



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 06:35 PM UTC

PDB ID : 5FCI / pdb\_00005fci  
Title : Structure of the vacant uL3 W255C mutant 80S yeast ribosome  
Authors : Mailliot, J.; Garreau de Loubresse, N.; Yusupova, G.; Dinman, J.D.; Yusupov, M.  
Deposited on : 2015-12-15  
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | <b>FAILED</b>                                                    |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

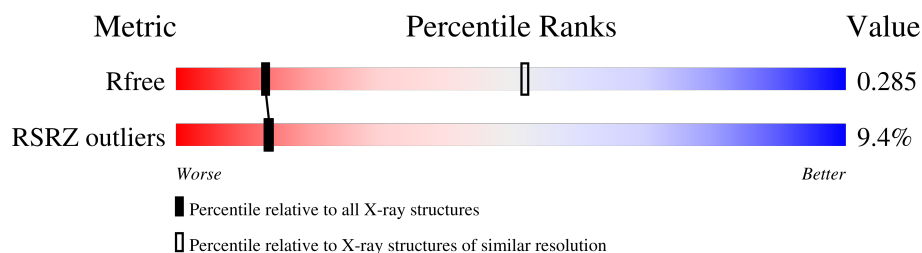
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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)) |
|---------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$    | 180053                      | 1001 (3.44-3.36)                                      |
| RSRZ outliers | 180081                      | 1001 (3.44-3.36)                                      |

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 85  | OHX  | 2     | 2022 | -         | -        | -       | X                |
| 86  | MG   | 1     | 3786 | -         | -        | -       | X                |
| 86  | MG   | 1     | 3809 | -         | -        | -       | X                |
| 86  | MG   | 1     | 3833 | -         | -        | -       | X                |
| 86  | MG   | 1     | 3834 | -         | -        | -       | X                |
| 86  | MG   | 1     | 3836 | -         | -        | -       | X                |
| 86  | MG   | 1     | 3841 | -         | -        | -       | X                |
| 86  | MG   | 1     | 3902 | -         | -        | -       | X                |
| 86  | MG   | 1     | 3920 | -         | -        | -       | X                |
| 86  | MG   | 1     | 3956 | -         | -        | -       | X                |
| 86  | MG   | 1     | 4086 | -         | -        | -       | X                |
| 86  | MG   | 1     | 4087 | -         | -        | -       | X                |
| 86  | MG   | 1     | 4089 | -         | -        | -       | X                |
| 86  | MG   | 1     | 4097 | -         | -        | -       | X                |
| 86  | MG   | 1     | 4098 | -         | -        | -       | X                |
| 86  | MG   | 1     | 4102 | -         | -        | -       | X                |
| 86  | MG   | 1     | 4105 | -         | -        | -       | X                |
| 86  | MG   | 1     | 4127 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 86  | MG   | 2     | 2055 | -         | -        | -       | X                |
| 86  | MG   | 2     | 2063 | -         | -        | -       | X                |
| 86  | MG   | 2     | 2064 | -         | -        | -       | X                |
| 86  | MG   | 2     | 2066 | -         | -        | -       | X                |
| 86  | MG   | 2     | 2081 | -         | -        | -       | X                |
| 86  | MG   | 2     | 2087 | -         | -        | -       | X                |
| 86  | MG   | 2     | 2093 | -         | -        | -       | X                |
| 86  | MG   | 2     | 2097 | -         | -        | -       | X                |
| 86  | MG   | 2     | 2101 | -         | -        | -       | X                |
| 86  | MG   | 2     | 2105 | -         | -        | -       | X                |
| 86  | MG   | 2     | 2109 | -         | -        | -       | X                |
| 86  | MG   | 2     | 2114 | -         | -        | -       | X                |
| 86  | MG   | 2     | 2124 | -         | -        | -       | X                |
| 86  | MG   | 5     | 3833 | -         | -        | -       | X                |
| 86  | MG   | 5     | 3846 | -         | -        | -       | X                |
| 86  | MG   | 5     | 3884 | -         | -        | -       | X                |
| 86  | MG   | 5     | 3957 | -         | -        | -       | X                |
| 86  | MG   | 5     | 3981 | -         | -        | -       | X                |
| 86  | MG   | 5     | 3994 | -         | -        | -       | X                |
| 86  | MG   | 5     | 4134 | -         | -        | -       | X                |
| 86  | MG   | 6     | 2064 | -         | -        | -       | X                |
| 86  | MG   | 6     | 2065 | -         | -        | -       | X                |
| 86  | MG   | 6     | 2089 | -         | -        | -       | X                |
| 86  | MG   | 6     | 2100 | -         | -        | -       | X                |
| 86  | MG   | 6     | 2102 | -         | -        | -       | X                |
| 86  | MG   | 6     | 2108 | -         | -        | -       | X                |
| 86  | MG   | 6     | 2113 | -         | -        | -       | X                |
| 86  | MG   | 6     | 2130 | -         | -        | -       | X                |
| 86  | MG   | 6     | 2134 | -         | -        | -       | X                |
| 86  | MG   | 6     | 2143 | -         | -        | -       | X                |
| 86  | MG   | 6     | 2163 | -         | -        | -       | X                |
| 86  | MG   | 6     | 2178 | -         | -        | -       | X                |
| 86  | MG   | 6     | 2179 | -         | -        | -       | X                |
| 86  | MG   | C2    | 201  | -         | -        | -       | X                |
| 86  | MG   | C2    | 204  | -         | -        | -       | X                |
| 86  | MG   | C2    | 208  | -         | -        | -       | X                |
| 86  | MG   | L2    | 302  | -         | -        | -       | X                |
| 86  | MG   | M1    | 201  | -         | -        | -       | X                |
| 86  | MG   | M7    | 203  | -         | -        | -       | X                |
| 86  | MG   | MG    | 2224 | -         | -        | -       | X                |
| 86  | MG   | Q1    | 101  | -         | -        | -       | X                |
| 86  | MG   | n0    | 204  | -         | -        | -       | X                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 86  | MG   | o4    | 202 | -         | -        | -       | X                |
| 86  | MG   | q1    | 101 | -         | -        | -       | X                |

## 2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 411776 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 18S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1   | 2     | 1781     | Total | C     | N    | O     | P    | 0       | 1       | 0     |
|     |       |          | 37970 | 16975 | 6720 | 12493 | 1782 |         |         |       |
| 1   | 6     | 1795     | Total | C     | N    | O     | P    | 0       | 1       | 0     |
|     |       |          | 38260 | 17105 | 6763 | 12596 | 1796 |         |         |       |

- Molecule 2 is a protein called 40S ribosomal protein S0-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | S0    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1612  | 1034 | 285 | 291 | 2 |         |         |       |
| 2   | s0    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1612  | 1034 | 285 | 291 | 2 |         |         |       |

- Molecule 3 is a protein called 40S ribosomal protein S1-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | S1    | 214      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1709  | 1084 | 310 | 311 | 4 |         |         |       |
| 3   | s1    | 216      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1722  | 1091 | 312 | 315 | 4 |         |         |       |

- Molecule 4 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | S2    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1635  | 1047 | 289 | 297 | 2 |         |         |       |
| 4   | s2    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1635  | 1047 | 289 | 297 | 2 |         |         |       |

- Molecule 5 is a protein called 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5   | S3    | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1734  | 1101 | 313 | 314 | 6 |         |         |       |
| 5   | s3    | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1734  | 1101 | 313 | 314 | 6 |         |         |       |

- Molecule 6 is a protein called 40S ribosomal protein S4-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 6   | S4    | 260      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2068  | 1316 | 389 | 360 | 3 |         |         |       |
| 6   | s4    | 260      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2068  | 1316 | 389 | 360 | 3 |         |         |       |

- Molecule 7 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 7   | S5    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1609  | 1007 | 300 | 299 | 3 |         |         |       |
| 7   | s5    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1609  | 1007 | 300 | 299 | 3 |         |         |       |

- Molecule 8 is a protein called 40S ribosomal protein S6-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 8   | S6    | 226      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1820  | 1142 | 350 | 325 | 3 |         |         |       |
| 8   | s6    | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1755  | 1102 | 337 | 313 | 3 |         |         |       |

- Molecule 9 is a protein called 40S ribosomal protein S7-A.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 9   | S7    | 184      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1481  | 951 | 265 | 265 |  |         |         |       |
| 9   | s7    | 186      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1492  | 957 | 267 | 268 |  |         |         |       |

- Molecule 10 is a protein called 40S ribosomal protein S8-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | S8    | 188      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1489  | 925 | 298 | 264 | 2 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | s8    | 188      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1489  | 925 | 298 | 264 | 2 |         |         |       |

- Molecule 11 is a protein called 40S ribosomal protein S9-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | S9    | 185      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1494  | 943 | 289 | 261 | 1 |         |         |       |
| 11  | s9    | 185      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1494  | 943 | 289 | 261 | 1 |         |         |       |

- Molecule 12 is a protein called 40S ribosomal protein S10-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | C0    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 772   | 499 | 126 | 145 | 2 |         |         |       |

- Molecule 13 is a protein called 40S ribosomal protein S11-A,40S ribosomal protein S11-A (uS17).

