61                | 0     |
| 55  | MG   | DA    | 3200 | 1/1   | 0.86 | 1.13 | 86,86,86,86                | 0     |
| 55  | MG   | DA    | 3090 | 1/1   | 0.86 | 0.34 | 54,54,54,54                | 0     |
| 55  | MG   | AA    | 3161 | 1/1   | 0.86 | 0.24 | 57,57,57,57                | 0     |
| 56  | OHX  | DA    | 3255 | 7/7   | 0.86 | 0.22 | 93,104,107,143             | 1     |
| 55  | MG   | AA    | 3287 | 1/1   | 0.86 | 0.32 | 66,66,66,66                | 0     |
| 55  | MG   | AA    | 3071 | 1/1   | 0.86 | 0.42 | 84,84,84,84                | 0     |
| 55  | MG   | BA    | 1676 | 1/1   | 0.86 | 0.40 | 78,78,78,78                | 0     |
| 55  | MG   | DA    | 3072 | 1/1   | 0.87 | 0.09 | 93,93,93,93                | 0     |
| 55  | MG   | AA    | 3110 | 1/1   | 0.87 | 0.39 | 76,76,76,76                | 0     |
| 55  | MG   | AA    | 3231 | 1/1   | 0.87 | 0.39 | 57,57,57,57                | 0     |
| 55  | MG   | AA    | 3233 | 1/1   | 0.87 | 0.26 | 82,82,82,82                | 0     |
| 56  | OHX  | CA    | 1789 | 7/7   | 0.87 | 0.12 | 152,164,170,204            | 1     |
| 55  | MG   | CA    | 1678 | 1/1   | 0.87 | 0.09 | 97,97,97,97                | 0     |
| 55  | MG   | DA    | 3276 | 1/1   | 0.87 | 0.40 | 78,78,78,78                | 0     |
| 55  | MG   | DA    | 3115 | 1/1   | 0.87 | 0.25 | 44,44,44,44                | 0     |
| 55  | MG   | DA    | 3066 | 1/1   | 0.87 | 0.31 | 77,77,77,77                | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 56  | OHX  | AA    | 3548 | 7/7   | 0.87 | 0.15 | 125,128,143,177            | 1     |
| 56  | OHX  | DA    | 3462 | 7/7   | 0.87 | 0.12 | 154,157,165,208            | 1     |
| 55  | MG   | DA    | 3102 | 1/1   | 0.87 | 0.25 | 76,76,76,76                | 0     |
| 55  | MG   | AA    | 3082 | 1/1   | 0.87 | 0.29 | 57,57,57,57                | 0     |
| 55  | MG   | DA    | 3020 | 1/1   | 0.87 | 0.60 | 60,60,60,60                | 0     |
| 55  | MG   | CA    | 1691 | 1/1   | 0.87 | 0.19 | 128,128,128,128            | 0     |
| 55  | MG   | AA    | 3174 | 1/1   | 0.87 | 0.15 | 91,91,91,91                | 0     |
| 55  | MG   | AA    | 3307 | 1/1   | 0.87 | 0.30 | 72,72,72,72                | 0     |
| 55  | MG   | AA    | 3203 | 1/1   | 0.87 | 0.45 | 72,72,72,72                | 0     |
| 55  | MG   | AA    | 3170 | 1/1   | 0.87 | 0.62 | 69,69,69,69                | 0     |
| 55  | MG   | AA    | 3160 | 1/1   | 0.87 | 0.38 | 69,69,69,69                | 0     |
| 55  | MG   | BA    | 1686 | 1/1   | 0.87 | 0.15 | 100,100,100,100            | 0     |
| 55  | MG   | DA    | 3238 | 1/1   | 0.87 | 0.42 | 67,67,67,67                | 0     |
| 56  | OHX  | DB    | 218  | 7/7   | 0.87 | 0.37 | 134,141,153,171            | 1     |
| 55  | MG   | BA    | 1697 | 1/1   | 0.87 | 0.48 | 74,74,74,74                | 0     |
| 56  | OHX  | AA    | 3511 | 7/7   | 0.87 | 0.14 | 133,137,167,178            | 2     |
| 55  | MG   | BA    | 1645 | 1/1   | 0.87 | 0.15 | 76,76,76,76                | 0     |
| 55  | MG   | AA    | 3182 | 1/1   | 0.87 | 0.46 | 66,66,66,66                | 0     |
| 55  | MG   | DA    | 3281 | 1/1   | 0.87 | 0.23 | 65,65,65,65                | 0     |
| 55  | MG   | DA    | 3055 | 1/1   | 0.87 | 0.41 | 54,54,54,54                | 0     |
| 55  | MG   | AA    | 3211 | 1/1   | 0.87 | 0.18 | 58,58,58,58                | 0     |
| 56  | OHX  | DA    | 3223 | 7/7   | 0.87 | 0.17 | 126,133,144,169            | 1     |
| 55  | MG   | AA    | 3172 | 1/1   | 0.87 | 0.58 | 71,71,71,71                | 0     |
| 56  | OHX  | AA    | 3528 | 7/7   | 0.87 | 0.27 | 119,125,142,174            | 1     |
| 55  | MG   | BB    | 101  | 1/1   | 0.87 | 0.11 | 95,95,95,95                | 0     |
| 55  | MG   | BA    | 1617 | 1/1   | 0.88 | 0.49 | 60,60,60,60                | 0     |
| 56  | OHX  | CR    | 101  | 7/7   | 0.88 | 0.32 | 143,150,160,179            | 1     |
| 55  | MG   | AA    | 3200 | 1/1   | 0.88 | 0.33 | 82,82,82,82                | 0     |
| 55  | MG   | AA    | 3318 | 1/1   | 0.88 | 0.24 | 75,75,75,75                | 0     |
| 55  | MG   | DA    | 3206 | 1/1   | 0.88 | 0.16 | 52,52,52,52                | 0     |
| 56  | OHX  | DA    | 3448 | 7/7   | 0.88 | 0.13 | 134,147,163,206            | 1     |
| 55  | MG   | DA    | 3022 | 1/1   | 0.88 | 0.70 | 63,63,63,63                | 0     |
| 55  | MG   | CC    | 106  | 1/1   | 0.88 | 0.61 | 75,75,75,75                | 0     |
| 55  | MG   | BA    | 1619 | 1/1   | 0.88 | 0.39 | 64,64,64,64                | 0     |
| 55  | MG   | AA    | 3317 | 1/1   | 0.88 | 0.21 | 55,55,55,55                | 0     |
| 55  | MG   | DA    | 3314 | 1/1   | 0.88 | 0.20 | 70,70,70,70                | 0     |
| 55  | MG   | AA    | 3304 | 1/1   | 0.88 | 0.17 | 55,55,55,55                | 0     |
| 55  | MG   | AA    | 3031 | 1/1   | 0.88 | 0.34 | 40,40,40,40                | 0     |
| 55  | MG   | BA    | 1707 | 1/1   | 0.88 | 0.11 | 63,63,63,63                | 0     |
| 55  | MG   | AA    | 3075 | 1/1   | 0.88 | 0.19 | 78,78,78,78                | 0     |
| 55  | MG   | BA    | 1692 | 1/1   | 0.88 | 0.15 | 73,73,73,73                | 0     |
| 55  | MG   | CA    | 1659 | 1/1   | 0.88 | 0.11 | 116,116,116,116            | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | AA    | 3151 | 1/1   | 0.88 | 0.32 | 46,46,46,46                 | 0     |
| 56  | OHX  | CA    | 1747 | 7/7   | 0.88 | 0.18 | 129,134,147,212             | 1     |
| 55  | MG   | DA    | 3312 | 1/1   | 0.88 | 0.29 | 81,81,81,81                 | 0     |
| 55  | MG   | BA    | 1649 | 1/1   | 0.88 | 0.41 | 92,92,92,92                 | 0     |
| 55  | MG   | AA    | 3264 | 1/1   | 0.88 | 0.28 | 51,51,51,51                 | 0     |
| 55  | MG   | CA    | 1707 | 1/1   | 0.88 | 0.18 | 97,97,97,97                 | 0     |
| 55  | MG   | BF    | 301  | 1/1   | 0.88 | 0.24 | 79,79,79,79                 | 0     |
| 55  | MG   | AA    | 3251 | 1/1   | 0.88 | 0.61 | 75,75,75,75                 | 0     |
| 56  | OHX  | D8    | 101  | 7/7   | 0.88 | 0.20 | 140,149,164,175             | 1     |
| 55  | MG   | CA    | 1615 | 1/1   | 0.88 | 0.20 | 109,109,109,109             | 0     |
| 55  | MG   | AA    | 3125 | 1/1   | 0.88 | 0.21 | 63,63,63,63                 | 0     |
| 55  | MG   | DA    | 3308 | 1/1   | 0.88 | 0.23 | 60,60,60,60                 | 0     |
| 55  | MG   | BA    | 1648 | 1/1   | 0.88 | 0.40 | 86,86,86,86                 | 0     |
| 56  | OHX  | DA    | 3473 | 7/7   | 0.88 | 0.10 | 138,151,163,196             | 1     |
| 55  | MG   | BA    | 1671 | 1/1   | 0.88 | 0.51 | 68,68,68,68                 | 0     |
| 56  | OHX  | AA    | 3557 | 7/7   | 0.88 | 0.23 | 89,102,113,146              | 1     |
| 56  | OHX  | BA    | 1803 | 7/7   | 0.88 | 0.08 | 211,214,221,256             | 1     |
| 55  | MG   | CA    | 1714 | 1/1   | 0.88 | 0.42 | 84,84,84,84                 | 0     |
| 56  | OHX  | CB    | 104  | 7/7   | 0.88 | 0.64 | 175,181,183,194             | 1     |
| 55  | MG   | DA    | 3155 | 1/1   | 0.88 | 0.30 | 58,58,58,58                 | 0     |
| 55  | MG   | BA    | 1681 | 1/1   | 0.88 | 0.32 | 64,64,64,64                 | 0     |
| 55  | MG   | AA    | 3254 | 1/1   | 0.88 | 0.35 | 43,43,43,43                 | 0     |
| 56  | OHX  | BB    | 115  | 7/7   | 0.88 | 0.25 | 90,109,116,116              | 3     |
| 55  | MG   | BA    | 1690 | 1/1   | 0.88 | 0.11 | 81,81,81,81                 | 0     |
| 56  | OHX  | DB    | 217  | 7/7   | 0.88 | 0.19 | 135,139,157,196             | 1     |
| 56  | OHX  | BA    | 1766 | 7/7   | 0.88 | 0.19 | 108,139,151,181             | 2     |
| 55  | MG   | DA    | 3045 | 1/1   | 0.88 | 0.15 | 61,61,61,61                 | 0     |
| 55  | MG   | BC    | 102  | 1/1   | 0.88 | 0.40 | 65,65,65,65                 | 0     |
| 56  | OHX  | AA    | 3529 | 7/7   | 0.88 | 0.21 | 114,130,134,179             | 1     |
| 56  | OHX  | DA    | 3413 | 7/7   | 0.88 | 0.29 | 103,122,138,176             | 1     |
| 55  | MG   | DA    | 3209 | 1/1   | 0.88 | 0.34 | 64,64,64,64                 | 0     |
| 55  | MG   | AA    | 3124 | 1/1   | 0.88 | 0.32 | 88,88,88,88                 | 0     |
| 56  | OHX  | CA    | 1785 | 7/7   | 0.88 | 0.18 | 125,126,143,155             | 1     |
| 55  | MG   | BB    | 107  | 1/1   | 0.89 | 0.16 | 80,80,80,80                 | 0     |
| 55  | MG   | CA    | 1684 | 1/1   | 0.89 | 0.46 | 82,82,82,82                 | 0     |
| 56  | OHX  | DA    | 3405 | 7/7   | 0.89 | 0.18 | 129,133,151,175             | 1     |
| 56  | OHX  | DA    | 3218 | 7/7   | 0.89 | 0.26 | 96,106,121,133              | 1     |
| 55  | MG   | AA    | 3072 | 1/1   | 0.89 | 0.36 | 73,73,73,73                 | 0     |
| 56  | OHX  | AA    | 3420 | 7/7   | 0.89 | 0.21 | 112,125,135,178             | 2     |
| 56  | OHX  | BA    | 1765 | 7/7   | 0.89 | 0.26 | 91,107,120,150              | 3     |
| 55  | MG   | BA    | 1634 | 1/1   | 0.89 | 0.14 | 73,73,73,73                 | 0     |
| 56  | OHX  | AB    | 216  | 7/7   | 0.89 | 0.19 | 106,124,147,185             | 1     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 55  | MG   | CA    | 1698 | 1/1   | 0.89 | 0.70 | 86,86,86,86                | 0     |
| 55  | MG   | AA    | 3239 | 1/1   | 0.89 | 0.57 | 52,52,52,52                | 0     |
| 55  | MG   | CA    | 1625 | 1/1   | 0.89 | 0.16 | 87,87,87,87                | 0     |
| 56  | OHX  | CA    | 1808 | 7/7   | 0.89 | 0.26 | 163,164,177,210            | 1     |
| 56  | OHX  | AA    | 3530 | 7/7   | 0.89 | 0.29 | 117,123,125,163            | 1     |
| 55  | MG   | DA    | 3114 | 1/1   | 0.89 | 0.39 | 37,37,37,37                | 0     |
| 56  | OHX  | CA    | 1778 | 7/7   | 0.89 | 0.09 | 148,157,164,202            | 1     |
| 55  | MG   | DA    | 3035 | 1/1   | 0.89 | 0.28 | 95,95,95,95                | 0     |
| 56  | OHX  | DB    | 214  | 7/7   | 0.89 | 0.13 | 145,149,169,184            | 1     |
| 56  | OHX  | AA    | 3476 | 7/7   | 0.89 | 0.23 | 88,98,119,157              | 1     |
| 56  | OHX  | AB    | 218  | 7/7   | 0.89 | 0.13 | 138,141,157,181            | 1     |
| 55  | MG   | DB    | 204  | 1/1   | 0.89 | 0.25 | 76,76,76,76                | 0     |
| 55  | MG   | DA    | 3031 | 1/1   | 0.89 | 0.18 | 77,77,77,77                | 0     |
| 56  | OHX  | DA    | 3478 | 7/7   | 0.89 | 0.19 | 106,110,128,170            | 1     |
| 55  | MG   | CA    | 1670 | 1/1   | 0.89 | 0.19 | 95,95,95,95                | 0     |
| 55  | MG   | CA    | 1610 | 1/1   | 0.89 | 0.41 | 87,87,87,87                | 0     |
| 55  | MG   | CA    | 1648 | 1/1   | 0.89 | 0.42 | 70,70,70,70                | 0     |
| 55  | MG   | DA    | 3260 | 1/1   | 0.89 | 0.30 | 68,68,68,68                | 0     |
| 56  | OHX  | AA    | 3512 | 7/7   | 0.89 | 0.18 | 110,115,138,180            | 2     |
| 56  | OHX  | DA    | 3385 | 7/7   | 0.89 | 0.16 | 78,128,134,201             | 1     |
| 55  | MG   | BA    | 1609 | 1/1   | 0.89 | 0.29 | 65,65,65,65                | 0     |
| 55  | MG   | DA    | 3116 | 1/1   | 0.89 | 0.28 | 62,62,62,62                | 0     |
| 55  | MG   | AA    | 3087 | 1/1   | 0.89 | 0.24 | 82,82,82,82                | 0     |
| 55  | MG   | DA    | 3286 | 1/1   | 0.89 | 0.11 | 77,77,77,77                | 0     |
| 55  | MG   | CA    | 1660 | 1/1   | 0.89 | 0.31 | 97,97,97,97                | 0     |
| 56  | OHX  | DA    | 3490 | 7/7   | 0.89 | 0.17 | 103,106,122,159            | 3     |
| 55  | MG   | BA    | 1693 | 1/1   | 0.89 | 0.13 | 68,68,68,68                | 0     |
| 55  | MG   | DA    | 3050 | 1/1   | 0.89 | 0.82 | 74,74,74,74                | 0     |
| 56  | OHX  | AA    | 3554 | 7/7   | 0.89 | 0.24 | 138,143,153,173            | 1     |
| 55  | MG   | CA    | 1701 | 1/1   | 0.89 | 0.23 | 109,109,109,109            | 0     |
| 56  | OHX  | DA    | 3468 | 7/7   | 0.89 | 0.17 | 143,146,150,189            | 1     |
| 55  | MG   | DA    | 3067 | 1/1   | 0.89 | 0.15 | 82,82,82,82                | 0     |
| 55  | MG   | DA    | 3023 | 1/1   | 0.89 | 0.55 | 70,70,70,70                | 0     |
| 56  | OHX  | AA    | 3549 | 7/7   | 0.89 | 0.27 | 96,102,109,128             | 2     |
| 56  | OHX  | AA    | 3515 | 7/7   | 0.89 | 0.24 | 93,97,116,159              | 2     |
| 56  | OHX  | AA    | 3480 | 7/7   | 0.89 | 0.24 | 111,119,135,158            | 2     |
| 56  | OHX  | AB    | 215  | 7/7   | 0.89 | 0.18 | 110,123,130,165            | 1     |
| 56  | OHX  | AA    | 3456 | 7/7   | 0.89 | 0.19 | 111,115,132,161            | 3     |
| 55  | MG   | DA    | 3177 | 1/1   | 0.89 | 0.47 | 61,61,61,61                | 0     |
| 55  | MG   | AA    | 3022 | 1/1   | 0.89 | 0.37 | 28,28,28,28                | 0     |
| 56  | OHX  | AA    | 3513 | 7/7   | 0.89 | 0.20 | 120,125,139,159            | 2     |
| 55  | MG   | AA    | 3058 | 1/1   | 0.89 | 0.12 | 61,61,61,61                | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 56  | OHX  | AA    | 3551 | 7/7   | 0.89 | 0.24 | 97,115,123,153             | 1     |
| 55  | MG   | AA    | 3266 | 1/1   | 0.89 | 0.43 | 62,62,62,62                | 0     |
| 55  | MG   | DA    | 3057 | 1/1   | 0.89 | 0.32 | 58,58,58,58                | 0     |
| 56  | OHX  | CA    | 1786 | 7/7   | 0.89 | 0.09 | 163,163,175,198            | 1     |
| 55  | MG   | DA    | 3205 | 1/1   | 0.89 | 0.13 | 106,106,106,106            | 0     |
| 55  | MG   | CA    | 1608 | 1/1   | 0.89 | 0.30 | 76,76,76,76                | 0     |
| 55  | MG   | AA    | 3199 | 1/1   | 0.90 | 0.51 | 75,75,75,75                | 0     |
| 55  | MG   | AA    | 3294 | 1/1   | 0.90 | 0.32 | 36,36,36,36                | 0     |
| 56  | OHX  | DA    | 3447 | 7/7   | 0.90 | 0.12 | 122,140,155,176            | 2     |
| 55  | MG   | AA    | 3325 | 1/1   | 0.90 | 0.42 | 75,75,75,75                | 0     |
| 55  | MG   | DA    | 3030 | 1/1   | 0.90 | 0.20 | 94,94,94,94                | 0     |
| 55  | MG   | CA    | 1647 | 1/1   | 0.90 | 0.46 | 70,70,70,70                | 0     |
| 56  | OHX  | AA    | 3544 | 7/7   | 0.90 | 0.23 | 118,127,137,169            | 1     |
| 56  | OHX  | AA    | 3417 | 7/7   | 0.90 | 0.23 | 90,102,131,147             | 3     |
| 55  | MG   | DA    | 3329 | 1/1   | 0.90 | 0.44 | 60,60,60,60                | 0     |
| 56  | OHX  | AB    | 213  | 7/7   | 0.90 | 0.15 | 88,108,129,159             | 3     |
| 55  | MG   | DA    | 3186 | 1/1   | 0.90 | 0.36 | 34,34,34,34                | 0     |
| 56  | OHX  | AA    | 3451 | 7/7   | 0.90 | 0.19 | 79,96,106,142              | 1     |
| 56  | OHX  | DA    | 3480 | 7/7   | 0.90 | 0.10 | 125,130,144,190            | 1     |
| 55  | MG   | DA    | 3315 | 1/1   | 0.90 | 0.44 | 78,78,78,78                | 0     |
| 56  | OHX  | AA    | 3523 | 7/7   | 0.90 | 0.16 | 112,123,137,155            | 1     |
| 55  | MG   | AA    | 3127 | 1/1   | 0.90 | 0.39 | 45,45,45,45                | 0     |
| 55  | MG   | DA    | 3283 | 1/1   | 0.90 | 0.31 | 86,86,86,86                | 0     |
| 56  | OHX  | CA    | 1811 | 7/7   | 0.90 | 0.18 | 126,129,137,159            | 1     |
| 55  | MG   | DA    | 3037 | 1/1   | 0.90 | 0.43 | 73,73,73,73                | 0     |
| 55  | MG   | AA    | 3099 | 1/1   | 0.90 | 0.34 | 60,60,60,60                | 0     |
| 55  | MG   | DA    | 3140 | 1/1   | 0.90 | 0.42 | 55,55,55,55                | 0     |
| 55  | MG   | AA    | 3176 | 1/1   | 0.90 | 0.43 | 46,46,46,46                | 0     |
| 55  | MG   | AA    | 3028 | 1/1   | 0.90 | 0.39 | 35,35,35,35                | 0     |
| 55  | MG   | AA    | 3165 | 1/1   | 0.90 | 0.68 | 79,79,79,79                | 0     |
| 56  | OHX  | AA    | 3492 | 7/7   | 0.90 | 0.10 | 139,142,151,196            | 1     |
| 55  | MG   | BA    | 1642 | 1/1   | 0.90 | 0.43 | 69,69,69,69                | 0     |
| 56  | OHX  | CA    | 1759 | 7/7   | 0.90 | 0.17 | 125,133,140,148            | 1     |
| 55  | MG   | AA    | 3085 | 1/1   | 0.90 | 0.29 | 74,74,74,74                | 0     |
| 55  | MG   | BA    | 1655 | 1/1   | 0.90 | 0.34 | 84,84,84,84                | 0     |
| 56  | OHX  | AA    | 3505 | 7/7   | 0.90 | 0.15 | 143,150,161,212            | 1     |
| 55  | MG   | AA    | 3240 | 1/1   | 0.90 | 0.50 | 56,56,56,56                | 0     |
| 56  | OHX  | AA    | 3500 | 7/7   | 0.90 | 0.13 | 118,131,153,193            | 1     |
| 56  | OHX  | DA    | 3253 | 7/7   | 0.90 | 0.14 | 141,144,160,190            | 1     |
| 55  | MG   | CA    | 1656 | 1/1   | 0.90 | 0.33 | 94,94,94,94                | 0     |
| 55  | MG   | AA    | 3113 | 1/1   | 0.90 | 0.24 | 88,88,88,88                | 0     |
| 55  | MG   | CA    | 1682 | 1/1   | 0.90 | 0.28 | 107,107,107,107            | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 56  | OHX  | CA    | 1783 | 7/7   | 0.90 | 0.20 | 113,117,137,164            | 1     |
| 56  | OHX  | AA    | 3503 | 7/7   | 0.90 | 0.29 | 99,108,119,150             | 1     |
| 56  | OHX  | A1    | 204  | 7/7   | 0.90 | 0.15 | 107,117,147,182            | 3     |
| 56  | OHX  | BA    | 1812 | 7/7   | 0.90 | 0.06 | 170,174,180,213            | 1     |
| 55  | MG   | AA    | 3249 | 1/1   | 0.90 | 0.22 | 81,81,81,81                | 0     |
| 55  | MG   | DA    | 3121 | 1/1   | 0.90 | 0.53 | 78,78,78,78                | 0     |
| 55  | MG   | AA    | 3226 | 1/1   | 0.90 | 0.52 | 68,68,68,68                | 0     |
| 55  | MG   | AA    | 3148 | 1/1   | 0.90 | 0.29 | 69,69,69,69                | 0     |
| 55  | MG   | CA    | 1705 | 1/1   | 0.90 | 0.48 | 73,73,73,73                | 0     |
| 56  | OHX  | BA    | 1790 | 7/7   | 0.90 | 0.09 | 163,166,178,211            | 1     |
| 55  | MG   | DA    | 3151 | 1/1   | 0.90 | 0.28 | 62,62,62,62                | 0     |
| 56  | OHX  | BA    | 1756 | 7/7   | 0.90 | 0.08 | 153,171,174,206            | 1     |
| 55  | MG   | BA    | 1614 | 1/1   | 0.90 | 0.13 | 73,73,73,73                | 0     |
| 56  | OHX  | DA    | 3111 | 7/7   | 0.90 | 0.19 | 118,129,134,197            | 1     |
| 55  | MG   | AA    | 3274 | 1/1   | 0.90 | 0.12 | 36,36,36,36                | 0     |
| 55  | MG   | BB    | 109  | 1/1   | 0.90 | 0.21 | 80,80,80,80                | 0     |
| 56  | OHX  | DA    | 3489 | 7/7   | 0.90 | 0.13 | 117,121,134,153            | 1     |
| 56  | OHX  | AA    | 3522 | 7/7   | 0.90 | 0.20 | 74,93,104,150              | 2     |
| 55  | MG   | BA    | 1607 | 1/1   | 0.90 | 0.11 | 102,102,102,102            | 0     |
| 55  | MG   | AA    | 3117 | 1/1   | 0.90 | 0.21 | 90,90,90,90                | 0     |
| 55  | MG   | AA    | 3126 | 1/1   | 0.90 | 0.32 | 54,54,54,54                | 0     |
| 55  | MG   | BA    | 1688 | 1/1   | 0.90 | 0.18 | 79,79,79,79                | 0     |
| 55  | MG   | DA    | 3033 | 1/1   | 0.90 | 0.24 | 82,82,82,82                | 0     |
| 55  | MG   | BC    | 101  | 1/1   | 0.90 | 0.35 | 62,62,62,62                | 0     |
| 56  | OHX  | AA    | 3498 | 7/7   | 0.90 | 0.34 | 120,126,136,160            | 2     |
| 56  | OHX  | BA    | 1795 | 7/7   | 0.90 | 0.11 | 152,159,163,204            | 1     |
| 55  | MG   | AA    | 3195 | 1/1   | 0.91 | 0.39 | 58,58,58,58                | 0     |
| 56  | OHX  | DA    | 3362 | 7/7   | 0.91 | 0.22 | 83,98,103,158              | 1     |
| 56  | OHX  | BA    | 1791 | 7/7   | 0.91 | 0.13 | 122,123,136,173            | 1     |
| 56  | OHX  | AA    | 3536 | 7/7   | 0.91 | 0.12 | 99,110,129,173             | 2     |
| 56  | OHX  | BA    | 1780 | 7/7   | 0.91 | 0.22 | 115,123,136,153            | 1     |
| 55  | MG   | AA    | 3171 | 1/1   | 0.91 | 0.34 | 59,59,59,59                | 0     |
| 56  | OHX  | CB    | 106  | 7/7   | 0.91 | 0.20 | 97,107,117,126             | 6     |
| 55  | MG   | AA    | 3285 | 1/1   | 0.91 | 0.37 | 77,77,77,77                | 0     |
| 56  | OHX  | CA    | 1787 | 7/7   | 0.91 | 0.16 | 117,122,135,155            | 1     |
| 56  | OHX  | AA    | 3439 | 7/7   | 0.91 | 0.17 | 114,122,140,194            | 1     |
| 56  | OHX  | CA    | 1775 | 7/7   | 0.91 | 0.10 | 139,154,159,200            | 1     |
| 56  | OHX  | AA    | 3502 | 7/7   | 0.91 | 0.10 | 128,135,148,184            | 1     |
| 56  | OHX  | DA    | 3433 | 7/7   | 0.91 | 0.21 | 104,114,132,147            | 1     |
| 55  | MG   | BC    | 103  | 1/1   | 0.91 | 0.51 | 70,70,70,70                | 0     |
| 56  | OHX  | BD    | 102  | 7/7   | 0.91 | 0.10 | 170,180,207,224            | 1     |
| 56  | OHX  | AA    | 3564 | 7/7   | 0.91 | 0.18 | 94,114,124,148             | 1     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | DA    | 3282 | 1/1   | 0.91 | 0.35 | 69,69,69,69                 | 0     |
| 55  | MG   | AA    | 3237 | 1/1   | 0.91 | 0.48 | 62,62,62,62                 | 0     |
| 55  | MG   | BA    | 1660 | 1/1   | 0.91 | 0.56 | 52,52,52,52                 | 0     |
| 56  | OHX  | AA    | 3482 | 7/7   | 0.91 | 0.19 | 85,96,105,135               | 1     |
| 55  | MG   | BA    | 1710 | 1/1   | 0.91 | 0.33 | 113,113,113,113             | 0     |
| 55  | MG   | AA    | 3090 | 1/1   | 0.91 | 0.39 | 78,78,78,78                 | 0     |
| 55  | MG   | BA    | 1632 | 1/1   | 0.91 | 0.21 | 73,73,73,73                 | 0     |
| 56  | OHX  | CA    | 1755 | 7/7   | 0.91 | 0.11 | 119,128,149,178             | 1     |
| 55  | MG   | BA    | 1667 | 1/1   | 0.91 | 0.52 | 73,73,73,73                 | 0     |
| 55  | MG   | AA    | 3100 | 1/1   | 0.91 | 0.29 | 58,58,58,58                 | 0     |
| 56  | OHX  | CA    | 1753 | 7/7   | 0.91 | 0.26 | 82,120,146,173              | 3     |
| 55  | MG   | AA    | 3155 | 1/1   | 0.91 | 0.11 | 79,79,79,79                 | 0     |
| 56  | OHX  | AA    | 3526 | 7/7   | 0.91 | 0.25 | 87,90,101,128               | 1     |
| 55  | MG   | BA    | 1661 | 1/1   | 0.91 | 0.49 | 61,61,61,61                 | 0     |
| 56  | OHX  | AA    | 3514 | 7/7   | 0.91 | 0.13 | 126,137,144,183             | 1     |
| 55  | MG   | AA    | 3276 | 1/1   | 0.91 | 0.36 | 76,76,76,76                 | 0     |
| 55  | MG   | DA    | 3317 | 1/1   | 0.91 | 0.35 | 85,85,85,85                 | 0     |
| 56  | OHX  | DA    | 3127 | 7/7   | 0.91 | 0.27 | 118,132,150,170             | 2     |
| 55  | MG   | CC    | 105  | 1/1   | 0.91 | 0.53 | 66,66,66,66                 | 0     |
| 55  | MG   | DA    | 3043 | 1/1   | 0.91 | 0.40 | 73,73,73,73                 | 0     |
| 56  | OHX  | BR    | 101  | 7/7   | 0.91 | 0.19 | 132,137,152,164             | 1     |
| 55  | MG   | DA    | 3153 | 1/1   | 0.91 | 0.45 | 69,69,69,69                 | 0     |
| 55  | MG   | DA    | 3239 | 1/1   | 0.91 | 0.20 | 79,79,79,79                 | 0     |
| 56  | OHX  | BA    | 1797 | 7/7   | 0.91 | 0.13 | 117,130,138,173             | 1     |
| 55  | MG   | DA    | 3088 | 1/1   | 0.91 | 0.31 | 47,47,47,47                 | 0     |
| 56  | OHX  | DA    | 3476 | 7/7   | 0.91 | 0.11 | 126,136,143,174             | 1     |
| 56  | OHX  | D5    | 102  | 7/7   | 0.91 | 0.28 | 114,129,141,158             | 1     |
| 56  | OHX  | DA    | 3475 | 7/7   | 0.91 | 0.21 | 126,139,148,175             | 1     |
| 55  | MG   | DA    | 3079 | 1/1   | 0.91 | 0.24 | 49,49,49,49                 | 0     |
| 56  | OHX  | DA    | 3467 | 7/7   | 0.91 | 0.12 | 133,139,156,192             | 1     |
| 55  | MG   | AA    | 3293 | 1/1   | 0.91 | 0.24 | 72,72,72,72                 | 0     |
| 56  | OHX  | AA    | 3527 | 7/7   | 0.91 | 0.10 | 147,148,161,187             | 1     |
| 55  | MG   | DA    | 3213 | 1/1   | 0.91 | 0.39 | 57,57,57,57                 | 0     |
| 56  | OHX  | BD    | 103  | 7/7   | 0.91 | 0.15 | 108,110,116,155             | 1     |
| 55  | MG   | BA    | 1610 | 1/1   | 0.91 | 0.15 | 75,75,75,75                 | 0     |
| 55  | MG   | AA    | 3167 | 1/1   | 0.91 | 0.16 | 51,51,51,51                 | 0     |
| 55  | MG   | DA    | 3235 | 1/1   | 0.91 | 0.47 | 66,66,66,66                 | 0     |
| 55  | MG   | CA    | 1713 | 1/1   | 0.91 | 0.18 | 114,114,114,114             | 0     |
| 55  | MG   | CA    | 1654 | 1/1   | 0.91 | 0.23 | 89,89,89,89                 | 0     |
| 55  | MG   | BA    | 1691 | 1/1   | 0.91 | 0.19 | 87,87,87,87                 | 0     |
| 56  | OHX  | DA    | 3450 | 7/7   | 0.91 | 0.13 | 133,139,150,199             | 1     |
| 56  | OHX  | BA    | 1786 | 7/7   | 0.91 | 0.20 | 133,136,154,188             | 1     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | BA    | 1654 | 1/1   | 0.91 | 0.35 | 64,64,64,64                 | 0     |
| 56  | OHX  | BA    | 1792 | 7/7   | 0.91 | 0.17 | 118,131,146,181             | 1     |
| 55  | MG   | BA    | 1672 | 1/1   | 0.91 | 0.25 | 82,82,82,82                 | 0     |
| 55  | MG   | AA    | 3357 | 1/1   | 0.91 | 0.37 | 69,69,69,69                 | 0     |
| 55  | MG   | DA    | 3107 | 1/1   | 0.91 | 0.28 | 42,42,42,42                 | 0     |
| 55  | MG   | AA    | 3267 | 1/1   | 0.91 | 0.26 | 37,37,37,37                 | 0     |
| 55  | MG   | BA    | 1662 | 1/1   | 0.91 | 0.32 | 56,56,56,56                 | 0     |
| 56  | OHX  | DA    | 3472 | 7/7   | 0.91 | 0.10 | 162,171,176,223             | 1     |
| 55  | MG   | DA    | 3210 | 1/1   | 0.91 | 0.75 | 73,73,73,73                 | 0     |
| 55  | MG   | DA    | 3113 | 1/1   | 0.91 | 0.20 | 73,73,73,73                 | 0     |
| 55  | MG   | CA    | 1630 | 1/1   | 0.91 | 0.43 | 86,86,86,86                 | 0     |
| 56  | OHX  | CA    | 1799 | 7/7   | 0.91 | 0.30 | 142,145,160,170             | 1     |
| 56  | OHX  | DA    | 3440 | 7/7   | 0.91 | 0.15 | 142,144,161,189             | 1     |
| 55  | MG   | CA    | 1666 | 1/1   | 0.91 | 0.30 | 75,75,75,75                 | 0     |
| 55  | MG   | DA    | 3104 | 1/1   | 0.91 | 0.38 | 64,64,64,64                 | 0     |
| 56  | OHX  | CA    | 1773 | 7/7   | 0.91 | 0.12 | 123,130,144,181             | 1     |
| 56  | OHX  | CA    | 1754 | 7/7   | 0.91 | 0.17 | 116,125,134,168             | 1     |
| 56  | OHX  | DA    | 3118 | 7/7   | 0.91 | 0.19 | 99,101,123,146              | 3     |
| 56  | OHX  | DA    | 3479 | 7/7   | 0.91 | 0.14 | 150,159,164,201             | 1     |
| 56  | OHX  | DA    | 3484 | 7/7   | 0.91 | 0.16 | 109,123,139,168             | 1     |
| 56  | OHX  | DA    | 3481 | 7/7   | 0.91 | 0.12 | 136,140,149,177             | 1     |
| 56  | OHX  | BA    | 1799 | 7/7   | 0.91 | 0.09 | 170,176,182,227             | 1     |
| 56  | OHX  | AB    | 214  | 7/7   | 0.91 | 0.14 | 125,133,135,173             | 1     |
| 56  | OHX  | DA    | 3220 | 7/7   | 0.91 | 0.12 | 141,154,156,201             | 1     |
| 55  | MG   | AA    | 3230 | 1/1   | 0.91 | 0.48 | 72,72,72,72                 | 0     |
| 56  | OHX  | CA    | 1788 | 7/7   | 0.91 | 0.17 | 138,144,149,176             | 1     |
| 56  | OHX  | AA    | 3454 | 7/7   | 0.91 | 0.16 | 103,116,132,145             | 1     |
| 56  | OHX  | DB    | 212  | 7/7   | 0.91 | 0.11 | 144,152,161,194             | 1     |
| 56  | OHX  | DA    | 3172 | 7/7   | 0.91 | 0.32 | 95,104,112,142              | 1     |
| 55  | MG   | DA    | 3323 | 1/1   | 0.91 | 0.54 | 100,100,100,100             | 0     |
| 55  | MG   | AA    | 3238 | 1/1   | 0.91 | 0.46 | 47,47,47,47                 | 0     |
| 56  | OHX  | BA    | 1777 | 7/7   | 0.92 | 0.07 | 176,178,192,246             | 1     |
| 56  | OHX  | DA    | 3455 | 7/7   | 0.92 | 0.08 | 139,144,150,194             | 1     |
| 56  | OHX  | BL    | 201  | 7/7   | 0.92 | 0.09 | 145,153,159,202             | 1     |
| 56  | OHX  | D3    | 101  | 7/7   | 0.92 | 0.14 | 129,139,156,171             | 2     |
| 56  | OHX  | AA    | 3495 | 7/7   | 0.92 | 0.19 | 106,114,133,188             | 1     |
| 56  | OHX  | DA    | 3491 | 7/7   | 0.92 | 0.11 | 104,107,129,176             | 1     |
| 55  | MG   | DA    | 3108 | 1/1   | 0.92 | 0.50 | 56,56,56,56                 | 0     |
| 56  | OHX  | AA    | 3485 | 7/7   | 0.92 | 0.18 | 103,114,131,163             | 1     |
| 56  | OHX  | BC    | 106  | 7/7   | 0.92 | 0.14 | 119,120,134,160             | 1     |
| 56  | OHX  | CA    | 1780 | 7/7   | 0.92 | 0.09 | 138,146,156,182             | 1     |
| 55  | MG   | AA    | 3114 | 1/1   | 0.92 | 0.39 | 62,62,62,62                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 55  | MG   | CA    | 1690 | 1/1   | 0.92 | 0.11 | 93,93,93,93                | 0     |
| 56  | OHX  | DA    | 3486 | 7/7   | 0.92 | 0.14 | 123,132,147,175            | 1     |
| 56  | OHX  | AA    | 3539 | 7/7   | 0.92 | 0.10 | 130,133,143,179            | 1     |
| 55  | MG   | DA    | 3025 | 1/1   | 0.92 | 0.17 | 59,59,59,59                | 0     |
| 55  | MG   | AA    | 3055 | 1/1   | 0.92 | 0.30 | 88,88,88,88                | 0     |
| 55  | MG   | BA    | 1627 | 1/1   | 0.92 | 0.21 | 58,58,58,58                | 0     |
| 55  | MG   | BA    | 1712 | 1/1   | 0.92 | 0.05 | 74,74,74,74                | 0     |
| 56  | OHX  | BA    | 1738 | 7/7   | 0.92 | 0.17 | 112,124,136,189            | 1     |
| 55  | MG   | AA    | 3313 | 1/1   | 0.92 | 0.39 | 82,82,82,82                | 0     |
| 55  | MG   | BA    | 1702 | 1/1   | 0.92 | 0.40 | 84,84,84,84                | 0     |
| 55  | MG   | DB    | 203  | 1/1   | 0.92 | 0.11 | 121,121,121,121            | 0     |
| 56  | OHX  | DA    | 3482 | 7/7   | 0.92 | 0.16 | 128,142,154,190            | 1     |
| 55  | MG   | AA    | 3234 | 1/1   | 0.92 | 0.08 | 68,68,68,68                | 0     |
| 55  | MG   | DA    | 3106 | 1/1   | 0.92 | 0.33 | 80,80,80,80                | 0     |
| 55  | MG   | AA    | 3273 | 1/1   | 0.92 | 0.44 | 60,60,60,60                | 0     |
| 56  | OHX  | AA    | 3484 | 7/7   | 0.92 | 0.14 | 123,137,150,203            | 1     |
| 55  | MG   | AA    | 3303 | 1/1   | 0.92 | 0.21 | 77,77,77,77                | 0     |
| 56  | OHX  | AA    | 3555 | 7/7   | 0.92 | 0.19 | 82,85,105,128              | 1     |
| 55  | MG   | CA    | 1688 | 1/1   | 0.92 | 0.17 | 79,79,79,79                | 0     |
| 56  | OHX  | DA    | 3469 | 7/7   | 0.92 | 0.20 | 116,119,133,163            | 1     |
| 56  | OHX  | DA    | 3173 | 7/7   | 0.92 | 0.10 | 157,163,175,202            | 1     |
| 56  | OHX  | DA    | 3415 | 7/7   | 0.92 | 0.16 | 128,140,160,189            | 1     |