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | C1    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1213  | 774 | 230 | 206 | 3 |         |         |       |
| 13  | c1    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1168  | 747 | 221 | 197 | 3 |         |         |       |

- Molecule 14 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14  | C2    | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 892   | 562 | 156 | 172 | 2 |         |         |       |
| 14  | c2    | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 892   | 562 | 156 | 172 | 2 |         |         |       |

- Molecule 15 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | C3    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1192  | 759 | 224 | 207 | 2 |         |         |       |
| 15  | c3    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1192  | 759 | 224 | 207 | 2 |         |         |       |

- Molecule 16 is a protein called 40S ribosomal protein S14-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | C4    | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 891   | 545 | 182 | 163 | 1 |         |         |       |
| 16  | c4    | 128      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 949   | 582 | 188 | 176 | 3 |         |         |       |

- Molecule 17 is a protein called 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | C5    | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 977   | 622 | 182 | 166 | 7 |         |         |       |
| 17  | c5    | 135      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1039  | 658 | 196 | 178 | 7 |         |         |       |

- Molecule 18 is a protein called 40S ribosomal protein S16-A.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 18  | C6    | 141      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1105  | 708 | 203 | 194 |  |         |         |       |
| 18  | c6    | 142      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1111  | 711 | 204 | 196 |  |         |         |       |

- Molecule 19 is a protein called 40S ribosomal protein S17-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | C7    | 120      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 965   | 603 | 183 | 177 | 2 |         |         |       |
| 19  | c7    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 944   | 591 | 179 | 172 | 2 |         |         |       |

- Molecule 20 is a protein called 40S ribosomal protein S18-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | C8    | 145      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1192  | 743 | 237 | 210 | 2 |         |         |       |
| 20  | c8    | 145      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1192  | 743 | 237 | 210 | 2 |         |         |       |

- Molecule 21 is a protein called 40S ribosomal protein S19-A.



| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21  | C9    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1112  | 694 | 208 | 208 | 2 |         |         |       |
| 21  | c9    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1112  | 694 | 208 | 208 | 2 |         |         |       |

- Molecule 22 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22  | D0    | 107      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 855   | 539 | 156 | 159 | 1 |         |         |       |
| 22  | d0    | 110      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 882   | 554 | 161 | 166 | 1 |         |         |       |

- Molecule 23 is a protein called 40S ribosomal protein S21-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 23  | D1    | 87       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 684   | 420 | 125 | 137 | 2 |         |         |       |
| 23  | d1    | 87       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 684   | 420 | 125 | 137 | 2 |         |         |       |

- Molecule 24 is a protein called 40S ribosomal protein S22-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24  | D2    | 129      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1021  | 650 | 188 | 180 | 3 |         |         |       |
| 24  | d2    | 129      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1021  | 650 | 188 | 180 | 3 |         |         |       |

- Molecule 25 is a protein called 40S ribosomal protein S23-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 25  | D3    | 144      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1121  | 708 | 220 | 191 | 2 |         |         |       |
| 25  | d3    | 144      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1121  | 708 | 220 | 191 | 2 |         |         |       |

- Molecule 26 is a protein called 40S ribosomal protein S24-A.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 26  | D4    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1073  | 676 | 208 | 189 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 26  | d4    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1073  | 676 | 208 | 189 |         |         |       |

- Molecule 27 is a protein called 40S ribosomal protein S25-A.

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 27  | D5    | 70       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 563   | 360 | 104 | 99 |         |         |       |
| 27  | d5    | 69       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 558   | 357 | 103 | 98 |         |         |       |

- Molecule 28 is a protein called 40S ribosomal protein S26-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28  | D6    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 769   | 475 | 160 | 129 | 5 |         |         |       |
| 28  | d6    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 769   | 475 | 160 | 129 | 5 |         |         |       |

- Molecule 29 is a protein called 40S ribosomal protein S27-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 29  | D7    | 81       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 610   | 382 | 110 | 113 | 5 |         |         |       |
| 29  | d7    | 81       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 610   | 382 | 110 | 113 | 5 |         |         |       |

- Molecule 30 is a protein called 40S ribosomal protein S28-A.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 30  | D8    | 63       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 497   | 306 | 99 | 91 | 1 |         |         |       |
| 30  | d8    | 63       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 497   | 306 | 99 | 91 | 1 |         |         |       |

- Molecule 31 is a protein called 40S ribosomal protein S29-A.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 31  | D9    | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 443   | 275 | 92 | 72 | 4 |         |         |       |
| 31  | d9    | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 443   | 275 | 92 | 72 | 4 |         |         |       |

- Molecule 32 is a protein called 40S ribosomal protein S30-A.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 32  | E0    | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 475   | 299 | 98  | 77 | 1 |         |         |       |
| 32  | e0    | 62       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 491   | 309 | 101 | 80 | 1 |         |         |       |

- Molecule 33 is a protein called 40S ribosomal protein S31.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 33  | E1    | 71       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 566   | 362 | 106 | 94 | 4 |         |         |       |
| 33  | e1    | 76       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 608   | 388 | 117 | 99 | 4 |         |         |       |

- Molecule 34 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 34  | SR    | 318      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2441  | 1543 | 418 | 472 | 8 |         |         |       |
| 34  | sR    | 318      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2445  | 1546 | 419 | 472 | 8 |         |         |       |

- Molecule 35 is a protein called Suppressor protein STM1,Suppressor protein STM1.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 35  | SM    | 159      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1104  | 652 | 221 | 231 |  |         |         |       |
| 35  | sM    | 104      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 680   | 403 | 140 | 137 |  |         |         |       |

- Molecule 36 is a RNA chain called 25S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 36  | 1     | 3149     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 67355 | 30086 | 12142 | 21978 | 3149 |         |         |       |
| 36  | 5     | 3150     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 67377 | 30095 | 12145 | 21987 | 3150 |         |         |       |

- Molecule 37 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 37  | 3     | 121      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2579  | 1152 | 461 | 845 | 121 |         |         |       |
| 37  | 7     | 121      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2579  | 1152 | 461 | 845 | 121 |         |         |       |

- Molecule 38 is a RNA chain called 5.8S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |      |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|---------|-------|
| 38  | 4     | 158      | Total | C    | N   | O    | P   | 0       | 0       | 0     |
|     |       |          | 3353  | 1500 | 586 | 1109 | 158 |         |         |       |
| 38  | 8     | 158      | Total | C    | N   | O    | P   | 0       | 0       | 0     |
|     |       |          | 3353  | 1500 | 586 | 1109 | 158 |         |         |       |

- Molecule 39 is a protein called 60S ribosomal protein L2-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 39  | L2    | 252      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1918  | 1193 | 389 | 335 | 1 |         |         |       |
| 39  | l2    | 252      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1918  | 1193 | 389 | 335 | 1 |         |         |       |

- Molecule 40 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 40  | L3    | 386      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3073  | 1948 | 583 | 533 | 9 |         |         |       |
| 40  | l3    | 386      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3073  | 1948 | 583 | 533 | 9 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| L3    | 255     | CYS      | TRP    | engineered mutation | UNP P14126 |
| l3    | 255     | CYS      | TRP    | engineered mutation | UNP P14126 |

- Molecule 41 is a protein called 60S ribosomal protein L4-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 41  | L4    | 361      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2749  | 1730 | 522 | 494 | 3 |         |         |       |
| 41  | l4    | 361      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2749  | 1730 | 522 | 494 | 3 |         |         |       |

- Molecule 42 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 42  | L5    | 296      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2375  | 1501 | 414 | 458 | 2 |         |         |       |
| 42  | 15    | 294      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2359  | 1489 | 412 | 456 | 2 |         |         |       |

- Molecule 43 is a protein called 60S ribosomal protein L6-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43  | L6    | 156      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1239  | 800 | 222 | 216 | 1 |         |         |       |
| 43  | 16    | 157      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1248  | 806 | 224 | 217 | 1 |         |         |       |

- Molecule 44 is a protein called 60S ribosomal protein L7-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 44  | L7    | 222      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1784  | 1151 | 324 | 308 | 1 |         |         |       |
| 44  | 17    | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1791  | 1155 | 325 | 310 | 1 |         |         |       |

- Molecule 45 is a protein called 60S ribosomal protein L8-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 45  | L8    | 233      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1817  | 1159 | 326 | 329 | 3 |         |         |       |
| 45  | 18    | 231      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1763  | 1130 | 316 | 314 | 3 |         |         |       |

- Molecule 46 is a protein called 60S ribosomal protein L9-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46  | L9    | 191      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1518  | 963 | 274 | 277 | 4 |         |         |       |
| 46  | 19    | 191      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1518  | 963 | 274 | 277 | 4 |         |         |       |

- Molecule 47 is a protein called 60S ribosomal protein L10.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 47  | M0    | 211      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1717  | 1089 | 325 | 297 | 6 |         |         |       |
| 47  | m0    | 213      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1733  | 1101 | 327 | 299 | 6 |         |         |       |

- Molecule 48 is a protein called 60S ribosomal protein L11-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48  | M1    | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1353  | 847 | 253 | 249 | 4 |         |         |       |
| 48  | m1    | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1353  | 847 | 253 | 249 | 4 |         |         |       |

- Molecule 49 is a protein called 60S ribosomal protein L13-A.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 49  | M3    | 193      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1543  | 962 | 315 | 266 |  |         |         |       |
| 49  | m3    | 194      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1548  | 965 | 316 | 267 |  |         |         |       |

- Molecule 50 is a protein called 60S ribosomal protein L14-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 50  | M4    | 136      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1053  | 675 | 199 | 177 | 2 |         |         |       |
| 50  | m4    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1059  | 678 | 200 | 179 | 2 |         |         |       |

- Molecule 51 is a protein called 60S ribosomal protein L15-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 51  | M5    | 203      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1720  | 1077 | 361 | 281 | 1 |         |         |       |
| 51  | m5    | 203      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1720  | 1077 | 361 | 281 | 1 |         |         |       |

- Molecule 52 is a protein called 60S ribosomal protein L16-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 52  | M6    | 197      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1555  | 1003 | 289 | 262 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 52  | m6    | 197      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1555  | 1003 | 289 | 262 | 1 |         |         |       |

- Molecule 53 is a protein called 60S ribosomal protein L17-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 53  | M7    | 183      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1442  | 896 | 287 | 259 |   |         |         |       |
| 53  | m7    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1227  | 764 | 238 | 225 |   |         |         |       |

- Molecule 54 is a protein called 60S ribosomal protein L18-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 54  | M8    | 185      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1441  | 908 | 290 | 241 | 2 |         |         |       |
| 54  | m8    | 185      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1441  | 908 | 290 | 241 | 2 |         |         |       |

- Molecule 55 is a protein called 60S ribosomal protein L19-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 55  | M9    | 188      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1521  | 935 | 326 | 260 |   |         |         |       |
| 55  | m9    | 188      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1521  | 935 | 326 | 260 |   |         |         |       |

- Molecule 56 is a protein called 60S ribosomal protein L20-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 56  | N0    | 172      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1445  | 930 | 267 | 244 | 4 |         |         |       |
| 56  | n0    | 172      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1445  | 930 | 267 | 244 | 4 |         |         |       |

- Molecule 57 is a protein called 60S ribosomal protein L21-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 57  | N1    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1276  | 805 | 246 | 221 | 4 |         |         |       |
| 57  | n1    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1276  | 805 | 246 | 221 | 4 |         |         |       |

- Molecule 58 is a protein called 60S ribosomal protein L22-A.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 58  | N2    | 100      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 796   | 516 | 131 | 149 |         |         |       |
| 58  | n2    | 98       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 778   | 505 | 127 | 146 |         |         |       |

- Molecule 59 is a protein called 60S ribosomal protein L23-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 59  | N3    | 136      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1003  | 628 | 189 | 179 | 7 |         |         |       |
| 59  | n3    | 136      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1003  | 628 | 189 | 179 | 7 |         |         |       |

- Molecule 60 is a protein called 60S ribosomal protein L24-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 60  | N4    | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 800   | 508 | 159 | 132 | 1 |         |         |       |
| 60  | n4    | 135      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1089  | 682 | 219 | 187 | 1 |         |         |       |

- Molecule 61 is a protein called 60S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 61  | N5    | 121      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 623 | 170 | 173 | 2 |         |         |       |
| 61  | n5    | 120      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 959   | 617 | 168 | 172 | 2 |         |         |       |

- Molecule 62 is a protein called 60S ribosomal protein L26-A.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 62  | N6    | 126      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 993   | 625 | 192 | 176 |         |         |       |
| 62  | n6    | 126      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 993   | 625 | 192 | 176 |         |         |       |

- Molecule 63 is a protein called 60S ribosomal protein L27-A.



| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 63  | N7    | 135      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1092  | 710 | 202 | 180 |         |         |       |
| 63  | n7    | 135      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1092  | 710 | 202 | 180 |         |         |       |

- Molecule 64 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 64  | N8    | 148      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1173  | 749 | 231 | 190 | 3 |         |         |       |
| 64  | n8    | 148      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1173  | 749 | 231 | 190 | 3 |         |         |       |

- Molecule 65 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 65  | N9    | 58       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 462   | 289 | 100 | 73 |         |         |       |
| 65  | n9    | 58       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 462   | 289 | 100 | 73 |         |         |       |

- Molecule 66 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 66  | O0    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 743   | 479 | 124 | 139 | 1 |         |         |       |
| 66  | o0    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 767   | 492 | 128 | 146 | 1 |         |         |       |

- Molecule 67 is a protein called 60S ribosomal protein L31-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 67  | O1    | 109      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 890   | 565 | 168 | 156 | 1 |         |         |       |
| 67  | o1    | 109      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 890   | 565 | 168 | 156 | 1 |         |         |       |

- Molecule 68 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 68  | O2    | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1020  | 647 | 205 | 167 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 68  | o2    | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1020  | 647 | 205 | 167 | 1 |         |         |       |

- Molecule 69 is a protein called 60S ribosomal protein L33-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 69  | O3    | 106      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 850   | 540 | 165 | 144 | 1 |         |         |       |
| 69  | o3    | 106      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 850   | 540 | 165 | 144 | 1 |         |         |       |

- Molecule 70 is a protein called 60S ribosomal protein L34-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 70  | O4    | 112      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 881   | 546 | 179 | 152 | 4 |         |         |       |
| 70  | o4    | 112      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 881   | 546 | 179 | 152 | 4 |         |         |       |

- Molecule 71 is a protein called 60S ribosomal protein L35-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 71  | O5    | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 969   | 615 | 186 | 167 | 1 |         |         |       |
| 71  | o5    | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 969   | 615 | 186 | 167 | 1 |         |         |       |

- Molecule 72 is a protein called 60S ribosomal protein L36-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 72  | O6    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 771   | 481 | 156 | 132 | 2 |         |         |       |
| 72  | o6    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 771   | 481 | 156 | 132 | 2 |         |         |       |

- Molecule 73 is a protein called 60S ribosomal protein L37-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 73  | O7    | 87       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 681   | 414 | 148 | 114 | 5 |         |         |       |
| 73  | o7    | 87       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 681   | 414 | 148 | 114 | 5 |         |         |       |

- Molecule 74 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 74  | O8    | 77       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 612   | 391 | 115 | 106 |         |         |       |
| 74  | o8    | 77       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 612   | 391 | 115 | 106 |         |         |       |

- Molecule 75 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 75  | O9    | 50       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 436   | 272 | 97 | 65 | 2 |         |         |       |
| 75  | o9    | 50       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 436   | 272 | 97 | 65 | 2 |         |         |       |

- Molecule 76 is a protein called Ubiquitin-60S ribosomal protein L40.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 76  | Q0    | 52       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 417   | 259 | 86 | 67 | 5 |         |         |       |
| 76  | q0    | 52       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 417   | 259 | 86 | 67 | 5 |         |         |       |

- Molecule 77 is a protein called 60S ribosomal protein L41-A.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 77  | Q1    | 25       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 233   | 142 | 63 | 27 | 1 |         |         |       |
| 77  | q1    | 25       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 233   | 142 | 63 | 27 | 1 |         |         |       |

- Molecule 78 is a protein called 60S ribosomal protein L42-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 78  | Q2    | 105      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 847   | 534 | 170 | 138 | 5 |         |         |       |
| 78  | q2    | 105      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 847   | 534 | 170 | 138 | 5 |         |         |       |

- Molecule 79 is a protein called 60S ribosomal protein L43-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 79  | Q3    | 91       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 694   | 429 | 138 | 121 | 6 |         |         |       |
| 79  | q3    | 91       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 694   | 429 | 138 | 121 | 6 |         |         |       |

- Molecule 80 is a protein called 40S ribosomal protein S10-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 80  | c0    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 762   | 491 | 125 | 144 | 2 |         |         |       |

There are 12 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| c0    | 87      | UNK      | -      | expression tag | UNP Q08745 |
| c0    | 88      | UNK      | -      | expression tag | UNP Q08745 |
| c0    | 89      | UNK      | -      | expression tag | UNP Q08745 |
| c0    | 90      | UNK      | -      | expression tag | UNP Q08745 |
| c0    | 91      | UNK      | -      | expression tag | UNP Q08745 |
| c0    | 92      | UNK      | -      | expression tag | UNP Q08745 |
| c0    | 93      | UNK      | -      | expression tag | UNP Q08745 |
| c0    | 94      | UNK      | -      | expression tag | UNP Q08745 |
| c0    | 95      | UNK      | -      | expression tag | UNP Q08745 |
| c0    | 96      | UNK      | -      | expression tag | UNP Q08745 |
| c0    | 97      | UNK      | -      | expression tag | UNP Q08745 |
| c0    | 98      | UNK      | -      | expression tag | UNP Q08745 |

- Molecule 81 is a protein called 60S ribosomal protein L12-A (uL11).

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 81  | m2    | 150      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 750   | 450 | 150 | 150 |         |         |       |

- Molecule 82 is a protein called 60S acidic ribosomal protein P0.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 82  | p0    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1077  | 687 | 192 | 195 | 3 |         |         |       |

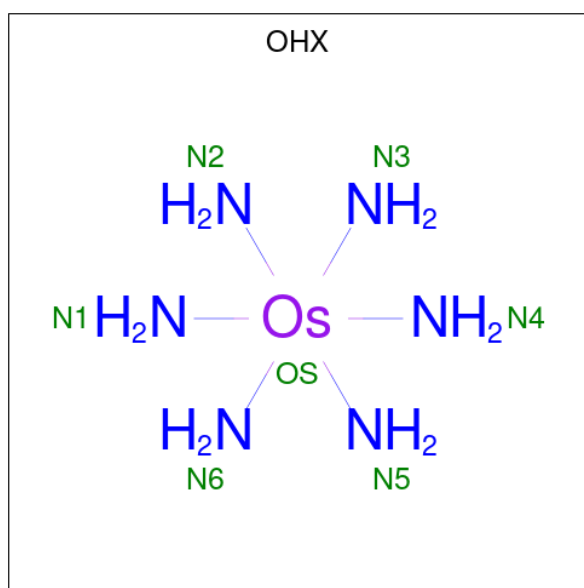
- Molecule 83 is a protein called 60S ribosomal protein P1 alpha.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 83  | p1    | 47       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 235   | 141 | 47 | 47 |         |         |       |

- Molecule 84 is a protein called 60S ribosomal protein P2 beta.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 84  | p2    | 46       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 230   | 138 | 46 | 46 |         |         |       |

- Molecule 85 is osmium (III) hexammine (CCD ID: OHX) (formula:  $\text{H}_{12}\text{N}_6\text{Os}$ ).



| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms      |        |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|---------|
| 85  | 2     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | 2     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | 2     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | 2     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | 2     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | 2     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | 2     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | 2     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | 2     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | 2     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | S6    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | S8    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | S9    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | C3    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | C5    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | C8    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | D9    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | SR    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | 1     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | 1     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | 1     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | 1     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 4     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 4     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 4     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 4     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 4     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 4     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 4     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 4     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 4     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 4     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 4     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 4     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | L3    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | L3    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | L4    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | M0    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | M5    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | M5    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | M7    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | M7    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | M9    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | N1    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | N9    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | O3    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | O4    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | O7    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | O7    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | Q2    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | s1    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | s1    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | s4    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | s8    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | s9    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | c1    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | c3    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | c5    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | c8    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | d4    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | d9    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | sR    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms      |        |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|---------|
| 85  | 8     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | 8     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | 8     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | 8     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | 8     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | 8     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | 8     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | 8     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | 13    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | 13    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | 14    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | 14    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | 15    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | 15    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | 15    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | 15    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | 19    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | m0    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | m0    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | m0    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 85  | m1    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 85  | m4    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | m5    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | n3    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | n5    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | n9    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | o2    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | o3    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | o4    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | o7    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 85  | q2    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