| 55  | MG   | DA    | 3028 | 1/1   | 0.92 | 0.45 | 44,44,44,44                | 0     |
| 56  | OHX  | CV    | 101  | 7/7   | 0.92 | 0.09 | 174,182,196,223            | 1     |
| 56  | OHX  | BA    | 1810 | 7/7   | 0.92 | 0.18 | 138,141,150,186            | 1     |
| 56  | OHX  | DA    | 3458 | 7/7   | 0.92 | 0.09 | 173,175,178,215            | 1     |
| 55  | MG   | BA    | 1684 | 1/1   | 0.92 | 0.21 | 67,67,67,67                | 0     |
| 56  | OHX  | CA    | 1809 | 7/7   | 0.92 | 0.07 | 150,160,169,213            | 1     |
| 56  | OHX  | DA    | 3176 | 7/7   | 0.92 | 0.19 | 162,165,176,192            | 1     |
| 56  | OHX  | DA    | 3258 | 7/7   | 0.92 | 0.19 | 103,111,118,148            | 1     |
| 56  | OHX  | DA    | 3442 | 7/7   | 0.92 | 0.15 | 135,142,161,190            | 1     |
| 56  | OHX  | DA    | 3457 | 7/7   | 0.92 | 0.10 | 149,156,166,200            | 1     |
| 56  | OHX  | AA    | 3543 | 7/7   | 0.92 | 0.10 | 145,150,162,204            | 1     |
| 55  | MG   | CA    | 1640 | 1/1   | 0.92 | 0.30 | 77,77,77,77                | 0     |
| 55  | MG   | AA    | 3128 | 1/1   | 0.92 | 0.34 | 53,53,53,53                | 0     |
| 56  | OHX  | BA    | 1750 | 7/7   | 0.92 | 0.16 | 112,129,139,168            | 1     |
| 55  | MG   | AA    | 3162 | 1/1   | 0.92 | 0.23 | 48,48,48,48                | 0     |
| 56  | OHX  | BA    | 1787 | 7/7   | 0.92 | 0.13 | 124,129,137,172            | 1     |
| 56  | OHX  | BA    | 1781 | 7/7   | 0.92 | 0.17 | 115,133,141,174            | 1     |
| 55  | MG   | DA    | 3044 | 1/1   | 0.92 | 0.30 | 100,100,100,100            | 0     |
| 56  | OHX  | AA    | 3501 | 7/7   | 0.92 | 0.12 | 104,117,124,169            | 1     |
| 56  | OHX  | DA    | 3226 | 7/7   | 0.92 | 0.16 | 120,131,144,175            | 1     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 55  | MG   | AA    | 3292 | 1/1   | 0.92 | 0.42 | 62,62,62,62                | 0     |
| 55  | MG   | DA    | 3187 | 1/1   | 0.92 | 0.28 | 55,55,55,55                | 0     |
| 56  | OHX  | DA    | 3171 | 7/7   | 0.92 | 0.20 | 95,116,127,171             | 1     |
| 55  | MG   | CA    | 1680 | 1/1   | 0.92 | 0.35 | 78,78,78,78                | 0     |
| 55  | MG   | AA    | 3081 | 1/1   | 0.92 | 0.21 | 81,81,81,81                | 0     |
| 56  | OHX  | BA    | 1807 | 7/7   | 0.92 | 0.15 | 133,136,150,177            | 1     |
| 56  | OHX  | CA    | 1810 | 7/7   | 0.92 | 0.10 | 113,132,142,167            | 1     |
| 56  | OHX  | BA    | 1757 | 7/7   | 0.92 | 0.20 | 86,113,131,156             | 4     |
| 55  | MG   | DA    | 3271 | 1/1   | 0.92 | 0.41 | 59,59,59,59                | 0     |
| 55  | MG   | AB    | 204  | 1/1   | 0.92 | 0.47 | 80,80,80,80                | 0     |
| 55  | MG   | BB    | 112  | 1/1   | 0.92 | 0.13 | 80,80,80,80                | 0     |
| 55  | MG   | AA    | 3309 | 1/1   | 0.92 | 0.41 | 77,77,77,77                | 0     |
| 56  | OHX  | AA    | 3559 | 7/7   | 0.92 | 0.22 | 123,137,143,179            | 1     |
| 55  | MG   | AA    | 3204 | 1/1   | 0.92 | 0.44 | 45,45,45,45                | 0     |
| 55  | MG   | AA    | 3312 | 1/1   | 0.92 | 0.25 | 71,71,71,71                | 0     |
| 55  | MG   | DA    | 3128 | 1/1   | 0.92 | 0.50 | 75,75,75,75                | 0     |
| 55  | MG   | DA    | 3060 | 1/1   | 0.92 | 0.46 | 77,77,77,77                | 0     |
| 55  | MG   | DA    | 3029 | 1/1   | 0.92 | 0.29 | 70,70,70,70                | 0     |
| 56  | OHX  | CA    | 1757 | 7/7   | 0.92 | 0.14 | 117,123,150,175            | 1     |
| 56  | OHX  | BA    | 1779 | 7/7   | 0.92 | 0.14 | 129,134,141,170            | 1     |
| 56  | OHX  | DA    | 3407 | 7/7   | 0.92 | 0.15 | 124,134,145,191            | 1     |
| 55  | MG   | BA    | 1631 | 1/1   | 0.92 | 0.10 | 85,85,85,85                | 0     |
| 56  | OHX  | BA    | 1737 | 7/7   | 0.92 | 0.13 | 120,131,149,172            | 1     |
| 55  | MG   | BA    | 1647 | 1/1   | 0.92 | 0.39 | 66,66,66,66                | 0     |
| 55  | MG   | DA    | 3179 | 1/1   | 0.92 | 0.42 | 46,46,46,46                | 0     |
| 55  | MG   | AA    | 3033 | 1/1   | 0.92 | 0.33 | 39,39,39,39                | 0     |
| 55  | MG   | DA    | 3017 | 1/1   | 0.92 | 0.41 | 66,66,66,66                | 0     |
| 55  | MG   | DA    | 3219 | 1/1   | 0.92 | 0.22 | 62,62,62,62                | 0     |
| 55  | MG   | DA    | 3326 | 1/1   | 0.92 | 0.42 | 90,90,90,90                | 0     |
| 56  | OHX  | CD    | 101  | 7/7   | 0.92 | 0.10 | 166,174,199,220            | 1     |
| 56  | OHX  | DA    | 3105 | 7/7   | 0.92 | 0.16 | 134,136,144,206            | 1     |
| 55  | MG   | AA    | 3169 | 1/1   | 0.92 | 0.54 | 47,47,47,47                | 0     |
| 55  | MG   | BA    | 1701 | 1/1   | 0.92 | 0.41 | 68,68,68,68                | 0     |
| 55  | MG   | BA    | 1605 | 1/1   | 0.92 | 0.12 | 81,81,81,81                | 0     |
| 56  | OHX  | AA    | 3509 | 7/7   | 0.92 | 0.20 | 91,109,142,150             | 3     |
| 56  | OHX  | CA    | 1769 | 7/7   | 0.92 | 0.11 | 141,144,170,199            | 1     |
| 55  | MG   | DA    | 3154 | 1/1   | 0.93 | 0.30 | 60,60,60,60                | 0     |
| 55  | MG   | CA    | 1602 | 1/1   | 0.93 | 0.42 | 58,58,58,58                | 0     |
| 56  | OHX  | AA    | 3473 | 7/7   | 0.93 | 0.21 | 104,114,132,167            | 1     |
| 55  | MG   | DA    | 3240 | 1/1   | 0.93 | 0.40 | 64,64,64,64                | 0     |
| 55  | MG   | AA    | 3194 | 1/1   | 0.93 | 0.42 | 56,56,56,56                | 0     |
| 56  | OHX  | AA    | 3408 | 7/7   | 0.93 | 0.14 | 107,111,135,163            | 1     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | BA    | 1682 | 1/1   | 0.93 | 0.08 | 68,68,68,68                 | 0     |
| 55  | MG   | BA    | 1700 | 1/1   | 0.93 | 0.05 | 119,119,119,119             | 0     |
| 55  | MG   | AA    | 3103 | 1/1   | 0.93 | 0.41 | 50,50,50,50                 | 0     |
| 55  | MG   | AA    | 3094 | 1/1   | 0.93 | 0.51 | 48,48,48,48                 | 0     |
| 56  | OHX  | BA    | 1775 | 7/7   | 0.93 | 0.15 | 113,130,145,176             | 1     |
| 56  | OHX  | CA    | 1802 | 7/7   | 0.93 | 0.10 | 130,138,148,200             | 1     |
| 55  | MG   | DA    | 3195 | 1/1   | 0.93 | 0.16 | 46,46,46,46                 | 0     |
| 55  | MG   | D0    | 201  | 1/1   | 0.93 | 0.14 | 51,51,51,51                 | 0     |
| 56  | OHX  | DA    | 3091 | 7/7   | 0.93 | 0.15 | 103,121,134,170             | 1     |
| 55  | MG   | A1    | 202  | 1/1   | 0.93 | 0.19 | 75,75,75,75                 | 0     |
| 56  | OHX  | BA    | 1725 | 7/7   | 0.93 | 0.15 | 95,114,126,182              | 1     |
| 56  | OHX  | AA    | 3448 | 7/7   | 0.93 | 0.10 | 141,143,155,200             | 1     |
| 56  | OHX  | AA    | 3541 | 7/7   | 0.93 | 0.39 | 131,134,141,173             | 1     |
| 56  | OHX  | DA    | 3463 | 7/7   | 0.93 | 0.20 | 142,149,156,188             | 1     |
| 55  | MG   | AA    | 3073 | 1/1   | 0.93 | 0.32 | 68,68,68,68                 | 0     |
| 56  | OHX  | AA    | 3524 | 7/7   | 0.93 | 0.13 | 115,120,140,187             | 1     |
| 56  | OHX  | CA    | 1781 | 7/7   | 0.93 | 0.13 | 153,161,166,239             | 1     |
| 55  | MG   | AA    | 3286 | 1/1   | 0.93 | 0.40 | 83,83,83,83                 | 0     |
| 55  | MG   | DA    | 3266 | 1/1   | 0.93 | 0.47 | 88,88,88,88                 | 0     |
| 56  | OHX  | AB    | 219  | 7/7   | 0.93 | 0.37 | 112,116,126,139             | 1     |
| 56  | OHX  | AA    | 3552 | 7/7   | 0.93 | 0.18 | 96,106,128,164              | 1     |
| 55  | MG   | DA    | 3272 | 1/1   | 0.93 | 0.10 | 57,57,57,57                 | 0     |
| 56  | OHX  | AA    | 3540 | 7/7   | 0.93 | 0.15 | 104,109,137,150             | 2     |
| 56  | OHX  | BA    | 1793 | 7/7   | 0.93 | 0.14 | 129,132,141,164             | 1     |
| 56  | OHX  | BA    | 1743 | 7/7   | 0.93 | 0.23 | 79,96,129,159               | 2     |
| 55  | MG   | DA    | 3334 | 1/1   | 0.93 | 0.34 | 75,75,75,75                 | 0     |
| 56  | OHX  | AA    | 3560 | 7/7   | 0.93 | 0.16 | 132,136,153,192             | 1     |
| 55  | MG   | BA    | 1618 | 1/1   | 0.93 | 0.33 | 71,71,71,71                 | 0     |
| 56  | OHX  | BA    | 1763 | 7/7   | 0.93 | 0.12 | 123,136,140,184             | 1     |
| 55  | MG   | BA    | 1713 | 1/1   | 0.93 | 0.45 | 81,81,81,81                 | 0     |
| 56  | OHX  | AA    | 3449 | 7/7   | 0.93 | 0.15 | 102,118,124,165             | 1     |
| 56  | OHX  | BA    | 1808 | 7/7   | 0.93 | 0.20 | 121,129,141,156             | 1     |
| 55  | MG   | AA    | 3004 | 1/1   | 0.93 | 0.36 | 32,32,32,32                 | 0     |
| 55  | MG   | AA    | 3029 | 1/1   | 0.93 | 0.29 | 59,59,59,59                 | 0     |
| 55  | MG   | AA    | 3297 | 1/1   | 0.93 | 0.07 | 80,80,80,80                 | 0     |
| 55  | MG   | CA    | 1645 | 1/1   | 0.93 | 0.50 | 58,58,58,58                 | 0     |
| 56  | OHX  | AA    | 3445 | 7/7   | 0.93 | 0.13 | 118,124,140,177             | 1     |
| 56  | OHX  | AA    | 3478 | 7/7   | 0.93 | 0.16 | 147,161,167,217             | 1     |
| 55  | MG   | AA    | 3086 | 1/1   | 0.93 | 0.32 | 73,73,73,73                 | 0     |
| 56  | OHX  | DA    | 3485 | 7/7   | 0.93 | 0.17 | 131,137,152,172             | 1     |
| 56  | OHX  | DA    | 3221 | 7/7   | 0.93 | 0.11 | 120,130,140,174             | 1     |
| 55  | MG   | DA    | 3098 | 1/1   | 0.93 | 0.16 | 63,63,63,63                 | 0     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 56  | OHX  | DA    | 3452 | 7/7   | 0.93 | 0.17 | 99,118,125,155             | 1     |
| 56  | OHX  | DA    | 3427 | 7/7   | 0.93 | 0.11 | 134,147,151,184            | 1     |
| 55  | MG   | DA    | 3194 | 1/1   | 0.93 | 0.45 | 48,48,48,48                | 0     |
| 56  | OHX  | AA    | 3443 | 7/7   | 0.93 | 0.15 | 110,114,126,149            | 2     |
| 56  | OHX  | DA    | 3159 | 7/7   | 0.93 | 0.19 | 75,86,105,131              | 3     |
| 56  | OHX  | AA    | 3499 | 7/7   | 0.93 | 0.15 | 107,112,120,152            | 1     |
| 55  | MG   | CA    | 1709 | 1/1   | 0.93 | 0.25 | 76,76,76,76                | 0     |
| 56  | OHX  | DA    | 3103 | 7/7   | 0.93 | 0.20 | 94,102,107,128             | 2     |
| 56  | OHX  | DA    | 3434 | 7/7   | 0.93 | 0.13 | 127,134,154,190            | 1     |
| 55  | MG   | CA    | 1673 | 1/1   | 0.93 | 0.33 | 76,76,76,76                | 0     |
| 56  | OHX  | DA    | 3453 | 7/7   | 0.93 | 0.26 | 145,153,160,191            | 1     |
| 56  | OHX  | DA    | 3437 | 7/7   | 0.93 | 0.15 | 113,120,134,160            | 1     |
| 55  | MG   | AO    | 201  | 1/1   | 0.93 | 0.14 | 66,66,66,66                | 0     |
| 56  | OHX  | DA    | 3444 | 7/7   | 0.93 | 0.14 | 123,132,145,175            | 1     |
| 55  | MG   | AA    | 3066 | 1/1   | 0.93 | 0.30 | 62,62,62,62                | 0     |
| 55  | MG   | BA    | 1668 | 1/1   | 0.93 | 0.34 | 64,64,64,64                | 0     |
| 56  | OHX  | DA    | 3438 | 7/7   | 0.93 | 0.13 | 120,135,146,170            | 1     |
| 55  | MG   | DA    | 3189 | 1/1   | 0.93 | 0.62 | 56,56,56,56                | 0     |
| 55  | MG   | DA    | 3032 | 1/1   | 0.93 | 0.11 | 38,38,38,38                | 0     |
| 56  | OHX  | BA    | 1785 | 7/7   | 0.93 | 0.13 | 117,124,136,144            | 2     |
| 55  | MG   | AA    | 3177 | 1/1   | 0.93 | 0.26 | 46,46,46,46                | 0     |
| 56  | OHX  | DA    | 3376 | 7/7   | 0.93 | 0.20 | 38,106,133,165             | 3     |
| 56  | OHX  | BA    | 1769 | 7/7   | 0.93 | 0.09 | 159,168,172,218            | 1     |
| 56  | OHX  | CA    | 1784 | 7/7   | 0.93 | 0.15 | 127,135,151,190            | 1     |
| 56  | OHX  | AA    | 3553 | 7/7   | 0.93 | 0.12 | 160,165,172,209            | 1     |
| 56  | OHX  | DB    | 215  | 7/7   | 0.93 | 0.16 | 147,149,158,191            | 1     |
| 55  | MG   | DA    | 3267 | 1/1   | 0.93 | 0.34 | 82,82,82,82                | 0     |
| 55  | MG   | AA    | 3049 | 1/1   | 0.93 | 0.13 | 66,66,66,66                | 0     |
| 55  | MG   | CA    | 1679 | 1/1   | 0.93 | 0.17 | 87,87,87,87                | 0     |
| 56  | OHX  | AA    | 3367 | 7/7   | 0.93 | 0.25 | 69,72,90,147               | 3     |
| 55  | MG   | AA    | 3079 | 1/1   | 0.93 | 0.38 | 67,67,67,67                | 0     |
| 55  | MG   | AA    | 3118 | 1/1   | 0.93 | 0.23 | 69,69,69,69                | 0     |
| 55  | MG   | BA    | 1611 | 1/1   | 0.93 | 0.37 | 47,47,47,47                | 0     |
| 55  | MG   | CA    | 1694 | 1/1   | 0.93 | 0.37 | 89,89,89,89                | 0     |
| 55  | MG   | BA    | 1663 | 1/1   | 0.93 | 0.74 | 80,80,80,80                | 0     |
| 55  | MG   | AA    | 3135 | 1/1   | 0.93 | 0.35 | 66,66,66,66                | 0     |
| 56  | OHX  | AA    | 3521 | 7/7   | 0.93 | 0.12 | 103,107,119,167            | 2     |
| 55  | MG   | CA    | 1631 | 1/1   | 0.93 | 0.34 | 74,74,74,74                | 0     |
| 55  | MG   | BA    | 1629 | 1/1   | 0.93 | 0.14 | 79,79,79,79                | 0     |
| 56  | OHX  | DA    | 3421 | 7/7   | 0.93 | 0.17 | 96,112,124,166             | 1     |
| 56  | OHX  | BA    | 1742 | 7/7   | 0.93 | 0.11 | 149,155,172,201            | 1     |
| 55  | MG   | AA    | 3319 | 1/1   | 0.93 | 0.09 | 63,63,63,63                | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | OHX  | BA    | 1798 | 7/7   | 0.93 | 0.11 | 135,136,153,212             | 1     |
| 55  | MG   | AA    | 3133 | 1/1   | 0.93 | 0.34 | 45,45,45,45                 | 0     |
| 55  | MG   | DA    | 3185 | 1/1   | 0.93 | 0.40 | 49,49,49,49                 | 0     |
| 56  | OHX  | DA    | 3459 | 7/7   | 0.94 | 0.16 | 85,104,120,156              | 1     |
| 55  | MG   | CA    | 1675 | 1/1   | 0.94 | 0.40 | 94,94,94,94                 | 0     |
| 55  | MG   | AA    | 3283 | 1/1   | 0.94 | 0.10 | 21,21,21,21                 | 0     |
| 56  | OHX  | DA    | 3423 | 7/7   | 0.94 | 0.09 | 127,140,151,201             | 1     |
| 55  | MG   | DA    | 3309 | 1/1   | 0.94 | 0.17 | 68,68,68,68                 | 0     |
| 55  | MG   | CA    | 1606 | 1/1   | 0.94 | 0.16 | 70,70,70,70                 | 0     |
| 55  | MG   | AA    | 3101 | 1/1   | 0.94 | 0.32 | 47,47,47,47                 | 0     |
| 55  | MG   | DA    | 3139 | 1/1   | 0.94 | 0.45 | 54,54,54,54                 | 0     |
| 55  | MG   | AA    | 3005 | 1/1   | 0.94 | 0.39 | 48,48,48,48                 | 0     |
| 55  | MG   | AA    | 3056 | 1/1   | 0.94 | 0.23 | 55,55,55,55                 | 0     |
| 56  | OHX  | CA    | 1812 | 7/7   | 0.94 | 0.11 | 134,141,149,203             | 1     |
| 55  | MG   | CA    | 1655 | 1/1   | 0.94 | 0.33 | 70,70,70,70                 | 0     |
| 56  | OHX  | BA    | 1754 | 7/7   | 0.94 | 0.08 | 136,144,152,183             | 1     |
| 55  | MG   | CA    | 1661 | 1/1   | 0.94 | 0.52 | 83,83,83,83                 | 0     |
| 56  | OHX  | DA    | 3165 | 7/7   | 0.94 | 0.20 | 123,135,143,168             | 1     |
| 55  | MG   | DA    | 3047 | 1/1   | 0.94 | 0.15 | 79,79,79,79                 | 0     |
| 55  | MG   | AA    | 3219 | 1/1   | 0.94 | 0.30 | 65,65,65,65                 | 0     |