- Molecule 86 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 86  | 2     | 92       | Total | Mg | 0       | 0       |
|     |       |          | 92    | 92 |         |         |
| 86  | S4    | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 86  | S8    | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 86  | C2    | 8        | Total | Mg | 0       | 0       |
|     |       |          | 8     | 8  |         |         |
| 86  | C9    | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 86  | D1    | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 86  | D3    | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 86  | D9    | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 86  | SM    | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 86  | 1     | 395      | Total<br>395 | Mg<br>395 | 0       | 0       |
| 86  | 3     | 8        | Total<br>8   | Mg<br>8   | 0       | 0       |
| 86  | 4     | 16       | Total<br>16  | Mg<br>16  | 0       | 0       |
| 86  | L2    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 86  | L3    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 86  | L4    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 86  | L5    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | L7    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | L9    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | M0    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | M1    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | M3    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | M4    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | M5    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | M6    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 86  | M7    | 6        | Total<br>6   | Mg<br>6   | 0       | 0       |
| 86  | M8    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | M9    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | N0    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | N3    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 86  | N4    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 86  | N6    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | N8    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | N9    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | O1    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | O2    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | O5    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | O7    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 86  | Q1    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | Q2    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 86  | 6     | 136      | Total<br>136 | Mg<br>136 | 0       | 0       |
| 86  | s4    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | s6    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | c1    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | c8    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | sM    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 86  | 5     | 428      | Total<br>428 | Mg<br>428 | 0       | 0       |
| 86  | 7     | 11       | Total<br>11  | Mg<br>11  | 0       | 0       |
| 86  | 8     | 10       | Total<br>10  | Mg<br>10  | 0       | 0       |
| 86  | 13    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 86  | 14    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 86  | 17    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 86  | l9    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 86  | m0    | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 86  | m1    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 86  | m3    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 86  | m4    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 86  | m6    | 4        | Total<br>4 | Mg<br>4 | 0       | 0       |
| 86  | m7    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 86  | n0    | 4        | Total<br>4 | Mg<br>4 | 0       | 0       |
| 86  | n3    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 86  | n6    | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 86  | n8    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 86  | n9    | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 86  | o1    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 86  | o2    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 86  | o3    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 86  | o4    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 86  | q0    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 86  | q1    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 86  | p0    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 86  | MG    | 6        | Total<br>6 | Mg<br>6 | 0       | 0       |

- Molecule 87 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 87  | D6    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 87  | D7    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 87  | D9    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 87  | E1    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 87  | O7    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 87  | Q0    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 87  | Q2    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 87  | Q3    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 87  | d6    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 87  | d7    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 87  | d9    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 87  | e1    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 87  | o7    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 87  | q0    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 87  | q2    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 87  | q3    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |

MolProbity failed to run properly - this section is therefore empty.

### 3 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 435.45Å 287.66Å 303.76Å<br>90.00° 98.92° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 49.99 – 3.40<br>49.99 – 3.40                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 97.7 (49.99-3.40)<br>84.6 (49.99-3.40)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.35                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 0.57 (at 3.40Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX                                                      | Depositor        |
| R, $R_{free}$                                                           | 0.234 , 0.284<br>0.238 , 0.285                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 20186 reflections (2.00%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 67.8                                                        | Xtriage          |
| Anisotropy                                                              | 0.230                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 64.6                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.87                                                        | EDS              |
| Total number of atoms                                                   | 411776                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 78.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% 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.

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

MolProbity failed to run properly - this section is therefore empty.

### 4.3 Torsion angles [i](#)

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

MolProbity failed to run properly - this section is therefore empty.

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

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

### 4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 4.6 Ligand geometry [i](#)

Of 2303 ligands modelled in this entry, 1214 are monoatomic - leaving 1089 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 | $\# Z  > 2$ |
| 85  | OHX  | 5     | 3442 | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 5     | 3586 | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 5     | 3633 | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 1     | 3639 | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 2     | 1961 | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 5     | 3429 | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 8     | 204  | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 5     | 3545 | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 5     | 3594 | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 3     | 203  | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 1     | 3624 | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 6     | 2012 | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 7     | 205  | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 6     | 1928 | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 1     | 3607 | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 1     | 3447 | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 1     | 3728 | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 3     | 210  | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 5     | 3427 | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 1     | 3686 | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 1     | 3652 | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 5     | 3650 | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | M5    | 302  | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 5     | 3661 | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 1     | 3468 | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 5     | 3726 | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 6     | 1948 | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 1     | 3663 | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 5     | 3664 | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 5     | 3525 | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | D9    | 102  | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 14    | 401  | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 5     | 3599 | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 1     | 3674 | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 2     | 1954 | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 2     | 1983 | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 1     | 3502 | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 5     | 3455 | -    | 0,6,6        | -    | -           | -           |      |             |
| 85  | OHX  | 5     | 3695 | -    | 0,6,6        | -    | -           | -           |      |             |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 85  | OHX  | 6     | 1970 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3602 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3573 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | SR    | 401  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3486 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3418 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3465 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3716 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | M9    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3731 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3444 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1973 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3659 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3639 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3608 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3568 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3644 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1918 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 8     | 205  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1929 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3582 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | m0    | 302  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3549 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3658 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3454 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1998 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3601 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2018 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3718 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3598 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2023 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 4     | 214  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2036 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3421 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3414 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3616 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3460 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2006 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1991 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3746 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3433 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3469 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3585 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 85  | OHX  | 6     | 1983 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3409 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 8     | 203  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3406 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 4     | 206  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3546 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3632 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1934 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 7     | 212  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3581 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2036 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3592 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1921 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2041 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3413 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3567 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3673 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3503 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3420 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3653 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3481 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 15    | 302  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3403 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3415 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1987 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | N1    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3434 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3422 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1951 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3435 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 4     | 203  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3645 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3477 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 3     | 211  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3607 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3401 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1971 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1925 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1909 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3723 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3589 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3663 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3701 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 85  | OHX  | 6     | 2007 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3635 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1944 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1921 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3461 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1968 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3471 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | d9    | 102  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3712 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2031 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3735 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3554 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3404 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3535 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3429 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3648 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3709 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3546 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1915 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3629 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3538 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | L3    | 402  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3703 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3475 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1958 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 3     | 204  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3623 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3446 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1901 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3452 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3533 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3528 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1997 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3483 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | d4    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3651 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3722 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1996 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3462 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3467 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 8     | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3718 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3598 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 85  | OHX  | 5     | 3606 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1961 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3649 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1906 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3460 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3513 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3634 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1930 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3690 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3579 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3419 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2016 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3541 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3664 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | c3    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1972 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1920 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3701 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1981 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1957 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | s1    | 302  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3478 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3491 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3489 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3675 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3705 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | s9    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2014 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | S8    | 301  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | c5    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3455 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3724 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3621 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2041 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3622 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1954 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1955 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3734 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3583 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3520 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2015 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1992 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1998 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 85  | OHX  | 5     | 3432 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2021 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3450 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3551 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2024 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3681 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2019 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1907 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3569 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3676 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3449 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3676 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | c1    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3745 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3446 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3458 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3514 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3488 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1950 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3610 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3495 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1902 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1929 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1946 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | N9    | 102  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | O3    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1989 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3412 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3513 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3704 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2004 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3521 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3644 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1948 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3554 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3589 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3674 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3559 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 7     | 204  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1960 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3479 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3630 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1958 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 85  | OHX  | 1     | 3587 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3472 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2023 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3564 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | m4    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 7     | 207  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3418 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2014 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3528 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3547 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3462 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 4     | 213  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3431 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1923 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1910 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3606 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3566 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3722 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3492 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1913 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1980 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 7     | 203  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3537 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3611 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2016 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3565 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3577 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2027 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1986 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3580 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2022 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3449 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3500 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3710 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3595 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3626 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3585 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1971 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3471 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2001 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3659 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3733 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1931 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 85  | OHX  | 1     | 3681 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1925 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3518 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3470 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3517 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3530 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3677 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3463 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1959 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1975 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3657 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3699 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3726 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3448 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3713 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2027 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1922 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3506 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3464 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3615 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1989 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3409 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2017 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1935 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3683 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3686 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 8     | 208  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3436 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2020 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3545 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3699 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1938 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1908 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1927 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3642 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3534 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3524 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3690 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3459 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2009 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1993 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3466 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2038 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 85  | OHX  | 1     | 3487 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3714 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3403 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3717 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | o2    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3509 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3519 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3617 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3525 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1904 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3433 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3529 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3577 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 3     | 205  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3600 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3558 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3637 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3430 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2034 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3711 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2001 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3543 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3490 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1931 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1947 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1978 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3439 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3510 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3602 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3522 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3635 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 8     | 209  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | s4    | 301  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3547 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3719 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3637 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3731 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1976 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2043 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1901 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3442 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2009 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1937 | -    | 0,6,6        | -    | -        | -           |      |          |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 85  | OHX  | 5     | 3590 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3741 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3404 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3535 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3640 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3669 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3629 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2047 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3632 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1992 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3581 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | c8    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 7     | 202  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | o7    | 502  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2000 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3536 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2015 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1962 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1978 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3505 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3555 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3693 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2025 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3627 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | C5    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1939 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3693 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3472 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1953 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3477 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2008 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3457 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1924 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1946 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2035 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 4     | 202  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3482 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2013 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1960 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3669 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3743 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3665 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3619 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 85  | OHX  | 2     | 2018 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3522 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3630 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3655 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3441 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3642 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3464 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3526 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3739 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 8     | 202  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2008 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1950 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1926 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3517 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3466 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3670 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3724 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3709 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3621 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3408 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3640 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3714 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3405 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 7     | 206  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3476 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2044 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3450 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1906 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1962 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3422 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3425 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3536 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 3     | 208  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 8     | 206  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3441 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3500 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1943 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3610 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3684 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 8     | 210  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3575 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2002 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | M0    | 301  | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 85  | OHX  | 1     | 3625 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1905 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 7     | 209  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3479 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3593 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1967 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3571 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3493 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1915 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3428 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3457 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1932 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | O7    | 102  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1935 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3572 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1938 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3619 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3706 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1927 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3597 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3515 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3509 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3697 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3732 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3638 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | M7    | 202  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1908 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3520 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1940 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3426 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3492 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3527 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3511 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3667 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3537 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3737 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | s8    | 301  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3548 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3569 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3613 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1955 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3480 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3710 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 85  | OHX  | 1     | 3539 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1977 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | Q2    | 502  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3549 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3574 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3495 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1984 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3715 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3530 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3682 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3512 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3469 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3556 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3668 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3402 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1986 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1907 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1990 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | C8    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3684 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2049 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3504 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3544 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3564 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3588 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3448 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3489 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 7     | 208  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1965 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2039 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3592 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1937 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3578 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1919 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3685 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1973 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2045 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3591 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1947 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3534 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2035 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3425 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3614 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 85  | OHX  | 5     | 3603 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3720 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | O7    | 103  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2028 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3423 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3428 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3515 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2020 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3407 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2025 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1979 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2010 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3562 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1939 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3604 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2042 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3688 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3612 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3516 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3617 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3721 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3558 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3465 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3734 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | S6    | 301  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1916 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3636 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1964 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1917 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3463 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1945 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2031 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2038 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3531 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3551 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3565 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3725 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2004 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3506 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3504 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3556 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3480 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 15    | 304  | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 85  | OHX  | 8     | 211  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3601 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1981 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3419 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3493 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1949 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3518 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3438 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2024 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3443 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3496 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2010 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3696 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3641 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1920 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2040 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3437 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3501 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1995 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2043 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2013 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3675 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3524 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3668 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1949 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 4     | 207  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3643 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3456 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3634 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3735 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3740 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3410 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3474 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1956 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1952 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3612 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3720 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3593 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3415 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3692 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3700 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3540 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3672 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 85  | OHX  | 1     | 3459 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3729 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1905 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3679 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1918 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1941 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1936 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | n9    | 101  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3440 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3613 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3519 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3614 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3405 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3531 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3532 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1902 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3590 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1974 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | n3    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3521 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3680 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3633 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3562 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1917 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3727 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2021 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3543 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1922 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3618 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | s1    | 301  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3439 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3697 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3470 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2011 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3476 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3426 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3438 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3501 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1975 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3719 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3514 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3691 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3402 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 85  | OHX  | 1     | 3643 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1965 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 3     | 207  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3636 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3708 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3704 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3657 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3510 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3561 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | m0    | 303  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2005 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3631 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1959 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3584 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3467 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3443 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1976 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1984 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3453 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3587 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3678 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1979 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 8     | 218  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3605 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | C3    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3666 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1909 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3505 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3579 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3627 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3641 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3571 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3694 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3707 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3553 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3557 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3552 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3679 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2032 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3572 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3444 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1930 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3484 | -    | 0,6,6        | -    | -        | -           |      |          |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 85  | OHX  | 1     | 3616 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | L4    | 401  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3482 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1967 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 15    | 303  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3638 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2011 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 4     | 208  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2030 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1982 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3733 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3540 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3508 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2042 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3548 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3736 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 14    | 402  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1933 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3499 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3539 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3624 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 4     | 204  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1964 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3445 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3416 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3631 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2029 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1988 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3512 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3413 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3488 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1953 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3485 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3496 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3563 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3487 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3742 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3618 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3417 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2003 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3451 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3588 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1911 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 85  | OHX  | 2     | 1987 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3678 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3494 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 4     | 211  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1991 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3575 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3723 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3692 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1990 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2040 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3628 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3646 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1966 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1969 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1995 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3527 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3698 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 8     | 213  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3461 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3711 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1943 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3737 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3511 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3440 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3604 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3721 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2046 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | n5    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1993 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3605 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2029 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3660 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3542 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3732 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1985 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3694 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3702 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3623 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1910 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | O4    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1941 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3728 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3533 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 85  | OHX  | 2     | 2002 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1951 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 7     | 211  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3445 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3730 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3574 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3473 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3596 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3538 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3430 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3591 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3502 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1932 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3578 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3529 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3717 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3609 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3451 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2022 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3436 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3427 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3411 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3744 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3580 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3661 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3683 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3498 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 3     | 202  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1940 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3423 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 8     | 217  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1903 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | m5    | 501  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3456 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3608 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3685 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1926 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2037 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3568 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3582 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3474 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3553 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3454 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 85  | OHX  | 6     | 2005 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3560 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3689 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3499 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 8     | 212  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3654 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1977 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1916 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3671 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3526 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 3     | 206  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1956 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1952 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3570 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3662 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1919 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | sR    | 401  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3656 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 4     | 212  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3408 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1972 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3532 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1994 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3667 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2032 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3421 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3447 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3552 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1963 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3609 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1936 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3420 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3561 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3523 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3596 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3620 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3652 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3406 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3544 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1982 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3687 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2019 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 15    | 301  | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 85  | OHX  | 5     | 3542 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | m1    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3435 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 19    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3576 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3696 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1969 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3550 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2028 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3458 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 8     | 215  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3708 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1997 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3503 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3424 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1988 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3729 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3566 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1933 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3600 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1996 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3497 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2026 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3584 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3486 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3573 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3702 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3453 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3738 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2006 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | o3    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2003 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3648 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3700 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3680 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3655 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1913 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3595 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3478 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3727 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3414 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1966 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1911 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 85  | OHX  | S9    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1928 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3712 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3620 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3670 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3483 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3611 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 8     | 207  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3599 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 4     | 205  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3437 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3689 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3703 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 4     | 209  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | o4    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3615 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1923 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1912 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3412 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3576 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3736 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3673 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | l3    | 402  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3550 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3570 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3653 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3603 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3665 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1914 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | M7    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3434 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3677 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | l3    | 401  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3645 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3586 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3491 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1985 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3706 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2033 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3713 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3594 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3401 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2037 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 85  | OHX  | 5     | 3649 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3672 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3622 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3725 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3583 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1945 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3494 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3541 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3407 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1912 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3490 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2033 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3484 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 8     | 214  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3666 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 8     | 216  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3698 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3707 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3597 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1914 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3557 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3567 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1934 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 3     | 209  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1980 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3475 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3497 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | m0    | 301  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3650 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3507 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3432 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3647 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3656 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1942 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3416 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 7     | 210  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3452 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3559 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3651 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1999 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3682 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3523 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3691 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 85  | OHX  | 2     | 1957 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3508 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3410 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2034 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1994 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | M5    | 303  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3555 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3687 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3730 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | L3    | 401  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2012 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3473 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1944 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3468 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1999 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3716 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1963 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1903 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2007 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 4     | 210  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2000 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3424 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3485 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1968 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3563 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3658 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3411 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 4     | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3705 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3498 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3417 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1974 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3625 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2050 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3626 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | q2    | 502  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3662 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2039 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2017 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 2030 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3628 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3646 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3431 | -    | 0,6,6        | -    | -        | -           |      |          |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 85  | OHX  | 1     | 3695 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3481 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1942 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 2     | 1970 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3688 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3560 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2026 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1924 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 1904 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 6     | 2048 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3660 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3654 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3516 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 7     | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3507 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3647 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 1     | 3671 | -    | 0,6,6        | -    | -        | -           |      |          |
| 85  | OHX  | 5     | 3715 | -    | 0,6,6        | -    | -        | -           |      |          |

There are no bond length outliers.

There are no bond angle outliers.

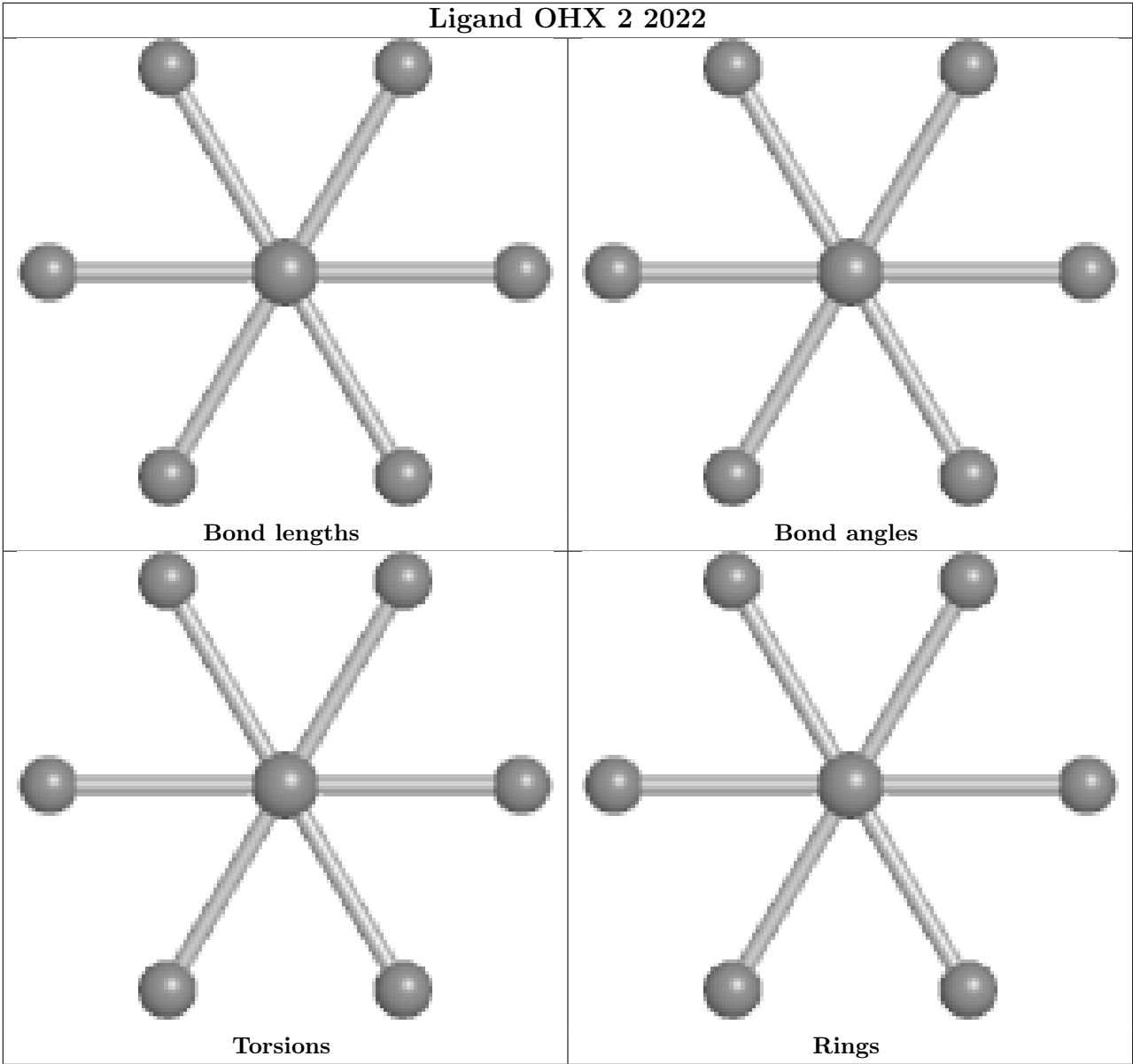
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.