| 55  | MG   | AA    | 3225 | 1/1   | 0.94 | 0.52 | 52,52,52,52                 | 0     |
| 56  | OHX  | DB    | 209  | 7/7   | 0.94 | 0.15 | 130,143,158,186             | 1     |
| 55  | MG   | AA    | 3252 | 1/1   | 0.94 | 0.38 | 52,52,52,52                 | 0     |
| 56  | OHX  | BA    | 1761 | 7/7   | 0.94 | 0.08 | 136,147,154,197             | 1     |
| 56  | OHX  | AO    | 203  | 7/7   | 0.94 | 0.13 | 83,92,110,152               | 1     |
| 55  | MG   | AA    | 3261 | 1/1   | 0.94 | 0.23 | 53,53,53,53                 | 0     |
| 56  | OHX  | DA    | 3477 | 7/7   | 0.94 | 0.07 | 153,157,164,211             | 1     |
| 56  | OHX  | DA    | 3214 | 7/7   | 0.94 | 0.21 | 82,92,98,133                | 2     |
| 55  | MG   | BA    | 1616 | 1/1   | 0.94 | 0.06 | 101,101,101,101             | 0     |
| 55  | MG   | DA    | 3101 | 1/1   | 0.94 | 0.22 | 59,59,59,59                 | 0     |
| 56  | OHX  | CA    | 1777 | 7/7   | 0.94 | 0.09 | 157,162,168,202             | 1     |
| 56  | OHX  | BA    | 1748 | 7/7   | 0.94 | 0.14 | 124,127,141,171             | 1     |
| 55  | MG   | AA    | 3268 | 1/1   | 0.94 | 0.16 | 38,38,38,38                 | 0     |
| 56  | OHX  | DA    | 3487 | 7/7   | 0.94 | 0.18 | 106,108,129,150             | 1     |
| 55  | MG   | DA    | 3204 | 1/1   | 0.94 | 0.30 | 58,58,58,58                 | 0     |
| 55  | MG   | CA    | 1601 | 1/1   | 0.94 | 0.38 | 75,75,75,75                 | 0     |
| 55  | MG   | BA    | 1620 | 1/1   | 0.94 | 0.26 | 73,73,73,73                 | 0     |
| 55  | MG   | AA    | 3220 | 1/1   | 0.94 | 0.20 | 38,38,38,38                 | 0     |
| 56  | OHX  | AA    | 3462 | 7/7   | 0.94 | 0.17 | 105,108,119,142             | 2     |
| 56  | OHX  | BA    | 1783 | 7/7   | 0.94 | 0.10 | 121,130,148,178             | 1     |
| 55  | MG   | DB    | 202  | 1/1   | 0.94 | 0.14 | 98,98,98,98                 | 0     |
| 56  | OHX  | BA    | 1782 | 7/7   | 0.94 | 0.11 | 137,145,154,180             | 1     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 56  | OHX  | BA    | 1749 | 7/7   | 0.94 | 0.17 | 112,116,136,168            | 1     |
| 55  | MG   | AA    | 3108 | 1/1   | 0.94 | 0.11 | 54,54,54,54                | 0     |
| 55  | MG   | DA    | 3076 | 1/1   | 0.94 | 0.64 | 54,54,54,54                | 0     |
| 55  | MG   | AA    | 3109 | 1/1   | 0.94 | 0.37 | 38,38,38,38                | 0     |
| 55  | MG   | DA    | 3277 | 1/1   | 0.94 | 0.10 | 89,89,89,89                | 0     |
| 56  | OHX  | DA    | 3169 | 7/7   | 0.94 | 0.17 | 110,124,136,172            | 1     |
| 55  | MG   | AB    | 205  | 1/1   | 0.94 | 0.23 | 68,68,68,68                | 0     |
| 55  | MG   | CA    | 1650 | 1/1   | 0.94 | 0.28 | 66,66,66,66                | 0     |
| 56  | OHX  | DA    | 3431 | 7/7   | 0.94 | 0.14 | 139,144,155,180            | 1     |
| 56  | OHX  | CA    | 1798 | 7/7   | 0.94 | 0.17 | 116,126,129,163            | 1     |
| 56  | OHX  | A1    | 203  | 7/7   | 0.94 | 0.16 | 97,103,123,154             | 1     |
| 56  | OHX  | BA    | 1796 | 7/7   | 0.94 | 0.24 | 119,126,142,152            | 1     |
| 55  | MG   | DA    | 3011 | 1/1   | 0.94 | 0.09 | 84,84,84,84                | 0     |
| 55  | MG   | AA    | 3080 | 1/1   | 0.94 | 0.21 | 63,63,63,63                | 0     |
| 56  | OHX  | BA    | 1794 | 7/7   | 0.94 | 0.09 | 156,163,165,204            | 1     |
| 55  | MG   | DA    | 3125 | 1/1   | 0.94 | 0.33 | 54,54,54,54                | 0     |
| 55  | MG   | DA    | 3321 | 1/1   | 0.94 | 0.20 | 56,56,56,56                | 0     |
| 56  | OHX  | CA    | 1792 | 7/7   | 0.94 | 0.11 | 189,191,192,232            | 1     |
| 56  | OHX  | CA    | 1793 | 7/7   | 0.94 | 0.08 | 142,146,153,194            | 1     |
| 56  | OHX  | A6    | 101  | 7/7   | 0.94 | 0.15 | 112,127,141,158            | 2     |
| 55  | MG   | AB    | 202  | 1/1   | 0.94 | 0.18 | 80,80,80,80                | 0     |
| 56  | OHX  | DA    | 3424 | 7/7   | 0.94 | 0.15 | 124,129,137,157            | 2     |
| 56  | OHX  | AA    | 3504 | 7/7   | 0.94 | 0.20 | 101,103,116,145            | 2     |
| 56  | OHX  | AA    | 3569 | 7/7   | 0.94 | 0.13 | 134,142,144,168            | 1     |
| 55  | MG   | DA    | 3077 | 1/1   | 0.94 | 0.56 | 52,52,52,52                | 0     |
| 55  | MG   | AA    | 3131 | 1/1   | 0.94 | 0.55 | 62,62,62,62                | 0     |
| 56  | OHX  | DA    | 3392 | 7/7   | 0.94 | 0.12 | 115,117,129,183            | 1     |
| 55  | MG   | BA    | 1638 | 1/1   | 0.94 | 0.35 | 104,104,104,104            | 0     |
| 56  | OHX  | DA    | 3435 | 7/7   | 0.94 | 0.19 | 86,99,124,155              | 1     |
| 56  | OHX  | BA    | 1747 | 7/7   | 0.94 | 0.20 | 117,129,140,148            | 1     |
| 56  | OHX  | CA    | 1790 | 7/7   | 0.94 | 0.17 | 99,111,123,147             | 2     |
| 56  | OHX  | DA    | 3460 | 7/7   | 0.94 | 0.13 | 111,124,134,174            | 1     |
| 56  | OHX  | DA    | 3394 | 7/7   | 0.94 | 0.12 | 127,139,150,223            | 0     |
| 56  | OHX  | DA    | 3411 | 7/7   | 0.94 | 0.14 | 104,112,132,163            | 1     |
| 56  | OHX  | AA    | 3532 | 7/7   | 0.94 | 0.13 | 136,144,160,202            | 1     |
| 56  | OHX  | AA    | 3425 | 7/7   | 0.94 | 0.10 | 158,168,177,207            | 1     |
| 55  | MG   | AA    | 3159 | 1/1   | 0.94 | 0.43 | 81,81,81,81                | 0     |
| 56  | OHX  | DA    | 3245 | 7/7   | 0.94 | 0.13 | 95,128,139,165             | 1     |
| 55  | MG   | AA    | 3178 | 1/1   | 0.94 | 0.42 | 76,76,76,76                | 0     |
| 56  | OHX  | BA    | 1811 | 7/7   | 0.94 | 0.13 | 110,118,135,147            | 1     |
| 55  | MG   | BD    | 101  | 1/1   | 0.94 | 0.21 | 103,103,103,103            | 0     |
| 56  | OHX  | BA    | 1731 | 7/7   | 0.94 | 0.25 | 99,107,129,161             | 1     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | AF    | 301  | 1/1   | 0.94 | 0.07 | 74,74,74,74                 | 0     |
| 56  | OHX  | AA    | 3568 | 7/7   | 0.94 | 0.16 | 101,109,114,153             | 1     |
| 55  | MG   | DA    | 3014 | 1/1   | 0.94 | 0.35 | 55,55,55,55                 | 0     |
| 55  | MG   | AA    | 3263 | 1/1   | 0.94 | 0.32 | 39,39,39,39                 | 0     |
| 56  | OHX  | DA    | 3461 | 7/7   | 0.94 | 0.08 | 171,173,180,211             | 1     |
| 56  | OHX  | DB    | 213  | 7/7   | 0.94 | 0.16 | 125,144,157,169             | 2     |
| 56  | OHX  | DA    | 3465 | 7/7   | 0.94 | 0.15 | 123,136,143,165             | 1     |
| 55  | MG   | AA    | 3104 | 1/1   | 0.94 | 0.28 | 62,62,62,62                 | 0     |
| 55  | MG   | AA    | 3210 | 1/1   | 0.94 | 0.55 | 43,43,43,43                 | 0     |
| 56  | OHX  | DA    | 3087 | 7/7   | 0.94 | 0.16 | 102,119,134,177             | 1     |
| 55  | MG   | AA    | 3243 | 1/1   | 0.94 | 0.40 | 62,62,62,62                 | 0     |
| 55  | MG   | AA    | 3321 | 1/1   | 0.94 | 0.35 | 41,41,41,41                 | 0     |
| 57  | PAR  | CA    | 1722 | 42/42 | 0.94 | 0.15 | 72,88,95,97                 | 0     |
| 55  | MG   | A5    | 101  | 1/1   | 0.94 | 0.33 | 43,43,43,43                 | 0     |
| 55  | MG   | AA    | 3314 | 1/1   | 0.94 | 0.15 | 63,63,63,63                 | 0     |
| 56  | OHX  | BB    | 114  | 7/7   | 0.94 | 0.29 | 176,178,180,206             | 1     |
| 55  | MG   | AA    | 3132 | 1/1   | 0.94 | 0.54 | 48,48,48,48                 | 0     |
| 56  | OHX  | BA    | 1752 | 7/7   | 0.94 | 0.09 | 168,174,177,207             | 1     |
| 56  | OHX  | DA    | 3432 | 7/7   | 0.94 | 0.10 | 116,131,140,173             | 1     |
| 55  | MG   | CA    | 1706 | 1/1   | 0.94 | 0.60 | 85,85,85,85                 | 0     |
| 55  | MG   | DA    | 3250 | 1/1   | 0.94 | 0.37 | 64,64,64,64                 | 0     |
| 56  | OHX  | CA    | 1800 | 7/7   | 0.94 | 0.08 | 165,167,172,220             | 1     |
| 56  | OHX  | A3    | 102  | 7/7   | 0.94 | 0.19 | 106,109,134,147             | 2     |
| 55  | MG   | DA    | 3229 | 1/1   | 0.94 | 0.44 | 45,45,45,45                 | 0     |
| 56  | OHX  | CA    | 1806 | 7/7   | 0.94 | 0.12 | 138,150,153,181             | 1     |
| 55  | MG   | DA    | 3216 | 1/1   | 0.94 | 0.43 | 71,71,71,71                 | 0     |
| 55  | MG   | BA    | 1658 | 1/1   | 0.94 | 0.43 | 47,47,47,47                 | 0     |
| 56  | OHX  | DA    | 3470 | 7/7   | 0.94 | 0.17 | 152,169,191,193             | 1     |
| 55  | MG   | AA    | 3059 | 1/1   | 0.94 | 0.32 | 77,77,77,77                 | 0     |
| 55  | MG   | DA    | 3016 | 1/1   | 0.94 | 0.59 | 51,51,51,51                 | 0     |
| 55  | MG   | CA    | 1619 | 1/1   | 0.94 | 0.21 | 92,92,92,92                 | 0     |
| 55  | MG   | DA    | 3265 | 1/1   | 0.94 | 0.18 | 73,73,73,73                 | 0     |
| 56  | OHX  | CA    | 1801 | 7/7   | 0.94 | 0.10 | 137,140,148,200             | 1     |
| 56  | OHX  | CA    | 1813 | 7/7   | 0.94 | 0.41 | 138,144,151,179             | 1     |
| 55  | MG   | DA    | 3142 | 1/1   | 0.94 | 0.41 | 76,76,76,76                 | 0     |
| 55  | MG   | AA    | 3057 | 1/1   | 0.94 | 0.18 | 56,56,56,56                 | 0     |
| 56  | OHX  | AA    | 3472 | 7/7   | 0.94 | 0.26 | 95,115,124,169              | 1     |
| 56  | OHX  | AA    | 3481 | 7/7   | 0.94 | 0.15 | 88,92,119,127               | 2     |
| 56  | OHX  | DA    | 3446 | 7/7   | 0.94 | 0.11 | 118,121,142,162             | 1     |
| 56  | OHX  | CA    | 1751 | 7/7   | 0.94 | 0.19 | 102,126,129,174             | 1     |
| 55  | MG   | DA    | 3228 | 1/1   | 0.94 | 0.44 | 58,58,58,58                 | 0     |
| 55  | MG   | AA    | 3356 | 1/1   | 0.94 | 0.58 | 70,70,70,70                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 56  | OHX  | DA    | 3464 | 7/7   | 0.94 | 0.25 | 117,129,143,171            | 1     |
| 56  | OHX  | CA    | 1765 | 7/7   | 0.94 | 0.06 | 169,177,182,233            | 1     |
| 55  | MG   | AA    | 3041 | 1/1   | 0.94 | 0.25 | 59,59,59,59                | 0     |
| 56  | OHX  | AA    | 3494 | 7/7   | 0.94 | 0.12 | 112,122,130,153            | 1     |
| 56  | OHX  | BA    | 1745 | 7/7   | 0.95 | 0.13 | 119,123,132,169            | 1     |
| 55  | MG   | DA    | 3137 | 1/1   | 0.95 | 0.42 | 51,51,51,51                | 0     |
| 56  | OHX  | AA    | 3496 | 7/7   | 0.95 | 0.12 | 107,119,130,176            | 1     |
| 55  | MG   | AA    | 3039 | 1/1   | 0.95 | 0.39 | 50,50,50,50                | 0     |
| 56  | OHX  | CA    | 1770 | 7/7   | 0.95 | 0.09 | 143,153,167,200            | 1     |
| 56  | OHX  | AA    | 3488 | 7/7   | 0.95 | 0.14 | 155,156,163,203            | 1     |
| 55  | MG   | DA    | 3038 | 1/1   | 0.95 | 0.23 | 77,77,77,77                | 0     |
| 55  | MG   | CA    | 1702 | 1/1   | 0.95 | 0.48 | 59,59,59,59                | 0     |
| 56  | OHX  | DA    | 3416 | 7/7   | 0.95 | 0.17 | 112,112,142,167            | 1     |
| 56  | OHX  | DA    | 3456 | 7/7   | 0.95 | 0.10 | 133,142,150,207            | 1     |
| 56  | OHX  | AA    | 3374 | 7/7   | 0.95 | 0.20 | 32,70,109,140              | 3     |
| 56  | OHX  | DA    | 3388 | 7/7   | 0.95 | 0.15 | 108,118,139,160            | 1     |
| 55  | MG   | DA    | 3291 | 1/1   | 0.95 | 0.20 | 66,66,66,66                | 0     |
| 55  | MG   | DA    | 3021 | 1/1   | 0.95 | 0.25 | 62,62,62,62                | 0     |
| 56  | OHX  | DA    | 3217 | 7/7   | 0.95 | 0.10 | 144,149,153,189            | 1     |
| 56  | OHX  | DA    | 3425 | 7/7   | 0.95 | 0.09 | 125,134,139,188            | 1     |
| 55  | MG   | AA    | 3074 | 1/1   | 0.95 | 0.11 | 90,90,90,90                | 0     |
| 55  | MG   | DA    | 3184 | 1/1   | 0.95 | 0.54 | 37,37,37,37                | 0     |
| 55  | MG   | CA    | 1642 | 1/1   | 0.95 | 0.57 | 69,69,69,69                | 0     |
| 55  | MG   | AA    | 3130 | 1/1   | 0.95 | 0.38 | 43,43,43,43                | 0     |
| 56  | OHX  | AA    | 3534 | 7/7   | 0.95 | 0.12 | 103,124,138,161            | 2     |
| 56  | OHX  | AW    | 101  | 7/7   | 0.95 | 0.17 | 112,118,129,149            | 1     |
| 56  | OHX  | BC    | 105  | 7/7   | 0.95 | 0.15 | 129,141,151,159            | 1     |
| 56  | OHX  | CA    | 1749 | 7/7   | 0.95 | 0.13 | 124,137,161,188            | 2     |
| 55  | MG   | AA    | 3224 | 1/1   | 0.95 | 0.24 | 79,79,79,79                | 0     |
| 56  | OHX  | AB    | 210  | 7/7   | 0.95 | 0.10 | 101,108,128,154            | 1     |
| 56  | OHX  | AA    | 3459 | 7/7   | 0.95 | 0.15 | 91,107,133,162             | 1     |
| 56  | OHX  | BA    | 1771 | 7/7   | 0.95 | 0.18 | 101,104,120,152            | 2     |
| 56  | OHX  | DA    | 3391 | 7/7   | 0.95 | 0.11 | 117,125,144,183            | 1     |
| 56  | OHX  | DA    | 3243 | 7/7   | 0.95 | 0.22 | 74,100,112,145             | 2     |
| 56  | OHX  | CA    | 1758 | 7/7   | 0.95 | 0.08 | 150,162,166,191            | 1     |
| 55  | MG   | BA    | 1678 | 1/1   | 0.95 | 0.33 | 44,44,44,44                | 0     |
| 56  | OHX  | AB    | 217  | 7/7   | 0.95 | 0.24 | 100,108,115,151            | 1     |
| 56  | OHX  | DA    | 3428 | 7/7   | 0.95 | 0.15 | 93,108,120,163             | 1     |
| 55  | MG   | DA    | 3247 | 1/1   | 0.95 | 0.33 | 48,48,48,48                | 0     |
| 56  | OHX  | CA    | 1807 | 7/7   | 0.95 | 0.27 | 109,119,124,150            | 1     |
| 56  | OHX  | CA    | 1782 | 7/7   | 0.95 | 0.18 | 134,137,147,160            | 1     |
| 55  | MG   | AA    | 3003 | 1/1   | 0.95 | 0.33 | 39,39,39,39                | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | OHX  | AA    | 3433 | 7/7   | 0.95 | 0.15 | 77,91,106,131               | 2     |
| 55  | MG   | DA    | 3122 | 1/1   | 0.95 | 0.37 | 30,30,30,30                 | 0     |
| 56  | OHX  | BA    | 1764 | 7/7   | 0.95 | 0.14 | 147,152,158,209             | 1     |
| 56  | OHX  | DA    | 3166 | 7/7   | 0.95 | 0.11 | 159,166,176,197             | 1     |
| 55  | MG   | DA    | 3225 | 1/1   | 0.95 | 0.42 | 55,55,55,55                 | 0     |
| 56  | OHX  | DA    | 3248 | 7/7   | 0.95 | 0.14 | 110,118,139,156             | 1     |
| 55  | MG   | AA    | 3149 | 1/1   | 0.95 | 0.36 | 58,58,58,58                 | 0     |
| 55  | MG   | DA    | 3299 | 1/1   | 0.95 | 0.29 | 67,67,67,67                 | 0     |
| 55  | MG   | DA    | 3006 | 1/1   | 0.95 | 0.25 | 63,63,63,63                 | 0     |
| 55  | MG   | CA    | 1603 | 1/1   | 0.95 | 0.29 | 62,62,62,62                 | 0     |
| 56  | OHX  | DA    | 3449 | 7/7   | 0.95 | 0.10 | 147,154,162,185             | 1     |
| 56  | OHX  | DA    | 3409 | 7/7   | 0.95 | 0.18 | 103,117,129,162             | 1     |
| 56  | OHX  | DA    | 3398 | 7/7   | 0.95 | 0.13 | 119,127,142,162             | 1     |
| 56  | OHX  | CA    | 1794 | 7/7   | 0.95 | 0.16 | 102,115,122,149             | 1     |
| 55  | MG   | DA    | 3152 | 1/1   | 0.95 | 0.39 | 57,57,57,57                 | 0     |
| 56  | OHX  | AA    | 3489 | 7/7   | 0.95 | 0.11 | 136,140,156,178             | 1     |
| 55  | MG   | DA    | 3126 | 1/1   | 0.95 | 0.51 | 63,63,63,63                 | 0     |
| 55  | MG   | AA    | 3255 | 1/1   | 0.95 | 0.24 | 47,47,47,47                 | 0     |
| 55  | MG   | DA    | 3275 | 1/1   | 0.95 | 0.45 | 53,53,53,53                 | 0     |
| 56  | OHX  | DB    | 210  | 7/7   | 0.95 | 0.12 | 119,127,150,173             | 2     |
| 56  | OHX  | AA    | 3371 | 7/7   | 0.95 | 0.18 | 65,79,88,136                | 2     |
| 56  | OHX  | AA    | 3464 | 7/7   | 0.95 | 0.13 | 105,115,140,175             | 1     |
| 56  | OHX  | DA    | 3430 | 7/7   | 0.95 | 0.07 | 176,181,185,214             | 1     |
| 55  | MG   | DA    | 3056 | 1/1   | 0.95 | 0.28 | 48,48,48,48                 | 0     |
| 56  | OHX  | DA    | 3224 | 7/7   | 0.95 | 0.23 | 104,110,126,166             | 1     |
| 55  | MG   | DA    | 3097 | 1/1   | 0.95 | 0.40 | 67,67,67,67                 | 0     |
| 55  | MG   | AA    | 3116 | 1/1   | 0.95 | 0.24 | 63,63,63,63                 | 0     |
| 56  | OHX  | DA    | 3163 | 7/7   | 0.95 | 0.20 | 124,127,154,166             | 1     |
| 55  | MG   | DA    | 3191 | 1/1   | 0.95 | 0.35 | 66,66,66,66                 | 0     |
| 55  | MG   | AA    | 3260 | 1/1   | 0.95 | 0.38 | 53,53,53,53                 | 0     |
| 55  | MG   | BA    | 1669 | 1/1   | 0.95 | 0.31 | 68,68,68,68                 | 0     |
| 56  | OHX  | DB    | 211  | 7/7   | 0.95 | 0.13 | 105,121,145,156             | 2     |
| 56  | OHX  | AA    | 3457 | 7/7   | 0.95 | 0.12 | 86,94,124,185               | 1     |
| 55  | MG   | BA    | 1623 | 1/1   | 0.95 | 0.45 | 39,39,39,39                 | 0     |
| 55  | MG   | DA    | 3297 | 1/1   | 0.95 | 0.28 | 70,70,70,70                 | 0     |
| 55  | MG   | AB    | 206  | 1/1   | 0.95 | 0.45 | 77,77,77,77                 | 0     |
| 56  | OHX  | DA    | 3466 | 7/7   | 0.95 | 0.18 | 116,124,134,165             | 2     |
| 56  | OHX  | AA    | 3516 | 7/7   | 0.95 | 0.18 | 90,98,116,166               | 1     |
| 55  | MG   | AA    | 3034 | 1/1   | 0.95 | 0.31 | 50,50,50,50                 | 0     |
| 55  | MG   | DA    | 3129 | 1/1   | 0.95 | 0.37 | 68,68,68,68                 | 0     |
| 56  | OHX  | AA    | 3517 | 7/7   | 0.95 | 0.08 | 125,127,137,177             | 1     |
| 55  | MG   | BA    | 1606 | 1/1   | 0.95 | 0.23 | 70,70,70,70                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | OHX  | AA    | 3563 | 7/7   | 0.95 | 0.22 | 128,136,143,179             | 1     |
| 56  | OHX  | AB    | 208  | 7/7   | 0.95 | 0.14 | 95,117,137,155              | 2     |
| 55  | MG   | DA    | 3230 | 1/1   | 0.95 | 0.24 | 51,51,51,51                 | 0     |
| 55  | MG   | DA    | 3262 | 1/1   | 0.95 | 0.23 | 59,59,59,59                 | 0     |
| 56  | OHX  | BA    | 1802 | 7/7   | 0.95 | 0.09 | 100,117,125,149             | 1     |
| 55  | MG   | DA    | 3156 | 1/1   | 0.95 | 0.19 | 73,73,73,73                 | 0     |
| 56  | OHX  | AB    | 209  | 7/7   | 0.95 | 0.14 | 98,103,137,147              | 3     |
| 55  | MG   | DA    | 3063 | 1/1   | 0.95 | 0.55 | 59,59,59,59                 | 0     |
| 56  | OHX  | DA    | 3390 | 7/7   | 0.95 | 0.13 | 117,127,135,170             | 1     |
| 56  | OHX  | DA    | 3215 | 7/7   | 0.95 | 0.14 | 97,115,127,150              | 3     |
| 55  | MG   | DA    | 3040 | 1/1   | 0.95 | 0.18 | 66,66,66,66                 | 0     |
| 55  | MG   | AA    | 3115 | 1/1   | 0.95 | 0.39 | 57,57,57,57                 | 0     |
| 55  | MG   | DA    | 3301 | 1/1   | 0.95 | 0.29 | 60,60,60,60                 | 0     |
| 55  | MG   | CA    | 1607 | 1/1   | 0.95 | 0.28 | 86,86,86,86                 | 0     |
| 55  | MG   | CA    | 1717 | 1/1   | 0.95 | 0.28 | 64,64,64,64                 | 0     |
| 55  | MG   | CA    | 1695 | 1/1   | 0.95 | 0.14 | 94,94,94,94                 | 0     |
| 56  | OHX  | DA    | 3174 | 7/7   | 0.95 | 0.16 | 100,112,120,180             | 1     |
| 56  | OHX  | BA    | 1744 | 7/7   | 0.95 | 0.13 | 134,144,157,183             | 1     |
| 56  | OHX  | AA    | 3426 | 7/7   | 0.95 | 0.11 | 104,117,127,168             | 3     |
| 55  | MG   | CA    | 1604 | 1/1   | 0.95 | 0.17 | 72,72,72,72                 | 0     |
| 55  | MG   | AA    | 3067 | 1/1   | 0.95 | 0.17 | 50,50,50,50                 | 0     |
| 55  | MG   | AA    | 3188 | 1/1   | 0.95 | 0.16 | 29,29,29,29                 | 0     |
| 55  | MG   | AA    | 3119 | 1/1   | 0.95 | 0.24 | 86,86,86,86                 | 0     |
| 55  | MG   | AA    | 3069 | 1/1   | 0.95 | 0.23 | 54,54,54,54                 | 0     |
| 56  | OHX  | AA    | 3394 | 7/7   | 0.95 | 0.14 | 113,123,125,181             | 1     |
| 55  | MG   | DA    | 3305 | 1/1   | 0.95 | 0.20 | 48,48,48,48                 | 0     |
| 56  | OHX  | AA    | 3561 | 7/7   | 0.95 | 0.14 | 86,92,112,144               | 2     |
| 55  | MG   | AA    | 3064 | 1/1   | 0.95 | 0.25 | 52,52,52,52                 | 0     |
| 55  | MG   | AA    | 3244 | 1/1   | 0.95 | 0.34 | 41,41,41,41                 | 0     |
| 55  | MG   | AA    | 3053 | 1/1   | 0.95 | 0.21 | 77,77,77,77                 | 0     |
| 56  | OHX  | AA    | 3423 | 7/7   | 0.95 | 0.12 | 100,115,121,157             | 1     |
| 55  | MG   | CA    | 1613 | 1/1   | 0.95 | 0.28 | 73,73,73,73                 | 0     |
| 56  | OHX  | CA    | 1795 | 7/7   | 0.95 | 0.12 | 115,125,132,165             | 1     |
| 56  | OHX  | DA    | 3414 | 7/7   | 0.95 | 0.12 | 126,128,140,174             | 1     |
| 56  | OHX  | AA    | 3362 | 7/7   | 0.95 | 0.15 | 104,116,120,168             | 1     |
| 56  | OHX  | AA    | 3436 | 7/7   | 0.95 | 0.21 | 90,93,119,164               | 1     |
| 55  | MG   | DA    | 3149 | 1/1   | 0.95 | 0.23 | 53,53,53,53                 | 0     |
| 55  | MG   | AA    | 3198 | 1/1   | 0.95 | 0.28 | 34,34,34,34                 | 0     |
| 55  | MG   | AA    | 3320 | 1/1   | 0.95 | 0.20 | 45,45,45,45                 | 0     |
| 56  | OHX  | AA    | 3447 | 7/7   | 0.95 | 0.10 | 110,120,136,163             | 1     |
| 55  | MG   | DA    | 3086 | 1/1   | 0.95 | 0.44 | 51,51,51,51                 | 0     |
| 55  | MG   | AA    | 3137 | 1/1   | 0.95 | 0.31 | 74,74,74,74                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 56  | OHX  | DA    | 3400 | 7/7   | 0.95 | 0.17 | 113,116,126,149            | 1     |
| 56  | OHX  | CK    | 201  | 7/7   | 0.95 | 0.19 | 143,148,155,179            | 1     |
| 55  | MG   | AA    | 3032 | 1/1   | 0.95 | 0.29 | 37,37,37,37                | 0     |
| 55  | MG   | AA    | 3299 | 1/1   | 0.95 | 0.32 | 41,41,41,41                | 0     |
| 56  | OHX  | CA    | 1761 | 7/7   | 0.95 | 0.09 | 133,143,154,174            | 1     |
| 56  | OHX  | AB    | 211  | 7/7   | 0.95 | 0.11 | 124,127,142,178            | 1     |
| 55  | MG   | CA    | 1700 | 1/1   | 0.95 | 0.31 | 97,97,97,97                | 0     |
| 56  | OHX  | CA    | 1745 | 7/7   | 0.95 | 0.14 | 117,120,127,165            | 1     |
| 56  | OHX  | D1    | 201  | 7/7   | 0.95 | 0.15 | 110,112,135,162            | 1     |
| 55  | MG   | BA    | 1665 | 1/1   | 0.95 | 0.24 | 53,53,53,53                | 0     |
| 56  | OHX  | DA    | 3483 | 7/7   | 0.95 | 0.12 | 103,116,126,199            | 1     |
| 55  | MG   | AE    | 302  | 1/1   | 0.95 | 0.17 | 74,74,74,74                | 0     |
| 56  | OHX  | AA    | 3547 | 7/7   | 0.95 | 0.11 | 80,87,107,118              | 1     |
| 56  | OHX  | CA    | 1731 | 7/7   | 0.95 | 0.19 | 90,118,129,156             | 1     |
| 55  | MG   | DA    | 3178 | 1/1   | 0.95 | 0.65 | 58,58,58,58                | 0     |
| 55  | MG   | CA    | 1644 | 1/1   | 0.95 | 0.35 | 89,89,89,89                | 0     |
| 56  | OHX  | AA    | 3395 | 7/7   | 0.95 | 0.19 | 100,109,130,162            | 1     |
| 55  | MG   | AA    | 3140 | 1/1   | 0.95 | 0.36 | 70,70,70,70                | 0     |
| 55  | MG   | CA    | 1639 | 1/1   | 0.95 | 0.46 | 69,69,69,69                | 0     |
| 55  | MG   | DA    | 3093 | 1/1   | 0.95 | 0.15 | 46,46,46,46                | 0     |
| 56  | OHX  | CA    | 1763 | 7/7   | 0.96 | 0.09 | 142,143,157,189            | 1     |
| 55  | MG   | AA    | 3093 | 1/1   | 0.96 | 0.42 | 35,35,35,35                | 0     |
| 55  | MG   | DA    | 3208 | 1/1   | 0.96 | 0.45 | 61,61,61,61                | 0     |
| 56  | OHX  | AA    | 3474 | 7/7   | 0.96 | 0.12 | 113,120,132,160            | 1     |
| 56  | OHX  | AA    | 3475 | 7/7   | 0.96 | 0.08 | 132,134,145,192            | 1     |
| 56  | OHX  | AA    | 3550 | 7/7   | 0.96 | 0.09 | 118,128,136,169            | 1     |
| 56  | OHX  | DA    | 3168 | 7/7   | 0.96 | 0.17 | 129,143,154,181            | 1     |
| 55  | MG   | AA    | 3023 | 1/1   | 0.96 | 0.30 | 35,35,35,35                | 0     |
| 55  | MG   | AA    | 3298 | 1/1   | 0.96 | 0.26 | 45,45,45,45                | 0     |
| 56  | OHX  | AA    | 3435 | 7/7   | 0.96 | 0.15 | 83,103,126,156             | 2     |
| 56  | OHX  | AA    | 3421 | 7/7   | 0.96 | 0.17 | 78,84,91,130               | 1     |
| 56  | OHX  | AB    | 212  | 7/7   | 0.96 | 0.12 | 91,105,122,151             | 3     |
| 56  | OHX  | AA    | 3405 | 7/7   | 0.96 | 0.12 | 100,103,111,158            | 1     |
| 56  | OHX  | AA    | 3465 | 7/7   | 0.96 | 0.22 | 82,99,109,148              | 1     |
| 56  | OHX  | AA    | 3535 | 7/7   | 0.96 | 0.15 | 94,101,108,146             | 1     |
| 55  | MG   | AA    | 3147 | 1/1   | 0.96 | 0.39 | 49,49,49,49                | 0     |
| 55  | MG   | AA    | 3001 | 1/1   | 0.96 | 0.35 | 32,32,32,32                | 0     |
| 56  | OHX  | DA    | 3445 | 7/7   | 0.96 | 0.10 | 121,130,142,174            | 1     |
| 56  | OHX  | CA    | 1803 | 7/7   | 0.96 | 0.09 | 137,147,156,198            | 1     |
| 56  | OHX  | AA    | 3470 | 7/7   | 0.96 | 0.08 | 116,126,152,171            | 1     |
| 56  | OHX  | AA    | 3416 | 7/7   | 0.96 | 0.18 | 108,113,125,155            | 1     |
| 56  | OHX  | CA    | 1776 | 7/7   | 0.96 | 0.16 | 112,115,132,151            | 1     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | CA    | 1637 | 1/1   | 0.96 | 0.53 | 69,69,69,69                 | 0     |
| 55  | MG   | AA    | 3206 | 1/1   | 0.96 | 0.23 | 37,37,37,37                 | 0     |
| 56  | OHX  | AA    | 3404 | 7/7   | 0.96 | 0.09 | 108,112,133,175             | 1     |
| 56  | OHX  | BA    | 1773 | 7/7   | 0.96 | 0.11 | 135,139,146,167             | 1     |
| 55  | MG   | AA    | 3065 | 1/1   | 0.96 | 0.25 | 46,46,46,46                 | 0     |
| 56  | OHX  | DA    | 3081 | 7/7   | 0.96 | 0.15 | 99,102,113,145              | 1     |
| 55  | MG   | AA    | 3262 | 1/1   | 0.96 | 0.28 | 62,62,62,62                 | 0     |
| 56  | OHX  | AA    | 3463 | 7/7   | 0.96 | 0.14 | 94,102,127,154              | 1     |
| 55  | MG   | AA    | 3050 | 1/1   | 0.96 | 0.39 | 45,45,45,45                 | 0     |
| 55  | MG   | DA    | 3133 | 1/1   | 0.96 | 0.26 | 51,51,51,51                 | 0     |
| 56  | OHX  | CA    | 1772 | 7/7   | 0.96 | 0.09 | 142,144,153,197             | 1     |
| 55  | MG   | AA    | 3011 | 1/1   | 0.96 | 0.27 | 44,44,44,44                 | 0     |
| 56  | OHX  | CA    | 1752 | 7/7   | 0.96 | 0.15 | 139,147,150,191             | 1     |
| 55  | MG   | DA    | 3273 | 1/1   | 0.96 | 0.37 | 41,41,41,41                 | 0     |
| 56  | OHX  | BA    | 1751 | 7/7   | 0.96 | 0.18 | 101,112,132,168             | 2     |
| 55  | MG   | AA    | 3275 | 1/1   | 0.96 | 0.59 | 71,71,71,71                 | 0     |
| 55  | MG   | DA    | 3285 | 1/1   | 0.96 | 0.40 | 57,57,57,57                 | 0     |
| 56  | OHX  | DA    | 3372 | 7/7   | 0.96 | 0.20 | 90,96,108,138               | 1     |
| 56  | OHX  | AA    | 3419 | 7/7   | 0.96 | 0.12 | 102,113,133,143             | 3     |
| 56  | OHX  | AA    | 3442 | 7/7   | 0.96 | 0.12 | 97,106,127,148              | 1     |
| 55  | MG   | DA    | 3274 | 1/1   | 0.96 | 0.39 | 69,69,69,69                 | 0     |
| 55  | MG   | AA    | 3205 | 1/1   | 0.96 | 0.13 | 42,42,42,42                 | 0     |
| 56  | OHX  | AA    | 3440 | 7/7   | 0.96 | 0.11 | 83,91,111,141               | 1     |
| 55  | MG   | AA    | 3102 | 1/1   | 0.96 | 0.37 | 52,52,52,52                 | 0     |
| 56  | OHX  | DA    | 3109 | 7/7   | 0.96 | 0.30 | 99,116,138,153              | 1     |
| 56  | OHX  | BA    | 1774 | 7/7   | 0.96 | 0.12 | 104,121,130,163             | 1     |
| 55  | MG   | DA    | 3058 | 1/1   | 0.96 | 0.41 | 70,70,70,70                 | 0     |
| 56  | OHX  | AA    | 3537 | 7/7   | 0.96 | 0.10 | 164,173,184,214             | 1     |
| 56  | OHX  | CA    | 1756 | 7/7   | 0.96 | 0.11 | 99,109,123,147              | 2     |
| 55  | MG   | CC    | 102  | 1/1   | 0.96 | 0.86 | 69,69,69,69                 | 0     |
| 55  | MG   | AA    | 3228 | 1/1   | 0.96 | 0.37 | 53,53,53,53                 | 0     |
| 56  | OHX  | CA    | 1805 | 7/7   | 0.96 | 0.13 | 128,130,148,187             | 1     |
| 56  | OHX  | AA    | 3491 | 7/7   | 0.96 | 0.17 | 96,99,117,169               | 1     |
| 55  | MG   | DA    | 3147 | 1/1   | 0.96 | 0.31 | 55,55,55,55                 | 0     |
| 55  | MG   | DA    | 3263 | 1/1   | 0.96 | 0.26 | 55,55,55,55                 | 0     |
| 55  | MG   | DA    | 3131 | 1/1   | 0.96 | 0.35 | 72,72,72,72                 | 0     |
| 55  | MG   | DA    | 3211 | 1/1   | 0.96 | 0.40 | 57,57,57,57                 | 0     |
| 55  | MG   | BA    | 1601 | 1/1   | 0.96 | 0.34 | 57,57,57,57                 | 0     |
| 55  | MG   | DA    | 3024 | 1/1   | 0.96 | 0.28 | 63,63,63,63                 | 0     |
| 55  | MG   | CA    | 1638 | 1/1   | 0.96 | 0.37 | 59,59,59,59                 | 0     |
| 55  | MG   | DA    | 3292 | 1/1   | 0.96 | 0.25 | 51,51,51,51                 | 0     |
| 56  | OHX  | AA    | 3510 | 7/7   | 0.96 | 0.13 | 98,106,123,159              | 1     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | OHX  | DA    | 3426 | 7/7   | 0.96 | 0.08 | 118,125,141,168             | 1     |
| 56  | OHX  | DA    | 3443 | 7/7   | 0.96 | 0.17 | 113,124,137,188             | 1     |
| 56  | OHX  | DA    | 3365 | 7/7   | 0.96 | 0.12 | 100,119,136,159             | 2     |
| 56  | OHX  | DA    | 3439 | 7/7   | 0.96 | 0.12 | 127,146,152,174             | 1     |
| 56  | OHX  | BA    | 1759 | 7/7   | 0.96 | 0.08 | 173,177,187,214             | 1     |
| 56  | OHX  | BA    | 1732 | 7/7   | 0.96 | 0.11 | 128,131,145,175             | 2     |
| 56  | OHX  | CA    | 1771 | 7/7   | 0.96 | 0.12 | 105,107,134,145             | 1     |
| 55  | MG   | DA    | 3241 | 1/1   | 0.96 | 0.17 | 47,47,47,47                 | 0     |
| 55  | MG   | DA    | 3120 | 1/1   | 0.96 | 0.32 | 52,52,52,52                 | 0     |
| 56  | OHX  | AA    | 3441 | 7/7   | 0.96 | 0.14 | 113,135,152,175             | 1     |
| 55  | MG   | DA    | 3269 | 1/1   | 0.96 | 0.42 | 52,52,52,52                 | 0     |
| 56  | OHX  | BA    | 1806 | 7/7   | 0.96 | 0.16 | 110,117,124,159             | 1     |
| 56  | OHX  | AA    | 3542 | 7/7   | 0.96 | 0.17 | 92,98,124,157               | 1     |
| 55  | MG   | AA    | 3145 | 1/1   | 0.96 | 0.33 | 27,27,27,27                 | 0     |
| 55  | MG   | DE    | 301  | 1/1   | 0.96 | 0.38 | 52,52,52,52                 | 0     |