4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 81  | m2    | 2                |
| 35  | sM    | 1                |
| 35  | SM    | 1                |

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| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 80  | c0    | 1                |
| 1   | 2     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | sM    | 139:UNK   | C      | 155:UNK   | N      | 37.65        |
| 1     | SM    | 141:ALA   | C      | 151:UNK   | N      | 26.56        |
| 1     | c0    | 84:GLU    | C      | 87:UNK    | N      | 8.21         |
| 1     | 2     | 1716:C    | O3'    | 1717:G    | P      | 4.60         |
| 1     | m2    | 23:UNK    | C      | 28:UNK    | N      | 4.05         |
| 1     | m2    | 52:UNK    | C      | 54:UNK    | N      | 3.55         |

## 5 Fit of model and data ⓘ

### 5.1 Protein, DNA and RNA chains ⓘ

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(Å²) | Q<0.9              |        |
|-----|-------|-----------------|--------|-----------|----|----------|--------------------|--------|
| 1   | 2     | 1781/1800 (98%) | 1.13   | 214 (12%) | 9  | 9        | 40, 97, 186, 235   | 1 (0%) |
| 1   | 6     | 1795/1800 (99%) | 0.87   | 121 (6%)  | 24 | 19       | 33, 82, 168, 218   | 1 (0%) |
| 2   | S0    | 206/251 (82%)   | 2.05   | 93 (45%)  | 0  | 1        | 108, 147, 226, 316 | 0      |
| 2   | s0    | 206/251 (82%)   | 1.48   | 46 (22%)  | 2  | 4        | 81, 112, 176, 255  | 0      |
| 3   | S1    | 214/254 (84%)   | 1.70   | 71 (33%)  | 1  | 1        | 111, 136, 156, 161 | 0      |
| 3   | s1    | 216/254 (85%)   | 0.84   | 11 (5%)   | 33 | 25       | 74, 87, 104, 112   | 0      |
| 4   | S2    | 217/253 (85%)   | 1.17   | 29 (13%)  | 7  | 8        | 81, 93, 115, 123   | 0      |
| 4   | s2    | 217/253 (85%)   | 0.85   | 22 (10%)  | 12 | 12       | 62, 74, 89, 98     | 0      |
| 5   | S3    | 223/239 (93%)   | 0.92   | 17 (7%)   | 20 | 17       | 81, 94, 124, 132   | 0      |
| 5   | s3    | 223/239 (93%)   | 1.04   | 17 (7%)   | 20 | 17       | 85, 109, 132, 140  | 0      |
| 6   | S4    | 260/260 (100%)  | 1.17   | 36 (13%)  | 6  | 8        | 72, 98, 110, 122   | 0      |
| 6   | s4    | 260/260 (100%)  | 0.86   | 14 (5%)   | 31 | 24       | 53, 79, 92, 115    | 0      |
| 7   | S5    | 206/224 (91%)   | 1.27   | 35 (16%)  | 4  | 5        | 101, 117, 125, 131 | 0      |
| 7   | s5    | 206/224 (91%)   | 1.05   | 20 (9%)   | 13 | 13       | 81, 101, 114, 117  | 0      |
| 8   | S6    | 226/236 (95%)   | 2.01   | 100 (44%) | 0  | 1        | 72, 126, 220, 365  | 0      |
| 8   | s6    | 218/236 (92%)   | 0.92   | 17 (7%)   | 19 | 16       | 54, 87, 104, 115   | 0      |
| 9   | S7    | 184/189 (97%)   | 1.21   | 26 (14%)  | 6  | 8        | 91, 117, 133, 136  | 0      |
| 9   | s7    | 186/189 (98%)   | 1.04   | 18 (9%)   | 13 | 13       | 72, 103, 131, 195  | 0      |
| 10  | S8    | 188/200 (94%)   | 1.25   | 30 (15%)  | 5  | 6        | 65, 84, 127, 136   | 0      |
| 10  | s8    | 188/200 (94%)   | 0.96   | 13 (6%)   | 23 | 18       | 49, 74, 126, 145   | 0      |
| 11  | S9    | 185/196 (94%)   | 1.29   | 35 (18%)  | 3  | 4        | 88, 103, 128, 145  | 0      |
| 11  | s9    | 185/196 (94%)   | 1.22   | 24 (12%)  | 7  | 8        | 67, 85, 114, 132   | 0      |
| 12  | C0    | 96/105 (91%)    | 1.19   | 18 (18%)  | 3  | 4        | 87, 106, 124, 135  | 0      |
| 13  | C1    | 146/155 (94%)   | 1.17   | 14 (9%)   | 13 | 13       | 68, 82, 105, 119   | 0      |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2  | OWAB(Å <sup>2</sup> ) |    | Q<0.9              |   |
|-----|-------|----------------|--------|----------|-----------------------|----|--------------------|---|
| 13  | c1    | 146/155 (94%)  | 1.13   | 23 (15%) | 5                     | 6  | 55, 69, 111, 187   | 0 |
| 14  | C2    | 109/142 (76%)  | 1.46   | 25 (22%) | 2                     | 4  | 139, 144, 148, 151 | 0 |
| 14  | c2    | 109/142 (76%)  | 1.93   | 50 (45%) | 0                     | 1  | 184, 196, 200, 201 | 0 |
| 15  | C3    | 150/150 (100%) | 1.04   | 13 (8%)  | 16                    | 14 | 73, 92, 108, 111   | 0 |
| 15  | c3    | 150/150 (100%) | 0.86   | 11 (7%)  | 21                    | 18 | 60, 77, 92, 103    | 0 |
| 16  | C4    | 127/136 (93%)  | 1.93   | 50 (39%) | 1                     | 1  | 82, 139, 149, 152  | 0 |
| 16  | c4    | 128/136 (94%)  | 1.00   | 11 (8%)  | 16                    | 15 | 60, 88, 93, 97     | 0 |
| 17  | C5    | 124/141 (87%)  | 1.06   | 17 (13%) | 6                     | 8  | 79, 96, 120, 131   | 0 |
| 17  | c5    | 135/141 (95%)  | 1.34   | 28 (20%) | 2                     | 4  | 71, 98, 118, 128   | 0 |
| 18  | C6    | 141/142 (99%)  | 1.56   | 37 (26%) | 1                     | 3  | 86, 109, 113, 116  | 0 |
| 18  | c6    | 142/142 (100%) | 1.54   | 37 (26%) | 1                     | 3  | 75, 97, 114, 131   | 0 |
| 19  | C7    | 120/136 (88%)  | 2.04   | 50 (41%) | 0                     | 1  | 99, 112, 309, 332  | 0 |
| 19  | c7    | 117/136 (86%)  | 2.06   | 48 (41%) | 0                     | 1  | 88, 102, 310, 364  | 0 |
| 20  | C8    | 145/145 (100%) | 1.24   | 22 (15%) | 5                     | 7  | 78, 103, 123, 127  | 0 |
| 20  | c8    | 145/145 (100%) | 1.03   | 16 (11%) | 10                    | 11 | 73, 92, 109, 115   | 0 |
| 21  | C9    | 143/143 (100%) | 1.91   | 51 (35%) | 1                     | 1  | 95, 103, 117, 124  | 0 |
| 21  | c9    | 143/143 (100%) | 1.06   | 14 (9%)  | 13                    | 13 | 76, 88, 102, 109   | 0 |
| 22  | D0    | 107/120 (89%)  | 1.63   | 33 (30%) | 1                     | 2  | 81, 109, 125, 128  | 0 |
| 22  | d0    | 110/120 (91%)  | 1.30   | 17 (15%) | 5                     | 7  | 79, 113, 136, 142  | 0 |
| 23  | D1    | 87/87 (100%)   | 1.08   | 9 (10%)  | 12                    | 12 | 102, 112, 163, 190 | 0 |
| 23  | d1    | 87/87 (100%)   | 0.78   | 5 (5%)   | 29                    | 22 | 74, 85, 129, 145   | 0 |
| 24  | D2    | 129/129 (100%) | 1.20   | 18 (13%) | 6                     | 8  | 76, 90, 98, 109    | 0 |
| 24  | d2    | 129/129 (100%) | 0.89   | 9 (6%)   | 22                    | 18 | 58, 70, 79, 92     | 0 |
| 25  | D3    | 144/144 (100%) | 0.93   | 15 (10%) | 11                    | 12 | 63, 69, 77, 86     | 0 |
| 25  | d3    | 144/144 (100%) | 0.66   | 4 (2%)   | 55                    | 41 | 48, 54, 64, 71     | 0 |
| 26  | D4    | 134/134 (100%) | 1.31   | 29 (21%) | 2                     | 4  | 86, 104, 115, 117  | 0 |
| 26  | d4    | 134/134 (100%) | 1.14   | 21 (15%) | 5                     | 6  | 62, 84, 97, 116    | 0 |
| 27  | D5    | 70/107 (65%)   | 1.29   | 12 (17%) | 4                     | 5  | 116, 124, 128, 128 | 0 |
| 27  | d5    | 69/107 (64%)   | 1.28   | 15 (21%) | 2                     | 4  | 92, 109, 115, 117  | 0 |
| 28  | D6    | 97/97 (100%)   | 1.50   | 21 (21%) | 2                     | 4  | 85, 101, 146, 147  | 0 |
| 28  | d6    | 97/97 (100%)   | 1.02   | 12 (12%) | 8                     | 9  | 63, 78, 96, 102    | 0 |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 29  | D7    | 81/81 (100%)    | 1.37   | 13 (16%) 5 6   | 93, 109, 126, 129     | 0     |
| 29  | d7    | 81/81 (100%)    | 1.06   | 8 (9%) 13 12   | 74, 89, 114, 118      | 0     |
| 30  | D8    | 63/66 (95%)     | 1.40   | 12 (19%) 3 4   | 108, 122, 128, 130    | 0     |
| 30  | d8    | 63/66 (95%)     | 1.07   | 7 (11%) 10 11  | 96, 107, 115, 118     | 0     |
| 31  | D9    | 53/55 (96%)     | 1.81   | 19 (35%) 1 1   | 84, 89, 106, 110      | 0     |
| 31  | d9    | 53/55 (96%)     | 1.73   | 20 (37%) 1 1   | 82, 94, 123, 130      | 0     |
| 32  | E0    | 60/62 (96%)     | 1.15   | 9 (15%) 5 7    | 69, 99, 123, 125      | 0     |
| 32  | e0    | 62/62 (100%)    | 0.87   | 7 (11%) 10 10  | 57, 82, 104, 111      | 0     |
| 33  | E1    | 71/76 (93%)     | 1.64   | 25 (35%) 1 1   | 96, 137, 146, 147     | 0     |
| 33  | e1    | 76/76 (100%)    | 2.21   | 37 (48%) 0 1   | 111, 170, 192, 197    | 0     |
| 34  | SR    | 318/318 (100%)  | 1.37   | 65 (20%) 3 4   | 110, 123, 140, 202    | 0     |
| 34  | sR    | 318/318 (100%)  | 1.41   | 59 (18%) 3 4   | 112, 128, 142, 186    | 0     |
| 35  | SM    | 133/182 (73%)   | 1.03   | 11 (8%) 17 15  | 57, 87, 146, 161      | 0     |
| 35  | sM    | 63/182 (34%)    | 1.03   | 12 (19%) 3 4   | 45, 97, 104, 108      | 0     |
| 36  | 1     | 3149/3396 (92%) | 0.52   | 125 (3%) 42 30 | 31, 57, 131, 226      | 0     |
| 36  | 5     | 3150/3396 (92%) | 0.45   | 94 (2%) 52 39  | 30, 54, 119, 190      | 0     |
| 37  | 3     | 121/121 (100%)  | 0.54   | 2 (1%) 69 54   | 41, 71, 88, 91        | 0     |
| 37  | 7     | 121/121 (100%)  | 0.41   | 2 (1%) 69 54   | 36, 55, 70, 74        | 0     |