| 56  | OHX  | DA    | 3410 | 7/7   | 0.96 | 0.13 | 107,112,124,146             | 1     |
| 55  | MG   | DA    | 3135 | 1/1   | 0.96 | 0.35 | 42,42,42,42                 | 0     |
| 55  | MG   | CA    | 1658 | 1/1   | 0.96 | 0.34 | 65,65,65,65                 | 0     |
| 55  | MG   | AA    | 3296 | 1/1   | 0.96 | 0.40 | 69,69,69,69                 | 0     |
| 55  | MG   | BA    | 1651 | 1/1   | 0.96 | 0.49 | 76,76,76,76                 | 0     |
| 56  | OHX  | CA    | 1762 | 7/7   | 0.96 | 0.08 | 148,151,154,182             | 1     |
| 56  | OHX  | AA    | 3460 | 7/7   | 0.96 | 0.13 | 131,133,148,193             | 1     |
| 56  | OHX  | BA    | 1809 | 7/7   | 0.96 | 0.09 | 159,162,164,206             | 1     |
| 55  | MG   | AA    | 3047 | 1/1   | 0.96 | 0.28 | 65,65,65,65                 | 0     |
| 56  | OHX  | DA    | 3099 | 7/7   | 0.96 | 0.27 | 104,109,114,163             | 1     |
| 56  | OHX  | BC    | 107  | 7/7   | 0.96 | 0.14 | 126,137,143,151             | 1     |
| 55  | MG   | AA    | 3250 | 1/1   | 0.96 | 0.36 | 55,55,55,55                 | 0     |
| 55  | MG   | AA    | 3339 | 1/1   | 0.96 | 0.52 | 58,58,58,58                 | 0     |
| 56  | OHX  | CA    | 1741 | 7/7   | 0.96 | 0.13 | 101,122,129,156             | 2     |
| 56  | OHX  | BA    | 1800 | 7/7   | 0.96 | 0.08 | 127,133,145,177             | 1     |
| 55  | MG   | AA    | 3016 | 1/1   | 0.96 | 0.38 | 29,29,29,29                 | 0     |
| 55  | MG   | AA    | 3045 | 1/1   | 0.96 | 0.19 | 33,33,33,33                 | 0     |
| 56  | OHX  | DA    | 3367 | 7/7   | 0.96 | 0.21 | 100,113,133,149             | 1     |
| 57  | PAR  | BA    | 1715 | 42/42 | 0.96 | 0.18 | 61,73,83,89                 | 0     |
| 55  | MG   | AA    | 3227 | 1/1   | 0.96 | 0.40 | 61,61,61,61                 | 0     |
| 56  | OHX  | DA    | 3399 | 7/7   | 0.96 | 0.22 | 104,107,123,144             | 2     |
| 56  | OHX  | AA    | 3386 | 7/7   | 0.96 | 0.17 | 75,83,104,131               | 1     |
| 55  | MG   | AA    | 3232 | 1/1   | 0.96 | 0.10 | 62,62,62,62                 | 0     |
| 56  | OHX  | DA    | 3396 | 7/7   | 0.96 | 0.19 | 96,99,105,140               | 1     |
| 56  | OHX  | DA    | 3094 | 7/7   | 0.96 | 0.18 | 110,121,124,149             | 1     |
| 56  | OHX  | AA    | 3479 | 7/7   | 0.96 | 0.17 | 94,103,125,176              | 3     |
| 56  | OHX  | AA    | 3381 | 7/7   | 0.96 | 0.11 | 127,136,147,180             | 1     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | AA    | 3002 | 1/1   | 0.96 | 0.41 | 34,34,34,34                 | 0     |
| 56  | OHX  | AA    | 3565 | 7/7   | 0.96 | 0.12 | 97,104,114,159              | 1     |
| 55  | MG   | BA    | 1673 | 1/1   | 0.96 | 0.42 | 75,75,75,75                 | 0     |
| 56  | OHX  | AA    | 3486 | 7/7   | 0.96 | 0.14 | 95,110,127,153              | 1     |
| 55  | MG   | AA    | 3021 | 1/1   | 0.96 | 0.34 | 35,35,35,35                 | 0     |
| 58  | ZN   | BG    | 301  | 1/1   | 0.96 | 0.30 | 84,84,84,84                 | 0     |
| 55  | MG   | CA    | 1611 | 1/1   | 0.96 | 0.20 | 81,81,81,81                 | 0     |
| 55  | MG   | AA    | 3246 | 1/1   | 0.96 | 0.28 | 44,44,44,44                 | 0     |
| 55  | MG   | DA    | 3222 | 1/1   | 0.96 | 0.34 | 83,83,83,83                 | 0     |
| 55  | MG   | AA    | 3036 | 1/1   | 0.96 | 0.44 | 48,48,48,48                 | 0     |
| 56  | OHX  | AA    | 3558 | 7/7   | 0.96 | 0.15 | 92,100,110,168              | 1     |
| 56  | OHX  | DA    | 3441 | 7/7   | 0.96 | 0.10 | 114,122,135,176             | 1     |
| 55  | MG   | CA    | 1616 | 1/1   | 0.96 | 0.41 | 100,100,100,100             | 0     |
| 56  | OHX  | DA    | 3162 | 7/7   | 0.96 | 0.14 | 128,132,141,207             | 0     |
| 55  | MG   | AA    | 3158 | 1/1   | 0.96 | 0.45 | 49,49,49,49                 | 0     |
| 56  | OHX  | BA    | 1758 | 7/7   | 0.96 | 0.07 | 153,155,160,202             | 1     |
| 55  | MG   | AA    | 3196 | 1/1   | 0.96 | 0.34 | 43,43,43,43                 | 0     |
| 56  | OHX  | AA    | 3483 | 7/7   | 0.96 | 0.17 | 106,109,118,158             | 2     |
| 55  | MG   | DA    | 3261 | 1/1   | 0.96 | 0.38 | 53,53,53,53                 | 0     |
| 56  | OHX  | CA    | 1764 | 7/7   | 0.96 | 0.16 | 113,122,135,168             | 1     |
| 56  | OHX  | AA    | 3545 | 7/7   | 0.96 | 0.12 | 92,105,127,145              | 2     |
| 56  | OHX  | AA    | 3467 | 7/7   | 0.96 | 0.12 | 72,88,95,139                | 1     |
| 56  | OHX  | DA    | 3436 | 7/7   | 0.96 | 0.12 | 121,133,143,171             | 1     |
| 55  | MG   | DA    | 3148 | 1/1   | 0.96 | 0.45 | 50,50,50,50                 | 0     |
| 55  | MG   | AA    | 3302 | 1/1   | 0.96 | 0.41 | 72,72,72,72                 | 0     |
| 55  | MG   | DA    | 3080 | 1/1   | 0.96 | 0.34 | 43,43,43,43                 | 0     |
| 55  | MG   | DA    | 3051 | 1/1   | 0.96 | 0.51 | 39,39,39,39                 | 0     |
| 56  | OHX  | BA    | 1753 | 7/7   | 0.96 | 0.13 | 103,110,125,169             | 1     |
| 56  | OHX  | AA    | 3525 | 7/7   | 0.96 | 0.10 | 118,124,140,179             | 1     |
| 55  | MG   | CN    | 201  | 1/1   | 0.96 | 0.12 | 79,79,79,79                 | 0     |
| 55  | MG   | AA    | 3144 | 1/1   | 0.96 | 0.34 | 43,43,43,43                 | 0     |
| 55  | MG   | DA    | 3005 | 1/1   | 0.96 | 0.28 | 41,41,41,41                 | 0     |
| 55  | MG   | DA    | 3009 | 1/1   | 0.96 | 0.31 | 50,50,50,50                 | 0     |
| 56  | OHX  | DA    | 3408 | 7/7   | 0.96 | 0.14 | 122,131,146,182             | 1     |
| 56  | OHX  | AA    | 3437 | 7/7   | 0.96 | 0.19 | 76,82,94,136                | 1     |
| 55  | MG   | AA    | 3208 | 1/1   | 0.96 | 0.37 | 62,62,62,62                 | 0     |
| 55  | MG   | AA    | 3112 | 1/1   | 0.96 | 0.15 | 87,87,87,87                 | 0     |
| 56  | OHX  | CA    | 1814 | 7/7   | 0.96 | 0.06 | 149,152,161,212             | 1     |
| 55  | MG   | AA    | 3095 | 1/1   | 0.96 | 0.40 | 42,42,42,42                 | 0     |
| 56  | OHX  | AA    | 3398 | 7/7   | 0.96 | 0.15 | 90,95,125,158               | 1     |
| 56  | OHX  | CA    | 1750 | 7/7   | 0.96 | 0.16 | 110,113,130,151             | 1     |
| 55  | MG   | DA    | 3207 | 1/1   | 0.97 | 0.34 | 37,37,37,37                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | AA    | 3153 | 1/1   | 0.97 | 0.44 | 40,40,40,40                 | 0     |
| 56  | OHX  | AA    | 3562 | 7/7   | 0.97 | 0.14 | 100,110,119,157             | 1     |
| 55  | MG   | AA    | 3123 | 1/1   | 0.97 | 0.18 | 65,65,65,65                 | 0     |
| 55  | MG   | DA    | 3182 | 1/1   | 0.97 | 0.26 | 52,52,52,52                 | 0     |
| 56  | OHX  | DA    | 3359 | 7/7   | 0.97 | 0.17 | 99,118,131,143              | 1     |
| 55  | MG   | DA    | 3130 | 1/1   | 0.97 | 0.21 | 48,48,48,48                 | 0     |
| 55  | MG   | AA    | 3006 | 1/1   | 0.97 | 0.38 | 40,40,40,40                 | 0     |
| 56  | OHX  | CA    | 1738 | 7/7   | 0.97 | 0.10 | 120,123,126,168             | 1     |
| 55  | MG   | CA    | 1663 | 1/1   | 0.97 | 0.14 | 65,65,65,65                 | 0     |
| 56  | OHX  | CA    | 1760 | 7/7   | 0.97 | 0.08 | 145,148,151,188             | 1     |
| 55  | MG   | DA    | 3167 | 1/1   | 0.97 | 0.28 | 61,61,61,61                 | 0     |
| 56  | OHX  | BA    | 1784 | 7/7   | 0.97 | 0.14 | 94,101,111,137              | 1     |
| 56  | OHX  | DA    | 3170 | 7/7   | 0.97 | 0.15 | 114,125,135,172             | 1     |
| 56  | OHX  | CA    | 1728 | 7/7   | 0.97 | 0.15 | 104,119,138,150             | 2     |
| 55  | MG   | DA    | 3089 | 1/1   | 0.97 | 0.45 | 54,54,54,54                 | 0     |
| 55  | MG   | AA    | 3253 | 1/1   | 0.97 | 0.38 | 49,49,49,49                 | 0     |
| 56  | OHX  | AA    | 3377 | 7/7   | 0.97 | 0.21 | 77,87,106,151               | 2     |
| 56  | OHX  | AA    | 3365 | 7/7   | 0.97 | 0.12 | 86,102,111,118              | 3     |
| 55  | MG   | AA    | 3214 | 1/1   | 0.97 | 0.38 | 41,41,41,41                 | 0     |
| 56  | OHX  | CA    | 1796 | 7/7   | 0.97 | 0.09 | 150,159,170,195             | 1     |
| 55  | MG   | DA    | 3316 | 1/1   | 0.97 | 0.25 | 51,51,51,51                 | 0     |
| 56  | OHX  | BA    | 1789 | 7/7   | 0.97 | 0.06 | 132,137,146,191             | 1     |
| 55  | MG   | CA    | 1697 | 1/1   | 0.97 | 0.17 | 66,66,66,66                 | 0     |
| 55  | MG   | DA    | 3004 | 1/1   | 0.97 | 0.23 | 32,32,32,32                 | 0     |
| 55  | MG   | AA    | 3054 | 1/1   | 0.97 | 0.24 | 83,83,83,83                 | 0     |
| 55  | MG   | BA    | 1694 | 1/1   | 0.97 | 0.23 | 60,60,60,60                 | 0     |
| 55  | MG   | AA    | 3070 | 1/1   | 0.97 | 0.18 | 56,56,56,56                 | 0     |
| 56  | OHX  | AA    | 3566 | 7/7   | 0.97 | 0.12 | 171,177,185,204             | 1     |
| 55  | MG   | AA    | 3221 | 1/1   | 0.97 | 0.29 | 41,41,41,41                 | 0     |
| 55  | MG   | BA    | 1679 | 1/1   | 0.97 | 0.42 | 60,60,60,60                 | 0     |
| 55  | MG   | AA    | 3012 | 1/1   | 0.97 | 0.29 | 45,45,45,45                 | 0     |
| 55  | MG   | DA    | 3188 | 1/1   | 0.97 | 0.35 | 38,38,38,38                 | 0     |
| 55  | MG   | BA    | 1646 | 1/1   | 0.97 | 0.31 | 48,48,48,48                 | 0     |
| 55  | MG   | AA    | 3068 | 1/1   | 0.97 | 0.16 | 92,92,92,92                 | 0     |
| 56  | OHX  | BA    | 1762 | 7/7   | 0.97 | 0.14 | 121,131,144,180             | 1     |
| 56  | OHX  | AA    | 3430 | 7/7   | 0.97 | 0.09 | 119,125,132,176             | 1     |
| 55  | MG   | CA    | 1649 | 1/1   | 0.97 | 0.34 | 92,92,92,92                 | 0     |
| 55  | MG   | CA    | 1669 | 1/1   | 0.97 | 0.37 | 48,48,48,48                 | 0     |
| 55  | MG   | AA    | 3163 | 1/1   | 0.97 | 0.40 | 34,34,34,34                 | 0     |
| 55  | MG   | DA    | 3193 | 1/1   | 0.97 | 0.34 | 43,43,43,43                 | 0     |
| 55  | MG   | DA    | 3001 | 1/1   | 0.97 | 0.35 | 39,39,39,39                 | 0     |
| 55  | MG   | AA    | 3152 | 1/1   | 0.97 | 0.41 | 50,50,50,50                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | AA    | 3150 | 1/1   | 0.97 | 0.23 | 53,53,53,53                 | 0     |
| 55  | MG   | AA    | 3258 | 1/1   | 0.97 | 0.31 | 39,39,39,39                 | 0     |
| 56  | OHX  | AA    | 3438 | 7/7   | 0.97 | 0.10 | 113,130,139,188             | 1     |
| 56  | OHX  | BA    | 1724 | 7/7   | 0.97 | 0.10 | 114,121,136,156             | 0     |
| 55  | MG   | AA    | 3063 | 1/1   | 0.97 | 0.35 | 45,45,45,45                 | 0     |
| 55  | MG   | DA    | 3143 | 1/1   | 0.97 | 0.31 | 38,38,38,38                 | 0     |
| 55  | MG   | BA    | 1641 | 1/1   | 0.97 | 0.32 | 54,54,54,54                 | 0     |
| 55  | MG   | AA    | 3280 | 1/1   | 0.97 | 0.40 | 61,61,61,61                 | 0     |
| 56  | OHX  | DA    | 3406 | 7/7   | 0.97 | 0.13 | 88,107,111,147              | 3     |
| 56  | OHX  | AA    | 3429 | 7/7   | 0.97 | 0.14 | 84,97,102,156               | 1     |
| 55  | MG   | AA    | 3218 | 1/1   | 0.97 | 0.31 | 35,35,35,35                 | 0     |
| 55  | MG   | DA    | 3161 | 1/1   | 0.97 | 0.37 | 41,41,41,41                 | 0     |
| 56  | OHX  | DA    | 3379 | 7/7   | 0.97 | 0.13 | 116,134,147,164             | 1     |
| 55  | MG   | AA    | 3248 | 1/1   | 0.97 | 0.30 | 28,28,28,28                 | 0     |
| 55  | MG   | CA    | 1634 | 1/1   | 0.97 | 0.60 | 64,64,64,64                 | 0     |
| 55  | MG   | DA    | 3141 | 1/1   | 0.97 | 0.29 | 64,64,64,64                 | 0     |
| 56  | OHX  | BA    | 1801 | 7/7   | 0.97 | 0.11 | 129,138,143,174             | 1     |
| 56  | OHX  | CA    | 1744 | 7/7   | 0.97 | 0.10 | 128,134,150,164             | 1     |
| 55  | MG   | AA    | 3166 | 1/1   | 0.97 | 0.35 | 41,41,41,41                 | 0     |
| 55  | MG   | CA    | 1612 | 1/1   | 0.97 | 0.26 | 95,95,95,95                 | 0     |
| 56  | OHX  | DA    | 3471 | 7/7   | 0.97 | 0.10 | 112,124,129,160             | 1     |
| 55  | MG   | DA    | 3190 | 1/1   | 0.97 | 0.62 | 44,44,44,44                 | 0     |
| 55  | MG   | CA    | 1664 | 1/1   | 0.97 | 0.17 | 57,57,57,57                 | 0     |
| 56  | OHX  | CA    | 1743 | 7/7   | 0.97 | 0.10 | 101,120,132,162             | 1     |
| 55  | MG   | DA    | 3010 | 1/1   | 0.97 | 0.36 | 47,47,47,47                 | 0     |
| 55  | MG   | AA    | 3186 | 1/1   | 0.97 | 0.17 | 57,57,57,57                 | 0     |
| 56  | OHX  | AA    | 3409 | 7/7   | 0.97 | 0.15 | 99,110,115,152              | 1     |
| 56  | OHX  | DA    | 3451 | 7/7   | 0.97 | 0.11 | 103,107,114,153             | 1     |
| 56  | OHX  | BA    | 1767 | 7/7   | 0.97 | 0.09 | 151,158,165,212             | 1     |
| 55  | MG   | AA    | 3015 | 1/1   | 0.97 | 0.30 | 44,44,44,44                 | 0     |
| 55  | MG   | AA    | 3027 | 1/1   | 0.97 | 0.28 | 35,35,35,35                 | 0     |
| 56  | OHX  | AA    | 3466 | 7/7   | 0.97 | 0.13 | 98,120,132,157              | 1     |
| 56  | OHX  | DA    | 3355 | 7/7   | 0.97 | 0.13 | 109,111,119,148             | 2     |
| 55  | MG   | DA    | 3280 | 1/1   | 0.97 | 0.46 | 63,63,63,63                 | 0     |
| 55  | MG   | AA    | 3216 | 1/1   | 0.97 | 0.48 | 33,33,33,33                 | 0     |
| 56  | OHX  | DA    | 3366 | 7/7   | 0.97 | 0.16 | 87,100,130,154              | 2     |
| 56  | OHX  | DA    | 3375 | 7/7   | 0.97 | 0.11 | 129,138,149,173             | 1     |
| 55  | MG   | AA    | 3315 | 1/1   | 0.97 | 0.17 | 50,50,50,50                 | 0     |
| 56  | OHX  | BA    | 1760 | 7/7   | 0.97 | 0.13 | 109,109,121,147             | 1     |
| 55  | MG   | AA    | 3213 | 1/1   | 0.97 | 0.22 | 60,60,60,60                 | 0     |
| 55  | MG   | DA    | 3070 | 1/1   | 0.97 | 0.19 | 69,69,69,69                 | 0     |
| 56  | OHX  | AA    | 3446 | 7/7   | 0.97 | 0.16 | 148,150,154,190             | 1     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 56  | OHX  | DA    | 3373 | 7/7   | 0.97 | 0.23 | 93,104,119,171             | 1     |
| 56  | OHX  | BA    | 1741 | 7/7   | 0.97 | 0.13 | 95,110,126,148             | 1     |
| 55  | MG   | DA    | 3008 | 1/1   | 0.97 | 0.22 | 43,43,43,43                | 0     |
| 56  | OHX  | CA    | 1766 | 7/7   | 0.97 | 0.08 | 116,126,135,171            | 1     |
| 55  | MG   | BA    | 1656 | 1/1   | 0.97 | 0.40 | 73,73,73,73                | 0     |
| 56  | OHX  | CA    | 1736 | 7/7   | 0.97 | 0.10 | 163,166,178,209            | 0     |
| 55  | MG   | AA    | 3044 | 1/1   | 0.97 | 0.47 | 42,42,42,42                | 0     |
| 56  | OHX  | AA    | 3388 | 7/7   | 0.97 | 0.12 | 106,112,125,156            | 1     |
| 56  | OHX  | CA    | 1742 | 7/7   | 0.97 | 0.11 | 153,166,169,174            | 1     |
| 56  | OHX  | CA    | 1733 | 7/7   | 0.97 | 0.14 | 109,120,127,147            | 1     |
| 56  | OHX  | DA    | 3257 | 7/7   | 0.97 | 0.19 | 107,112,124,148            | 1     |
| 56  | OHX  | DA    | 3254 | 7/7   | 0.97 | 0.27 | 126,129,138,165            | 1     |
| 55  | MG   | AA    | 3014 | 1/1   | 0.97 | 0.36 | 33,33,33,33                | 0     |
| 56  | OHX  | BA    | 1746 | 7/7   | 0.97 | 0.13 | 95,103,110,146             | 1     |
| 55  | MG   | BA    | 1652 | 1/1   | 0.97 | 0.41 | 68,68,68,68                | 0     |
| 55  | MG   | DA    | 3192 | 1/1   | 0.97 | 0.52 | 60,60,60,60                | 0     |
| 56  | OHX  | DA    | 3412 | 7/7   | 0.97 | 0.12 | 93,110,113,161             | 1     |
| 56  | OHX  | DO    | 201  | 7/7   | 0.97 | 0.15 | 112,117,125,146            | 1     |
| 56  | OHX  | DA    | 3083 | 7/7   | 0.97 | 0.13 | 104,111,120,146            | 1     |
| 55  | MG   | DA    | 3293 | 1/1   | 0.97 | 0.48 | 88,88,88,88                | 0     |
| 56  | OHX  | AA    | 3399 | 7/7   | 0.97 | 0.17 | 97,111,117,147             | 1     |
| 56  | OHX  | BG    | 302  | 7/7   | 0.97 | 0.09 | 138,141,145,177            | 1     |
| 56  | OHX  | DA    | 3403 | 7/7   | 0.97 | 0.13 | 99,105,122,140             | 1     |
| 56  | OHX  | DA    | 3132 | 7/7   | 0.97 | 0.10 | 185,187,192,225            | 1     |
| 55  | MG   | D5    | 101  | 1/1   | 0.97 | 0.25 | 43,43,43,43                | 0     |
| 56  | OHX  | AA    | 3412 | 7/7   | 0.97 | 0.10 | 119,122,141,174            | 1     |
| 55  | MG   | AA    | 3025 | 1/1   | 0.97 | 0.36 | 37,37,37,37                | 0     |
| 56  | OHX  | CA    | 1735 | 7/7   | 0.97 | 0.10 | 146,153,168,212            | 0     |
| 56  | OHX  | BA    | 1755 | 7/7   | 0.97 | 0.09 | 123,128,136,161            | 1     |
| 55  | MG   | DA    | 3012 | 1/1   | 0.97 | 0.31 | 44,44,44,44                | 0     |
| 56  | OHX  | DA    | 3393 | 7/7   | 0.97 | 0.11 | 133,134,150,191            | 1     |
| 55  | MG   | AA    | 3097 | 1/1   | 0.97 | 0.24 | 50,50,50,50                | 0     |
| 56  | OHX  | AA    | 3450 | 7/7   | 0.97 | 0.12 | 97,112,128,161             | 2     |
| 56  | OHX  | AO    | 202  | 7/7   | 0.97 | 0.11 | 93,104,115,140             | 1     |
| 56  | OHX  | DA    | 3404 | 7/7   | 0.97 | 0.12 | 107,121,131,166            | 1     |
| 55  | MG   | AA    | 3136 | 1/1   | 0.97 | 0.20 | 42,42,42,42                | 0     |
| 55  | MG   | AA    | 3077 | 1/1   | 0.97 | 0.42 | 39,39,39,39                | 0     |
| 56  | OHX  | DA    | 3402 | 7/7   | 0.97 | 0.10 | 122,136,148,204            | 1     |
| 55  | MG   | DA    | 3018 | 1/1   | 0.97 | 0.31 | 47,47,47,47                | 0     |
| 55  | MG   | AA    | 3241 | 1/1   | 0.97 | 0.34 | 52,52,52,52                | 0     |
| 55  | MG   | AA    | 3265 | 1/1   | 0.97 | 0.25 | 62,62,62,62                | 0     |
| 56  | OHX  | CA    | 1739 | 7/7   | 0.97 | 0.10 | 140,150,165,188            | 1     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 56  | OHX  | BA    | 1736 | 7/7   | 0.97 | 0.12 | 112,121,128,152            | 1     |
| 56  | OHX  | DA    | 3383 | 7/7   | 0.97 | 0.13 | 110,119,138,151            | 2     |
| 56  | OHX  | CA    | 1768 | 7/7   | 0.97 | 0.09 | 123,135,145,174            | 1     |
| 56  | OHX  | CA    | 1734 | 7/7   | 0.97 | 0.10 | 145,147,151,167            | 1     |
| 55  | MG   | AA    | 3026 | 1/1   | 0.97 | 0.30 | 43,43,43,43                | 0     |
| 56  | OHX  | AA    | 3428 | 7/7   | 0.97 | 0.08 | 114,120,124,169            | 1     |
| 56  | OHX  | BA    | 1734 | 7/7   | 0.97 | 0.16 | 92,99,114,146              | 1     |
| 55  | MG   | CA    | 1711 | 1/1   | 0.97 | 0.39 | 57,57,57,57                | 0     |
| 55  | MG   | AA    | 3179 | 1/1   | 0.97 | 0.33 | 39,39,39,39                | 0     |
| 55  | MG   | BA    | 1659 | 1/1   | 0.97 | 0.51 | 43,43,43,43                | 0     |
| 55  | MG   | DA    | 3236 | 1/1   | 0.97 | 0.49 | 62,62,62,62                | 0     |
| 55  | MG   | BA    | 1626 | 1/1   | 0.97 | 0.54 | 47,47,47,47                | 0     |
| 56  | OHX  | BA    | 1805 | 7/7   | 0.97 | 0.19 | 98,103,107,150             | 1     |
| 55  | MG   | AA    | 3271 | 1/1   | 0.97 | 0.45 | 63,63,63,63                | 0     |
| 55  | MG   | AA    | 3146 | 1/1   | 0.97 | 0.38 | 36,36,36,36                | 0     |
| 55  | MG   | AA    | 3098 | 1/1   | 0.97 | 0.31 | 29,29,29,29                | 0     |
| 55  | MG   | DA    | 3041 | 1/1   | 0.97 | 0.36 | 79,79,79,79                | 0     |
| 56  | OHX  | AA    | 3556 | 7/7   | 0.97 | 0.16 | 82,96,111,154              | 1     |
| 55  | MG   | AA    | 3256 | 1/1   | 0.97 | 0.43 | 52,52,52,52                | 0     |
| 55  | MG   | BA    | 1698 | 1/1   | 0.98 | 0.42 | 54,54,54,54                | 0     |
| 56  | OHX  | DA    | 3356 | 7/7   | 0.98 | 0.14 | 85,97,114,129              | 2     |
| 56  | OHX  | BA    | 1727 | 7/7   | 0.98 | 0.12 | 116,137,148,161            | 1     |
| 56  | OHX  | AA    | 3453 | 7/7   | 0.98 | 0.13 | 72,88,95,134               | 2     |
| 55  | MG   | A0    | 201  | 1/1   | 0.98 | 0.15 | 52,52,52,52                | 0     |
| 56  | OHX  | BA    | 1733 | 7/7   | 0.98 | 0.09 | 98,108,118,146             | 1     |
| 56  | OHX  | AA    | 3422 | 7/7   | 0.98 | 0.18 | 63,104,126,147             | 2     |
| 56  | OHX  | AA    | 3370 | 7/7   | 0.98 | 0.17 | 74,85,99,119               | 1     |
| 55  | MG   | AA    | 3288 | 1/1   | 0.98 | 0.31 | 55,55,55,55                | 0     |
| 56  | OHX  | AA    | 3385 | 7/7   | 0.98 | 0.17 | 73,87,109,139              | 2     |
| 55  | MG   | AA    | 3018 | 1/1   | 0.98 | 0.28 | 49,49,49,49                | 0     |
| 56  | OHX  | CA    | 1740 | 7/7   | 0.98 | 0.09 | 125,134,139,166            | 1     |
| 55  | MG   | AA    | 3129 | 1/1   | 0.98 | 0.22 | 43,43,43,43                | 0     |
| 56  | OHX  | DA    | 3068 | 7/7   | 0.98 | 0.12 | 102,127,131,147            | 0     |
| 56  | OHX  | BA    | 1768 | 7/7   | 0.98 | 0.15 | 87,95,105,130              | 2     |
| 56  | OHX  | BA    | 1729 | 7/7   | 0.98 | 0.11 | 110,115,135,137            | 1     |
| 55  | MG   | DA    | 3119 | 1/1   | 0.98 | 0.34 | 38,38,38,38                | 0     |
| 56  | OHX  | AA    | 3361 | 7/7   | 0.98 | 0.12 | 76,81,111,125              | 3     |
| 55  | MG   | DA    | 3197 | 1/1   | 0.98 | 0.28 | 49,49,49,49                | 0     |
| 56  | OHX  | DA    | 3084 | 7/7   | 0.98 | 0.14 | 132,139,149,176            | 1     |
| 56  | OHX  | AA    | 3458 | 7/7   | 0.98 | 0.18 | 96,103,139,158             | 1     |
| 55  | MG   | DA    | 3078 | 1/1   | 0.98 | 0.45 | 42,42,42,42                | 0     |
| 56  | OHX  | DA    | 3387 | 7/7   | 0.98 | 0.09 | 108,115,125,151            | 1     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | AA    | 3223 | 1/1   | 0.98 | 0.30 | 43,43,43,43                 | 0     |
| 56  | OHX  | AA    | 3461 | 7/7   | 0.98 | 0.12 | 102,110,120,148             | 1     |
| 56  | OHX  | CA    | 1748 | 7/7   | 0.98 | 0.08 | 137,145,152,186             | 1     |
| 56  | OHX  | AA    | 3369 | 7/7   | 0.98 | 0.11 | 76,100,116,143              | 1     |
| 56  | OHX  | BA    | 1720 | 7/7   | 0.98 | 0.13 | 95,108,133,161              | 2     |
| 56  | OHX  | DA    | 3364 | 7/7   | 0.98 | 0.17 | 75,93,104,118               | 1     |
| 55  | MG   | DA    | 3146 | 1/1   | 0.98 | 0.26 | 33,33,33,33                 | 0     |
| 56  | OHX  | AA    | 3360 | 7/7   | 0.98 | 0.14 | 88,94,111,129               | 2     |
| 55  | MG   | AA    | 3017 | 1/1   | 0.98 | 0.39 | 26,26,26,26                 | 0     |
| 56  | OHX  | BA    | 1730 | 7/7   | 0.98 | 0.12 | 106,118,135,150             | 1     |
| 55  | MG   | AA    | 3242 | 1/1   | 0.98 | 0.38 | 43,43,43,43                 | 0     |
| 56  | OHX  | AA    | 3452 | 7/7   | 0.98 | 0.10 | 92,103,111,136              | 1     |
| 56  | OHX  | BA    | 1728 | 7/7   | 0.98 | 0.08 | 140,147,157,166             | 1     |
| 55  | MG   | DA    | 3175 | 1/1   | 0.98 | 0.44 | 53,53,53,53                 | 0     |
| 56  | OHX  | AA    | 3424 | 7/7   | 0.98 | 0.15 | 84,93,116,147               | 1     |
| 55  | MG   | AA    | 3191 | 1/1   | 0.98 | 0.14 | 39,39,39,39                 | 0     |
| 56  | OHX  | AA    | 3401 | 7/7   | 0.98 | 0.12 | 101,105,125,153             | 1     |
| 55  | MG   | AA    | 3010 | 1/1   | 0.98 | 0.25 | 39,39,39,39                 | 0     |
| 56  | OHX  | DA    | 3363 | 7/7   | 0.98 | 0.12 | 95,105,122,123              | 2     |
| 55  | MG   | AA    | 3201 | 1/1   | 0.98 | 0.43 | 35,35,35,35                 | 0     |
| 55  | MG   | AA    | 3139 | 1/1   | 0.98 | 0.24 | 47,47,47,47                 | 0     |
| 56  | OHX  | CC    | 110  | 7/7   | 0.98 | 0.16 | 103,121,132,150             | 4     |
| 55  | MG   | DA    | 3026 | 1/1   | 0.98 | 0.28 | 55,55,55,55                 | 0     |
| 55  | MG   | CA    | 1635 | 1/1   | 0.98 | 0.34 | 51,51,51,51                 | 0     |
| 56  | OHX  | DA    | 3157 | 7/7   | 0.98 | 0.16 | 76,87,96,121                | 1     |
| 55  | MG   | DA    | 3015 | 1/1   | 0.98 | 0.28 | 56,56,56,56                 | 0     |
| 55  | MG   | DA    | 3095 | 1/1   | 0.98 | 0.22 | 58,58,58,58                 | 0     |
| 56  | OHX  | BA    | 1735 | 7/7   | 0.98 | 0.12 | 120,129,137,168             | 1     |
| 56  | OHX  | AA    | 3378 | 7/7   | 0.98 | 0.14 | 77,88,108,118               | 1     |
| 56  | OHX  | AA    | 3533 | 7/7   | 0.98 | 0.10 | 79,94,100,134               | 1     |
| 55  | MG   | DA    | 3007 | 1/1   | 0.98 | 0.29 | 43,43,43,43                 | 0     |
| 56  | OHX  | AA    | 3353 | 7/7   | 0.98 | 0.20 | 71,99,117,132               | 1     |
| 56  | OHX  | BA    | 1723 | 7/7   | 0.98 | 0.17 | 93,106,124,143              | 1     |
| 56  | OHX  | DA    | 3073 | 7/7   | 0.98 | 0.19 | 89,101,109,132              | 1     |
| 55  | MG   | DA    | 3198 | 1/1   | 0.98 | 0.40 | 44,44,44,44                 | 0     |
| 56  | OHX  | DA    | 3082 | 7/7   | 0.98 | 0.14 | 92,102,108,132              | 1     |
| 56  | OHX  | CA    | 1732 | 7/7   | 0.98 | 0.13 | 112,117,126,152             | 1     |
| 56  | OHX  | AA    | 3390 | 7/7   | 0.98 | 0.18 | 48,74,93,125                | 2     |
| 56  | OHX  | DA    | 3064 | 7/7   | 0.98 | 0.15 | 87,100,123,131              | 3     |
| 56  | OHX  | DA    | 3354 | 7/7   | 0.98 | 0.15 | 88,99,121,135               | 1     |
| 56  | OHX  | DA    | 3065 | 7/7   | 0.98 | 0.17 | 55,92,111,137               | 1     |
| 56  | OHX  | CA    | 1737 | 7/7   | 0.98 | 0.09 | 103,118,125,148             | 1     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 56  | OHX  | CA    | 1729 | 7/7   | 0.98 | 0.15 | 104,115,126,154            | 1     |
| 56  | OHX  | AA    | 3391 | 7/7   | 0.98 | 0.16 | 69,80,102,109              | 3     |
| 55  | MG   | DA    | 3231 | 1/1   | 0.98 | 0.41 | 50,50,50,50                | 0     |
| 55  | MG   | DA    | 3138 | 1/1   | 0.98 | 0.37 | 43,43,43,43                | 0     |
| 56  | OHX  | AA    | 3400 | 7/7   | 0.98 | 0.15 | 64,77,80,123               | 1     |
| 56  | OHX  | DA    | 3420 | 7/7   | 0.98 | 0.10 | 116,120,125,152            | 1     |
| 56  | OHX  | AA    | 3468 | 7/7   | 0.98 | 0.09 | 110,120,137,165            | 1     |
| 55  | MG   | DA    | 3034 | 1/1   | 0.98 | 0.15 | 69,69,69,69                | 0     |
| 55  | MG   | AA    | 3007 | 1/1   | 0.98 | 0.40 | 43,43,43,43                | 0     |
| 56  | OHX  | DA    | 3395 | 7/7   | 0.98 | 0.13 | 102,109,124,139            | 1     |
| 56  | OHX  | AA    | 3375 | 7/7   | 0.98 | 0.12 | 83,101,103,143             | 1     |
| 55  | MG   | AA    | 3187 | 1/1   | 0.98 | 0.26 | 40,40,40,40                | 0     |
| 55  | MG   | AA    | 3190 | 1/1   | 0.98 | 0.23 | 43,43,43,43                | 0     |
| 55  | MG   | BA    | 1604 | 1/1   | 0.98 | 0.20 | 69,69,69,69                | 0     |
| 56  | OHX  | DA    | 3369 | 7/7   | 0.98 | 0.15 | 89,100,105,125             | 1     |
| 56  | OHX  | AA    | 3387 | 7/7   | 0.98 | 0.11 | 110,123,134,164            | 1     |
| 55  | MG   | DA    | 3074 | 1/1   | 0.98 | 0.47 | 40,40,40,40                | 0     |
| 55  | MG   | AA    | 3184 | 1/1   | 0.98 | 0.38 | 35,35,35,35                | 0     |
| 56  | OHX  | AA    | 3366 | 7/7   | 0.98 | 0.17 | 79,94,104,141              | 1     |
| 55  | MG   | AA    | 3272 | 1/1   | 0.98 | 0.42 | 29,29,29,29                | 0     |
| 55  | MG   | AA    | 3134 | 1/1   | 0.98 | 0.44 | 48,48,48,48                | 0     |
| 56  | OHX  | AA    | 3354 | 7/7   | 0.98 | 0.14 | 96,105,128,164             | 0     |
| 56  | OHX  | DA    | 3381 | 7/7   | 0.98 | 0.13 | 111,118,134,167            | 1     |
| 56  | OHX  | AA    | 3380 | 7/7   | 0.98 | 0.15 | 86,90,110,143              | 1     |
| 56  | OHX  | DA    | 3397 | 7/7   | 0.98 | 0.09 | 104,119,125,149            | 1     |
| 56  | OHX  | DA    | 3382 | 7/7   | 0.98 | 0.17 | 67,85,95,136               | 2     |
| 56  | OHX  | DA    | 3246 | 7/7   | 0.98 | 0.14 | 89,97,107,138              | 1     |
| 56  | OHX  | AA    | 3469 | 7/7   | 0.98 | 0.09 | 103,113,128,153            | 1     |
| 55  | MG   | AA    | 3037 | 1/1   | 0.98 | 0.29 | 55,55,55,55                | 0     |
| 55  | MG   | AA    | 3197 | 1/1   | 0.98 | 0.25 | 57,57,57,57                | 0     |
| 56  | OHX  | AA    | 3487 | 7/7   | 0.98 | 0.13 | 73,82,95,140               | 2     |
| 56  | OHX  | AA    | 3427 | 7/7   | 0.98 | 0.12 | 131,132,136,155            | 1     |
| 56  | OHX  | DA    | 3422 | 7/7   | 0.98 | 0.14 | 92,100,111,154             | 1     |
| 56  | OHX  | AA    | 3471 | 7/7   | 0.98 | 0.14 | 80,105,117,155             | 1     |
| 56  | OHX  | DA    | 3429 | 7/7   | 0.98 | 0.09 | 118,130,143,180            | 1     |
| 56  | OHX  | DA    | 3389 | 7/7   | 0.98 | 0.12 | 82,85,99,113               | 1     |
| 56  | OHX  | AA    | 3410 | 7/7   | 0.98 | 0.14 | 91,99,106,125              | 1     |
| 56  | OHX  | DA    | 3348 | 7/7   | 0.98 | 0.13 | 97,115,128,140             | 1     |
| 56  | OHX  | DA    | 3377 | 7/7   | 0.98 | 0.16 | 91,105,111,146             | 2     |
| 55  | MG   | DA    | 3234 | 1/1   | 0.98 | 0.32 | 41,41,41,41                | 0     |
| 56  | OHX  | AA    | 3373 | 7/7   | 0.98 | 0.11 | 84,96,108,141              | 1     |
| 56  | OHX  | AA    | 3518 | 7/7   | 0.98 | 0.10 | 106,114,121,148            | 1     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | AA    | 3046 | 1/1   | 0.98 | 0.32 | 50,50,50,50                 | 0     |
| 55  | MG   | AE    | 303  | 1/1   | 0.98 | 0.24 | 36,36,36,36                 | 0     |
| 55  | MG   | CA    | 1633 | 1/1   | 0.98 | 0.53 | 46,46,46,46                 | 0     |
| 55  | MG   | CC    | 101  | 1/1   | 0.98 | 0.47 | 79,79,79,79                 | 0     |
| 56  | OHX  | AA    | 3364 | 7/7   | 0.98 | 0.15 | 72,81,97,125                | 1     |
| 56  | OHX  | BA    | 1770 | 7/7   | 0.98 | 0.11 | 114,115,121,163             | 1     |
| 56  | OHX  | AA    | 3477 | 7/7   | 0.98 | 0.14 | 81,92,107,133               | 2     |
| 55  | MG   | DA    | 3036 | 1/1   | 0.98 | 0.14 | 47,47,47,47                 | 0     |
| 56  | OHX  | DA    | 3384 | 7/7   | 0.98 | 0.13 | 89,92,105,143               | 2     |
| 56  | OHX  | AA    | 3397 | 7/7   | 0.98 | 0.12 | 96,102,109,143              | 1     |