| 38  | 4     | 158/158 (100%)  | 0.44   | 5 (3%) 50 37   | 37, 60, 97, 140       | 0     |
| 38  | 8     | 158/158 (100%)  | 0.56   | 6 (3%) 44 31   | 41, 63, 100, 119      | 0     |
| 39  | L2    | 252/253 (99%)   | 0.64   | 11 (4%) 39 28  | 41, 56, 73, 147       | 0     |
| 39  | l2    | 252/253 (99%)   | 0.85   | 18 (7%) 22 18  | 39, 57, 78, 146       | 0     |
| 40  | L3    | 386/386 (100%)  | 0.61   | 12 (3%) 51 38  | 36, 58, 75, 93        | 0     |
| 40  | l3    | 386/386 (100%)  | 0.40   | 12 (3%) 51 38  | 30, 44, 62, 97        | 0     |
| 41  | L4    | 361/361 (100%)  | 0.44   | 7 (1%) 66 51   | 34, 48, 64, 76        | 0     |
| 41  | l4    | 361/361 (100%)  | 0.47   | 9 (2%) 58 43   | 36, 50, 68, 80        | 0     |
| 42  | L5    | 296/296 (100%)  | 0.71   | 11 (3%) 45 32  | 52, 75, 96, 113       | 0     |
| 42  | l5    | 294/296 (99%)   | 0.71   | 16 (5%) 31 24  | 40, 58, 85, 120       | 0     |
| 43  | L6    | 156/175 (89%)   | 0.43   | 1 (0%) 85 75   | 43, 50, 67, 83        | 0     |
| 43  | l6    | 157/175 (89%)   | 0.44   | 2 (1%) 75 61   | 41, 50, 70, 79        | 0     |
| 44  | L7    | 222/243 (91%)   | 0.26   | 1 (0%) 87 78   | 36, 42, 65, 87        | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|----------------|-----------------------|-------|
| 44  | l7    | 223/243 (91%)  | 0.36   | 3 (1%) 75 61   | 33, 41, 72, 98        | 0     |
| 45  | L8    | 233/255 (91%)  | 1.15   | 35 (15%) 5 7   | 61, 81, 173, 291      | 0     |
| 45  | l8    | 231/255 (90%)  | 1.03   | 29 (12%) 8 9   | 68, 83, 110, 115      | 0     |
| 46  | L9    | 191/191 (100%) | 0.54   | 6 (3%) 51 38   | 48, 61, 73, 82        | 0     |
| 46  | l9    | 191/191 (100%) | 0.43   | 5 (2%) 57 42   | 40, 49, 64, 73        | 0     |
| 47  | M0    | 211/220 (95%)  | 0.45   | 8 (3%) 44 31   | 40, 50, 87, 161       | 0     |
| 47  | m0    | 213/220 (96%)  | 0.52   | 6 (2%) 55 41   | 35, 48, 82, 172       | 0     |
| 48  | M1    | 169/173 (97%)  | 0.98   | 17 (10%) 12 12 | 65, 81, 94, 100       | 0     |
| 48  | m1    | 169/173 (97%)  | 0.55   | 3 (1%) 67 53   | 46, 61, 70, 82        | 0     |
| 49  | M3    | 193/198 (97%)  | 0.61   | 6 (3%) 51 38   | 37, 59, 96, 119       | 0     |
| 49  | m3    | 194/198 (97%)  | 0.63   | 5 (2%) 57 42   | 38, 64, 96, 112       | 0     |
| 50  | M4    | 136/137 (99%)  | 0.46   | 5 (3%) 45 32   | 45, 50, 63, 71        | 0     |
| 50  | m4    | 137/137 (100%) | 0.41   | 5 (3%) 46 33   | 39, 45, 68, 80        | 0     |
| 51  | M5    | 203/203 (100%) | 0.89   | 13 (6%) 25 20  | 37, 53, 63, 68        | 0     |
| 51  | m5    | 203/203 (100%) | 1.04   | 22 (10%) 11 11 | 41, 58, 69, 73        | 0     |
| 52  | M6    | 197/198 (99%)  | 0.45   | 10 (5%) 33 25  | 35, 41, 60, 63        | 0     |
| 52  | m6    | 197/198 (99%)  | 0.38   | 7 (3%) 46 33   | 31, 35, 58, 62        | 0     |
| 53  | M7    | 183/183 (100%) | 0.78   | 20 (10%) 10 11 | 39, 50, 170, 329      | 0     |
| 53  | m7    | 155/183 (84%)  | 0.51   | 3 (1%) 66 51   | 35, 42, 53, 67        | 0     |
| 54  | M8    | 185/185 (100%) | 0.56   | 5 (2%) 56 42   | 38, 50, 66, 85        | 0     |
| 54  | m8    | 185/185 (100%) | 0.65   | 9 (4%) 35 26   | 36, 52, 64, 70        | 0     |
| 55  | M9    | 188/188 (100%) | 1.03   | 19 (10%) 12 12 | 64, 76, 138, 144      | 0     |
| 55  | m9    | 188/188 (100%) | 0.77   | 7 (3%) 45 32   | 55, 64, 120, 135      | 0     |
| 56  | N0    | 172/172 (100%) | 0.41   | 4 (2%) 61 46   | 39, 48, 61, 64        | 0     |
| 56  | n0    | 172/172 (100%) | 0.38   | 4 (2%) 61 46   | 35, 40, 51, 61        | 0     |
| 57  | N1    | 159/159 (100%) | 0.54   | 5 (3%) 51 38   | 41, 51, 87, 91        | 0     |
| 57  | n1    | 159/159 (100%) | 0.48   | 5 (3%) 51 38   | 38, 44, 80, 85        | 0     |
| 58  | N2    | 100/120 (83%)  | 1.15   | 12 (12%) 9 9   | 91, 102, 109, 112     | 0     |
| 58  | n2    | 98/120 (81%)   | 0.82   | 5 (5%) 33 25   | 75, 84, 92, 95        | 0     |
| 59  | N3    | 136/136 (100%) | 0.46   | 5 (3%) 45 32   | 43, 52, 61, 68        | 0     |
| 59  | n3    | 136/136 (100%) | 0.43   | 3 (2%) 62 47   | 31, 41, 54, 58        | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|----------------|-----------------------|-------|
| 60  | N4    | 98/155 (63%)   | 1.98   | 45 (45%) 0 1   | 52, 74, 448, 489      | 0     |
| 60  | n4    | 135/155 (87%)  | 1.21   | 33 (24%) 2 3   | 41, 94, 307, 436      | 0     |
| 61  | N5    | 121/141 (85%)  | 0.69   | 7 (5%) 29 22   | 52, 64, 84, 149       | 0     |
| 61  | n5    | 120/141 (85%)  | 0.92   | 12 (10%) 12 12 | 51, 67, 87, 95        | 0     |
| 62  | N6    | 126/126 (100%) | 0.78   | 7 (5%) 30 23   | 43, 59, 70, 76        | 0     |
| 62  | n6    | 126/126 (100%) | 0.92   | 9 (7%) 22 18   | 45, 60, 78, 83        | 0     |
| 63  | N7    | 135/135 (100%) | 0.95   | 11 (8%) 18 16  | 77, 89, 107, 114      | 0     |
| 63  | n7    | 135/135 (100%) | 1.17   | 15 (11%) 10 11 | 79, 90, 109, 117      | 0     |
| 64  | N8    | 148/148 (100%) | 0.58   | 7 (4%) 36 27   | 31, 52, 72, 81        | 0     |
| 64  | n8    | 148/148 (100%) | 0.53   | 1 (0%) 84 73   | 31, 53, 66, 70        | 0     |
| 65  | N9    | 58/58 (100%)   | 1.00   | 9 (15%) 5 7    | 37, 56, 94, 104       | 0     |
| 65  | n9    | 58/58 (100%)   | 1.02   | 5 (8%) 16 15   | 35, 53, 76, 80        | 0     |
| 66  | O0    | 97/104 (93%)   | 0.58   | 2 (2%) 63 48   | 75, 83, 96, 98        | 0     |
| 66  | o0    | 100/104 (96%)  | 0.70   | 5 (5%) 34 25   | 72, 80, 98, 104       | 0     |
| 67  | O1    | 109/112 (97%)  | 1.00   | 11 (10%) 12 12 | 54, 72, 123, 237      | 0     |
| 67  | o1    | 109/112 (97%)  | 0.72   | 5 (4%) 37 27   | 46, 58, 93, 168       | 0     |
| 68  | O2    | 127/129 (98%)  | 0.73   | 9 (7%) 22 18   | 31, 48, 57, 70        | 0     |
| 68  | o2    | 127/129 (98%)  | 0.62   | 6 (4%) 36 27   | 31, 50, 60, 70        | 0     |
| 69  | O3    | 106/106 (100%) | 0.56   | 4 (3%) 44 31   | 36, 43, 68, 83        | 0     |
| 69  | o3    | 106/106 (100%) | 0.34   | 2 (1%) 66 51   | 35, 40, 65, 72        | 0     |
| 70  | O4    | 112/120 (93%)  | 1.31   | 21 (18%) 3 4   | 55, 74, 101, 106      | 0     |
| 70  | o4    | 112/120 (93%)  | 1.21   | 17 (15%) 5 7   | 53, 71, 100, 105      | 0     |
| 71  | O5    | 119/119 (100%) | 0.85   | 9 (7%) 20 17   | 51, 67, 75, 81        | 0     |
| 71  | o5    | 119/119 (100%) | 0.84   | 11 (9%) 14 14  | 58, 68, 82, 90        | 0     |
| 72  | O6    | 99/99 (100%)   | 0.82   | 8 (8%) 18 16   | 57, 66, 91, 98        | 0     |
| 72  | o6    | 99/99 (100%)   | 0.93   | 12 (12%) 8 9   | 61, 72, 86, 100       | 0     |
| 73  | O7    | 87/87 (100%)   | 0.78   | 5 (5%) 29 22   | 39, 46, 70, 86        | 0     |
| 73  | o7    | 87/87 (100%)   | 0.93   | 9 (10%) 12 12  | 38, 47, 81, 114       | 0     |
| 74  | O8    | 77/77 (100%)   | 1.06   | 8 (10%) 11 12  | 84, 91, 99, 101       | 0     |
| 74  | o8    | 77/77 (100%)   | 1.05   | 7 (9%) 15 14   | 83, 91, 111, 122      | 0     |
| 75  | O9    | 50/50 (100%)   | 0.83   | 7 (14%) 6 8    | 48, 52, 60, 67        | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2         | OWAB(Å <sup>2</sup> ) | Q<0.9  |
|-----|-------|-------------------|--------|-----------------|-----------------------|--------|
| 75  | o9    | 50/50 (100%)      | 0.63   | 1 (2%) 65 49    | 48, 51, 61, 77        | 0      |
| 76  | Q0    | 52/52 (100%)      | 0.75   | 3 (5%) 29 22    | 48, 55, 66, 71        | 0      |
| 76  | q0    | 52/52 (100%)      | 0.32   | 1 (1%) 66 51    | 38, 41, 48, 54        | 0      |
| 77  | Q1    | 25/25 (100%)      | 1.61   | 6 (24%) 2 3     | 67, 68, 72, 73        | 0      |
| 77  | q1    | 25/25 (100%)      | 1.41   | 6 (24%) 2 3     | 54, 57, 67, 72        | 0      |
| 78  | Q2    | 105/105 (100%)    | 0.69   | 4 (3%) 44 31    | 44, 63, 74, 88        | 0      |
| 78  | q2    | 105/105 (100%)    | 0.71   | 5 (4%) 35 26    | 44, 56, 70, 88        | 0      |
| 79  | Q3    | 91/91 (100%)      | 0.56   | 1 (1%) 78 65    | 48, 58, 72, 82        | 0      |
| 79  | q3    | 91/91 (100%)      | 0.59   | 3 (3%) 49 36    | 46, 55, 71, 78        | 0      |
| 80  | c0    | 84/96 (87%)       | 1.73   | 32 (38%) 1 1    | 107, 133, 141, 144    | 0      |
| 81  | m2    | 0/150             | -      | -               | -                     | -      |
| 82  | p0    | 120/311 (38%)     | 1.17   | 11 (9%) 14 14   | 86, 103, 118, 125     | 0      |
| 83  | p1    | 0/47              | -      | -               | -                     | -      |
| 84  | p2    | 0/46              | -      | -               | -                     | -      |
| All | All   | 32953/35147 (93%) | 0.85   | 3085 (9%) 14 14 | 30, 72, 139, 489      | 2 (0%) |