| 56  | OHX  | AA    | 3383 | 7/7   | 0.98 | 0.13 | 91,96,109,133               | 1     |
| 56  | OHX  | DA    | 3358 | 7/7   | 0.98 | 0.11 | 107,117,135,165             | 2     |
| 56  | OHX  | AA    | 3493 | 7/7   | 0.98 | 0.10 | 102,115,123,140             | 1     |
| 55  | MG   | DA    | 3164 | 1/1   | 0.98 | 0.40 | 63,63,63,63                 | 0     |
| 56  | OHX  | DA    | 3136 | 7/7   | 0.98 | 0.15 | 95,108,117,144              | 1     |
| 56  | OHX  | CA    | 1746 | 7/7   | 0.98 | 0.09 | 112,115,128,150             | 1     |
| 55  | MG   | DA    | 3085 | 1/1   | 0.98 | 0.41 | 53,53,53,53                 | 0     |
| 56  | OHX  | AA    | 3406 | 7/7   | 0.98 | 0.11 | 93,96,102,133               | 1     |
| 55  | MG   | AA    | 3207 | 1/1   | 0.98 | 0.50 | 44,44,44,44                 | 0     |
| 56  | OHX  | BA    | 1739 | 7/7   | 0.98 | 0.12 | 109,119,131,155             | 1     |
| 55  | MG   | AA    | 3202 | 1/1   | 0.98 | 0.20 | 30,30,30,30                 | 0     |
| 56  | OHX  | AA    | 3414 | 7/7   | 0.98 | 0.15 | 92,104,120,143              | 1     |
| 55  | MG   | AA    | 3009 | 1/1   | 0.98 | 0.24 | 29,29,29,29                 | 0     |
| 56  | OHX  | DA    | 3368 | 7/7   | 0.98 | 0.11 | 86,101,103,132              | 2     |
| 55  | MG   | DA    | 3290 | 1/1   | 0.98 | 0.16 | 37,37,37,37                 | 0     |
| 56  | OHX  | DA    | 3370 | 7/7   | 0.98 | 0.14 | 94,102,123,149              | 1     |
| 56  | OHX  | CC    | 109  | 7/7   | 0.98 | 0.20 | 112,114,129,153             | 3     |
| 56  | OHX  | DA    | 3418 | 7/7   | 0.98 | 0.11 | 87,98,117,139               | 3     |
| 56  | OHX  | AA    | 3432 | 7/7   | 0.98 | 0.10 | 129,136,142,160             | 1     |
| 56  | OHX  | CA    | 1779 | 7/7   | 0.98 | 0.05 | 125,132,137,172             | 1     |
| 55  | MG   | DA    | 3150 | 1/1   | 0.98 | 0.17 | 46,46,46,46                 | 0     |
| 56  | OHX  | AA    | 3431 | 7/7   | 0.98 | 0.13 | 101,115,120,168             | 1     |
| 56  | OHX  | DA    | 3417 | 7/7   | 0.98 | 0.09 | 145,152,156,188             | 1     |
| 55  | MG   | AA    | 3040 | 1/1   | 0.98 | 0.29 | 59,59,59,59                 | 0     |
| 55  | MG   | DA    | 3123 | 1/1   | 0.98 | 0.29 | 38,38,38,38                 | 0     |
| 55  | MG   | DA    | 3052 | 1/1   | 0.98 | 0.47 | 42,42,42,42                 | 0     |
| 55  | MG   | CA    | 1636 | 1/1   | 0.98 | 0.19 | 82,82,82,82                 | 0     |
| 55  | MG   | AA    | 3106 | 1/1   | 0.98 | 0.24 | 72,72,72,72                 | 0     |
| 55  | MG   | BA    | 1603 | 1/1   | 0.98 | 0.19 | 40,40,40,40                 | 0     |
| 56  | OHX  | DA    | 3419 | 7/7   | 0.98 | 0.13 | 82,93,100,126               | 2     |
| 56  | OHX  | AA    | 3346 | 7/7   | 0.98 | 0.17 | 73,81,101,124               | 2     |
| 55  | MG   | DA    | 3232 | 1/1   | 0.98 | 0.62 | 63,63,63,63                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | DA    | 3144 | 1/1   | 0.98 | 0.56 | 44,44,44,44                 | 0     |
| 55  | MG   | AA    | 3019 | 1/1   | 0.98 | 0.30 | 42,42,42,42                 | 0     |
| 56  | OHX  | DA    | 3071 | 7/7   | 0.98 | 0.14 | 107,121,146,184             | 0     |
| 55  | MG   | DA    | 3227 | 1/1   | 0.98 | 0.31 | 44,44,44,44                 | 0     |
| 56  | OHX  | AA    | 3355 | 7/7   | 0.98 | 0.15 | 88,95,127,131               | 3     |
| 56  | OHX  | AA    | 3351 | 7/7   | 0.98 | 0.14 | 60,68,78,99                 | 3     |
| 55  | MG   | AA    | 3164 | 1/1   | 0.98 | 0.30 | 45,45,45,45                 | 0     |
| 56  | OHX  | DA    | 3062 | 7/7   | 0.98 | 0.18 | 70,95,103,114               | 1     |
| 55  | MG   | DA    | 3002 | 1/1   | 0.99 | 0.47 | 46,46,46,46                 | 0     |
| 56  | OHX  | DA    | 3249 | 7/7   | 0.99 | 0.13 | 93,103,118,149              | 1     |
| 55  | MG   | AA    | 3175 | 1/1   | 0.99 | 0.24 | 46,46,46,46                 | 0     |
| 56  | OHX  | AA    | 3332 | 7/7   | 0.99 | 0.16 | 40,73,95,99                 | 2     |
| 56  | OHX  | DA    | 3342 | 7/7   | 0.99 | 0.15 | 79,85,102,102               | 2     |
| 55  | MG   | AA    | 3051 | 1/1   | 0.99 | 0.37 | 69,69,69,69                 | 0     |
| 56  | OHX  | AA    | 3329 | 7/7   | 0.99 | 0.15 | 73,97,104,113               | 0     |
| 56  | OHX  | AA    | 3342 | 7/7   | 0.99 | 0.13 | 65,86,103,114               | 1     |
| 56  | OHX  | DA    | 3360 | 7/7   | 0.99 | 0.13 | 72,81,91,113                | 1     |
| 56  | OHX  | DA    | 3374 | 7/7   | 0.99 | 0.09 | 127,131,139,156             | 1     |
| 56  | OHX  | DA    | 3386 | 7/7   | 0.99 | 0.11 | 108,110,132,139             | 1     |
| 56  | OHX  | DA    | 3345 | 7/7   | 0.99 | 0.14 | 89,96,107,130               | 0     |
| 56  | OHX  | AE    | 304  | 7/7   | 0.99 | 0.11 | 73,87,113,116               | 2     |
| 56  | OHX  | DA    | 3134 | 7/7   | 0.99 | 0.13 | 114,120,126,150             | 1     |
| 56  | OHX  | DA    | 3343 | 7/7   | 0.99 | 0.15 | 93,113,122,129              | 0     |
| 56  | OHX  | AF    | 303  | 7/7   | 0.99 | 0.21 | 46,54,72,103                | 0     |
| 56  | OHX  | DB    | 208  | 7/7   | 0.99 | 0.10 | 120,124,144,144             | 2     |
| 56  | OHX  | BA    | 1722 | 7/7   | 0.99 | 0.08 | 114,116,123,159             | 0     |
| 56  | OHX  | AA    | 3407 | 7/7   | 0.99 | 0.16 | 53,82,90,103                | 2     |
| 56  | OHX  | AA    | 3348 | 7/7   | 0.99 | 0.15 | 75,81,98,100                | 3     |
| 56  | OHX  | BA    | 1726 | 7/7   | 0.99 | 0.09 | 134,139,145,195             | 0     |
| 56  | OHX  | DA    | 3338 | 7/7   | 0.99 | 0.17 | 72,79,93,112                | 0     |
| 55  | MG   | DA    | 3003 | 1/1   | 0.99 | 0.29 | 43,43,43,43                 | 0     |
| 56  | OHX  | AA    | 3359 | 7/7   | 0.99 | 0.12 | 91,110,118,137              | 1     |
| 56  | OHX  | AA    | 3368 | 7/7   | 0.99 | 0.09 | 104,115,121,140             | 1     |
| 56  | OHX  | DA    | 3335 | 7/7   | 0.99 | 0.17 | 87,96,112,126               | 0     |
| 55  | MG   | AA    | 3008 | 1/1   | 0.99 | 0.41 | 32,32,32,32                 | 0     |
| 56  | OHX  | DA    | 3351 | 7/7   | 0.99 | 0.13 | 87,96,108,109               | 1     |
| 56  | OHX  | BA    | 1740 | 7/7   | 0.99 | 0.13 | 107,110,122,131             | 1     |
| 56  | OHX  | AA    | 3335 | 7/7   | 0.99 | 0.24 | 62,76,78,127                | 0     |
| 56  | OHX  | AA    | 3490 | 7/7   | 0.99 | 0.11 | 85,93,105,125               | 1     |
| 56  | OHX  | CA    | 1727 | 7/7   | 0.99 | 0.09 | 114,118,131,143             | 0     |
| 58  | ZN   | BQ    | 101  | 1/1   | 0.99 | 0.07 | 135,135,135,135             | 0     |
| 55  | MG   | DA    | 3019 | 1/1   | 0.99 | 0.24 | 41,41,41,41                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 56  | OHX  | DA    | 3350 | 7/7   | 0.99 | 0.14 | 90,99,110,132              | 1     |
| 56  | OHX  | DA    | 3160 | 7/7   | 0.99 | 0.18 | 79,114,122,124             | 0     |
| 55  | MG   | AA    | 3185 | 1/1   | 0.99 | 0.41 | 35,35,35,35                | 0     |
| 56  | OHX  | AA    | 3415 | 7/7   | 0.99 | 0.08 | 90,93,100,146              | 1     |
| 56  | OHX  | DA    | 3357 | 7/7   | 0.99 | 0.12 | 100,118,130,150            | 1     |
| 56  | OHX  | AA    | 3376 | 7/7   | 0.99 | 0.11 | 96,107,117,142             | 1     |
| 55  | MG   | CA    | 1632 | 1/1   | 0.99 | 0.50 | 56,56,56,56                | 0     |
| 56  | OHX  | AA    | 3363 | 7/7   | 0.99 | 0.13 | 89,101,119,137             | 1     |
| 55  | MG   | DA    | 3013 | 1/1   | 0.99 | 0.42 | 40,40,40,40                | 0     |
| 56  | OHX  | AA    | 3341 | 7/7   | 0.99 | 0.19 | 77,80,88,124               | 1     |
| 56  | OHX  | CA    | 1791 | 7/7   | 0.99 | 0.11 | 100,118,129,154            | 1     |
| 55  | MG   | AA    | 3035 | 1/1   | 0.99 | 0.18 | 38,38,38,38                | 0     |
| 58  | ZN   | CQ    | 101  | 1/1   | 0.99 | 0.12 | 120,120,120,120            | 0     |
| 55  | MG   | AA    | 3121 | 1/1   | 0.99 | 0.35 | 65,65,65,65                | 0     |
| 56  | OHX  | DA    | 3340 | 7/7   | 0.99 | 0.14 | 86,102,124,126             | 1     |
| 56  | OHX  | AA    | 3402 | 7/7   | 0.99 | 0.13 | 73,86,98,123               | 1     |
| 56  | OHX  | CA    | 1723 | 7/7   | 0.99 | 0.20 | 84,100,111,141             | 0     |
| 56  | OHX  | BA    | 1717 | 7/7   | 0.99 | 0.17 | 81,90,105,119              | 0     |
| 56  | OHX  | AA    | 3396 | 7/7   | 0.99 | 0.10 | 93,107,119,142             | 1     |
| 56  | OHX  | AA    | 3327 | 7/7   | 0.99 | 0.21 | 38,70,106,113              | 0     |
| 56  | OHX  | AA    | 3403 | 7/7   | 0.99 | 0.18 | 59,89,94,139               | 1     |
| 56  | OHX  | DA    | 3378 | 7/7   | 0.99 | 0.09 | 153,156,169,185            | 0     |
| 56  | OHX  | DA    | 3347 | 7/7   | 0.99 | 0.12 | 89,99,108,134              | 0     |
| 56  | OHX  | DA    | 3075 | 7/7   | 0.99 | 0.16 | 89,91,114,123              | 1     |
| 56  | OHX  | AA    | 3350 | 7/7   | 0.99 | 0.13 | 95,103,113,148             | 1     |
| 58  | ZN   | CG    | 301  | 1/1   | 0.99 | 0.27 | 116,116,116,116            | 0     |
| 56  | OHX  | AA    | 3336 | 7/7   | 0.99 | 0.20 | 67,91,105,145              | 0     |
| 56  | OHX  | CA    | 1730 | 7/7   | 0.99 | 0.12 | 132,134,143,167            | 0     |
| 56  | OHX  | AA    | 3345 | 7/7   | 0.99 | 0.09 | 87,112,122,135             | 0     |
| 55  | MG   | AA    | 3013 | 1/1   | 0.99 | 0.37 | 27,27,27,27                | 0     |
| 55  | MG   | AA    | 3212 | 1/1   | 0.99 | 0.41 | 33,33,33,33                | 0     |
| 56  | OHX  | DA    | 3380 | 7/7   | 0.99 | 0.09 | 108,123,139,150            | 1     |
| 56  | OHX  | CA    | 1726 | 7/7   | 0.99 | 0.15 | 89,98,100,124              | 1     |
| 55  | MG   | AE    | 301  | 1/1   | 0.99 | 0.35 | 51,51,51,51                | 0     |
| 55  | MG   | AA    | 3192 | 1/1   | 0.99 | 0.38 | 34,34,34,34                | 0     |
| 56  | OHX  | AA    | 3344 | 7/7   | 0.99 | 0.12 | 86,92,112,118              | 1     |
| 56  | OHX  | AA    | 3330 | 7/7   | 0.99 | 0.18 | 81,85,101,147              | 0     |
| 56  | OHX  | BA    | 1718 | 7/7   | 0.99 | 0.21 | 68,82,103,130              | 2     |
| 56  | OHX  | CA    | 1724 | 7/7   | 0.99 | 0.12 | 88,111,121,131             | 0     |
| 56  | OHX  | DA    | 3401 | 7/7   | 0.99 | 0.12 | 108,115,120,150            | 1     |
| 56  | OHX  | DA    | 3353 | 7/7   | 0.99 | 0.14 | 102,117,129,132            | 1     |
| 56  | OHX  | AA    | 3418 | 7/7   | 0.99 | 0.17 | 96,110,119,135             | 1     |

*Continued on next page...*

*Continued from previous page...*

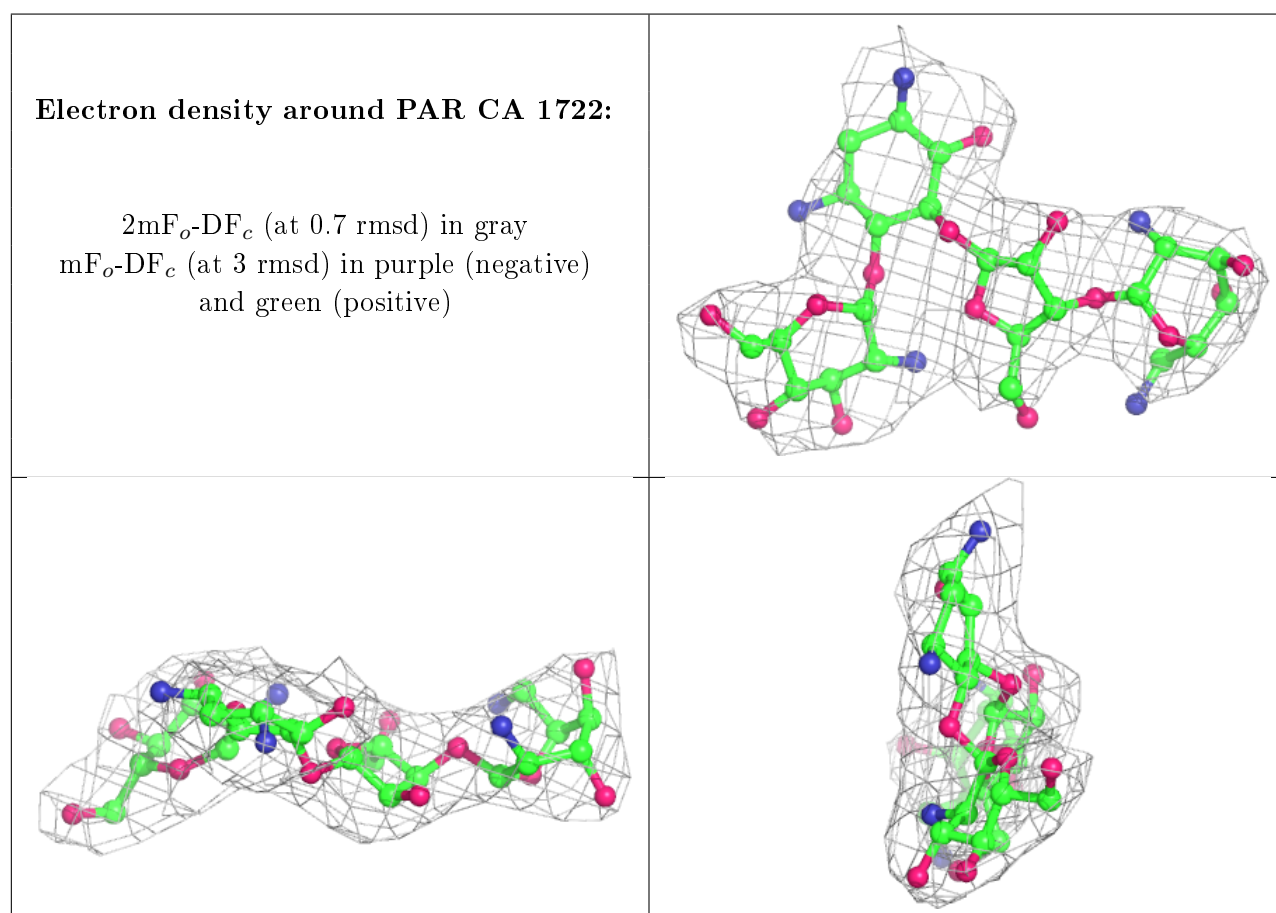
| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | AA    | 3180 | 1/1   | 0.99 | 0.47 | 42,42,42,42                 | 0     |
| 56  | OHX  | AA    | 3389 | 7/7   | 0.99 | 0.18 | 80,93,103,143               | 0     |
| 55  | MG   | AA    | 3024 | 1/1   | 0.99 | 0.42 | 45,45,45,45                 | 0     |
| 56  | OHX  | AA    | 3331 | 7/7   | 0.99 | 0.16 | 93,94,108,145               | 0     |
| 56  | OHX  | BA    | 1721 | 7/7   | 0.99 | 0.10 | 109,115,141,157             | 1     |
| 56  | OHX  | DF    | 301  | 7/7   | 0.99 | 0.12 | 53,80,83,83                 | 1     |
| 56  | OHX  | AA    | 3349 | 7/7   | 0.99 | 0.10 | 94,104,124,143              | 0     |
| 56  | OHX  | AA    | 3347 | 7/7   | 0.99 | 0.15 | 74,77,98,102                | 2     |
| 56  | OHX  | DA    | 3337 | 7/7   | 0.99 | 0.24 | 74,80,86,97                 | 1     |
| 56  | OHX  | BA    | 1814 | 7/7   | 0.99 | 0.11 | 88,100,109,173              | 0     |
| 55  | MG   | AA    | 3030 | 1/1   | 0.99 | 0.38 | 36,36,36,36                 | 0     |
| 55  | MG   | BA    | 1633 | 1/1   | 0.99 | 0.33 | 77,77,77,77                 | 0     |
| 56  | OHX  | DA    | 3371 | 7/7   | 0.99 | 0.11 | 119,121,131,160             | 1     |
| 56  | OHX  | AA    | 3328 | 7/7   | 0.99 | 0.16 | 67,76,86,89                 | 1     |
| 56  | OHX  | DA    | 3341 | 7/7   | 0.99 | 0.17 | 87,105,126,140              | 0     |
| 56  | OHX  | DA    | 3212 | 7/7   | 0.99 | 0.15 | 64,77,91,94                 | 1     |
| 56  | OHX  | AA    | 3434 | 7/7   | 0.99 | 0.17 | 98,102,107,132              | 1     |
| 56  | OHX  | AA    | 3411 | 7/7   | 0.99 | 0.08 | 107,117,135,154             | 0     |
| 56  | OHX  | AA    | 3393 | 7/7   | 0.99 | 0.15 | 50,81,89,115                | 2     |
| 56  | OHX  | CA    | 1725 | 7/7   | 0.99 | 0.11 | 108,111,122,123             | 1     |
| 56  | OHX  | AA    | 3326 | 7/7   | 0.99 | 0.17 | 75,76,87,119                | 0     |
| 55  | MG   | DA    | 3268 | 1/1   | 0.99 | 0.35 | 44,44,44,44                 | 0     |
| 56  | OHX  | AA    | 3444 | 7/7   | 0.99 | 0.14 | 79,89,101,122               | 2     |
| 56  | OHX  | BA    | 1716 | 7/7   | 0.99 | 0.17 | 73,86,99,116                | 0     |
| 55  | MG   | AA    | 3168 | 1/1   | 0.99 | 0.44 | 36,36,36,36                 | 0     |
| 55  | MG   | DA    | 3059 | 1/1   | 0.99 | 0.28 | 40,40,40,40                 | 0     |
| 56  | OHX  | AA    | 3352 | 7/7   | 0.99 | 0.17 | 80,86,96,122                | 1     |
| 56  | OHX  | DA    | 3344 | 7/7   | 0.99 | 0.16 | 93,104,111,114              | 1     |
| 56  | OHX  | AB    | 207  | 7/7   | 0.99 | 0.10 | 89,93,105,113               | 1     |
| 56  | OHX  | AA    | 3358 | 7/7   | 0.99 | 0.12 | 79,81,92,113                | 1     |
| 56  | OHX  | DA    | 3349 | 7/7   | 0.99 | 0.13 | 103,105,113,143             | 0     |
| 56  | OHX  | DA    | 3352 | 7/7   | 0.99 | 0.10 | 105,120,129,149             | 0     |
| 56  | OHX  | BA    | 1719 | 7/7   | 0.99 | 0.15 | 85,102,114,124              | 1     |
| 56  | OHX  | DA    | 3361 | 7/7   | 0.99 | 0.15 | 68,94,122,134               | 3     |
| 56  | OHX  | DA    | 3339 | 7/7   | 0.99 | 0.14 | 91,96,120,132               | 0     |
| 55  | MG   | AA    | 3042 | 1/1   | 0.99 | 0.30 | 42,42,42,42                 | 0     |
| 56  | OHX  | AA    | 3413 | 7/7   | 0.99 | 0.14 | 94,104,121,143              | 1     |
| 56  | OHX  | DA    | 3336 | 7/7   | 0.99 | 0.18 | 86,95,105,106               | 0     |
| 56  | OHX  | AA    | 3384 | 7/7   | 0.99 | 0.11 | 96,100,107,136              | 1     |
| 56  | OHX  | AA    | 3340 | 7/7   | 0.99 | 0.15 | 84,93,95,126                | 0     |
| 55  | MG   | AA    | 3020 | 1/1   | 0.99 | 0.43 | 42,42,42,42                 | 0     |
| 56  | OHX  | AA    | 3338 | 7/7   | 0.99 | 0.14 | 66,87,106,113               | 2     |

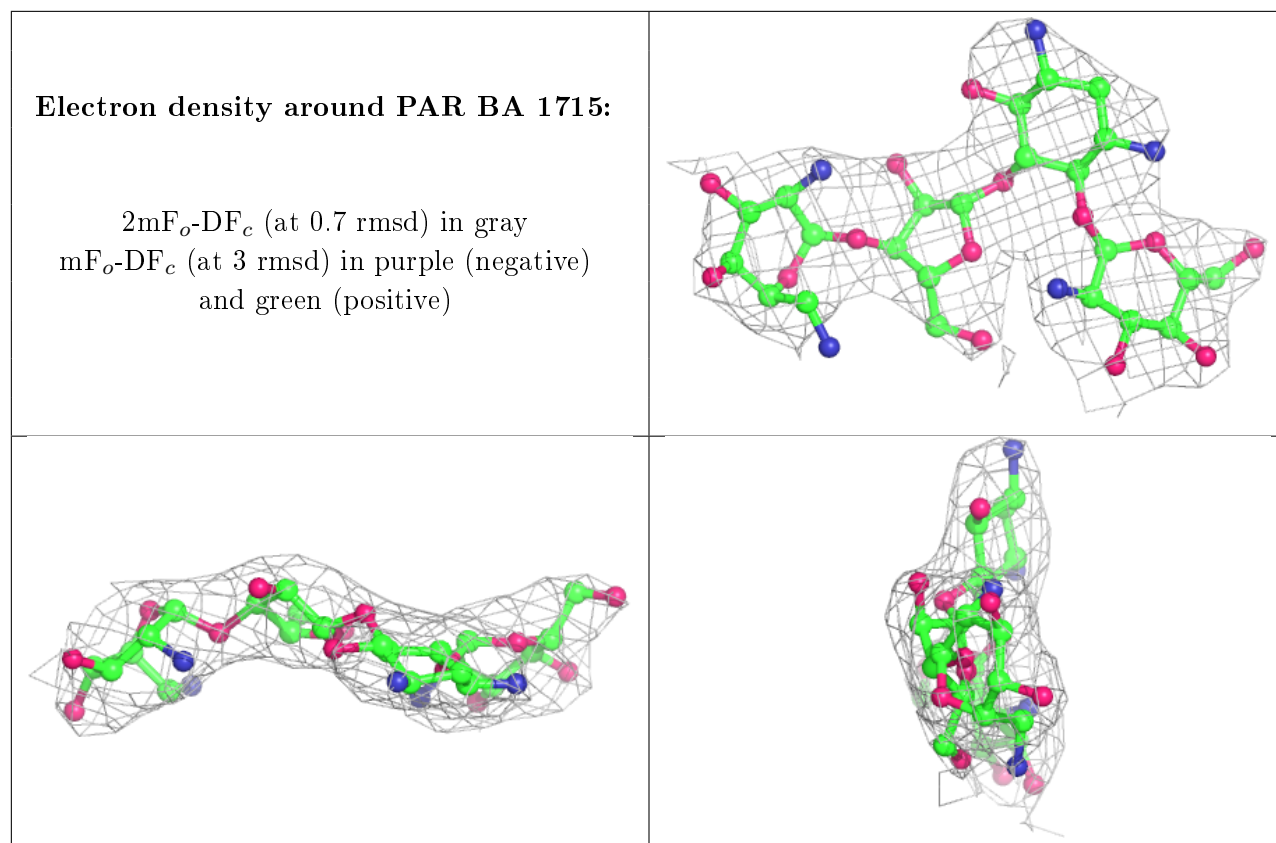
*Continued on next page...*

Continued from previous page...

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 56  | OHX  | AA    | 3333 | 7/7   | 0.99 | 0.14 | 99,103,122,123             | 0     |
| 56  | OHX  | DA    | 3061 | 7/7   | 1.00 | 0.13 | 81,86,92,106               | 0     |
| 56  | OHX  | AA    | 3382 | 7/7   | 1.00 | 0.16 | 65,73,84,93                | 0     |
| 56  | OHX  | DA    | 3346 | 7/7   | 1.00 | 0.11 | 107,113,126,132            | 0     |
| 56  | OHX  | AA    | 3379 | 7/7   | 1.00 | 0.23 | 20,47,62,138               | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.