All (3085) RSRZ outliers are listed below:

| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 2   | S0    | 40      | ALA  | 8.3  |
| 16  | C4    | 15      | GLY  | 7.7  |
| 18  | C6    | 20      | ALA  | 7.7  |
| 21  | C9    | 89      | ARG  | 7.6  |
| 19  | C7    | 125     | SER  | 7.3  |
| 33  | e1    | 145     | HIS  | 7.1  |
| 39  | l2    | 249     | SER  | 7.1  |
| 21  | C9    | 85      | SER  | 6.8  |
| 8   | S6    | 80      | ASN  | 6.7  |
| 1   | 6     | 656     | G    | 6.6  |
| 1   | 6     | 1756[A] | A    | 6.5  |
| 1   | 2     | 194     | U    | 6.5  |
| 16  | C4    | 16      | VAL  | 6.5  |
| 34  | sR    | 25      | THR  | 6.5  |
| 56  | N0    | 1       | MET  | 6.4  |
| 73  | o7    | 88      | ALA  | 6.4  |
| 39  | l2    | 253     | GLN  | 6.4  |
| 7   | S5    | 37      | GLN  | 6.3  |
| 21  | C9    | 92      | LYS  | 6.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 10  | S8    | 21   | PHE  | 6.2  |
| 31  | D9    | 4    | GLU  | 6.1  |
| 11  | s9    | 6    | ARG  | 6.1  |
| 14  | c2    | 30   | VAL  | 6.1  |
| 17  | c5    | 4    | ALA  | 6.1  |
| 1   | 2     | 1708 | U    | 6.0  |
| 1   | 6     | 1217 | A    | 6.0  |
| 1   | 2     | 1601 | G    | 6.0  |
| 33  | e1    | 80   | ARG  | 6.0  |
| 21  | C9    | 71   | VAL  | 5.9  |
| 19  | c7    | 25   | THR  | 5.8  |
| 4   | s2    | 92   | ALA  | 5.8  |
| 26  | d4    | 26   | ASP  | 5.8  |
| 21  | C9    | 90   | PRO  | 5.8  |
| 60  | N4    | 78   | ALA  | 5.8  |
| 60  | N4    | 76   | VAL  | 5.8  |
| 2   | S0    | 43   | ASP  | 5.8  |
| 19  | C7    | 110  | VAL  | 5.8  |
| 21  | C9    | 91   | TYR  | 5.6  |
| 9   | s7    | 52   | ALA  | 5.6  |
| 14  | c2    | 123  | VAL  | 5.6  |
| 2   | S0    | 107  | PHE  | 5.6  |
| 36  | 1     | 1349 | G    | 5.6  |
| 2   | S0    | 42   | PRO  | 5.6  |
| 70  | O4    | 2    | ALA  | 5.6  |
| 19  | C7    | 2    | GLY  | 5.6  |
| 36  | 1     | 2874 | G    | 5.6  |
| 17  | C5    | 104  | GLN  | 5.6  |
| 21  | C9    | 44   | GLU  | 5.5  |
| 19  | C7    | 53   | TYR  | 5.5  |
| 1   | 2     | 1709 | C    | 5.5  |
| 36  | 1     | 2772 | C    | 5.5  |
| 34  | SR    | 78   | ALA  | 5.5  |
| 18  | c6    | 19   | VAL  | 5.4  |
| 1   | 6     | 678  | A    | 5.4  |
| 60  | N4    | 75   | THR  | 5.4  |
| 21  | C9    | 86   | ARG  | 5.4  |
| 1   | 2     | 845  | G    | 5.3  |
| 53  | M7    | 168  | LEU  | 5.3  |
| 14  | c2    | 75   | VAL  | 5.3  |
| 22  | D0    | 120  | SER  | 5.3  |
| 56  | n0    | 2    | ALA  | 5.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | 2     | 280  | U    | 5.2  |
| 45  | l8    | 246  | MET  | 5.2  |
| 13  | c1    | 42   | PHE  | 5.1  |
| 19  | c7    | 53   | TYR  | 5.1  |
| 34  | SR    | 79   | TYR  | 5.1  |
| 6   | S4    | 25   | GLY  | 5.1  |
| 60  | N4    | 83   | THR  | 5.1  |
| 30  | D8    | 44   | VAL  | 5.1  |
| 11  | S9    | 181  | ALA  | 5.1  |
| 79  | q3    | 2    | ALA  | 5.1  |
| 5   | s3    | 145  | ALA  | 5.0  |
| 65  | N9    | 2    | ALA  | 5.0  |
| 39  | L2    | 253  | GLN  | 5.0  |
| 20  | c8    | 22   | VAL  | 5.0  |
| 1   | 6     | 676  | G    | 5.0  |
| 8   | S6    | 180  | THR  | 5.0  |
| 19  | c7    | 57   | LEU  | 5.0  |
| 21  | C9    | 5    | SER  | 4.9  |
| 21  | C9    | 41   | SER  | 4.9  |
| 26  | d4    | 69   | SER  | 4.9  |
| 3   | S1    | 96   | LEU  | 4.9  |
| 21  | C9    | 119  | LYS  | 4.9  |
| 1   | 2     | 217  | A    | 4.9  |
| 10  | S8    | 20   | GLN  | 4.9  |
| 19  | c7    | 65   | PRO  | 4.9  |
| 8   | S6    | 143  | LYS  | 4.9  |
| 4   | S2    | 86   | VAL  | 4.9  |
| 2   | s0    | 173  | ILE  | 4.9  |
| 31  | d9    | 16   | LYS  | 4.9  |
| 36  | 1     | 1103 | A    | 4.9  |
| 36  | 5     | 1103 | A    | 4.9  |
| 22  | D0    | 81   | THR  | 4.8  |
| 8   | S6    | 152  | ASP  | 4.8  |
| 1   | 2     | 1687 | U    | 4.8  |
| 21  | C9    | 83   | ALA  | 4.8  |
| 51  | m5    | 181  | ASN  | 4.8  |
| 2   | S0    | 50   | VAL  | 4.8  |
| 13  | C1    | 68   | GLY  | 4.8  |
| 8   | S6    | 182  | GLN  | 4.8  |
| 26  | d4    | 18   | LEU  | 4.8  |
| 34  | sR    | 62   | LYS  | 4.8  |
| 19  | c7    | 17   | ILE  | 4.7  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 19  | C7    | 117     | LEU  | 4.7  |
| 3   | S1    | 204     | ILE  | 4.7  |
| 54  | m8    | 14      | GLY  | 4.7  |
| 13  | C1    | 91      | LEU  | 4.7  |
| 10  | S8    | 8       | ARG  | 4.7  |
| 2   | S0    | 44      | GLY  | 4.7  |
| 31  | D9    | 5       | ASN  | 4.7  |
| 2   | S0    | 138     | TYR  | 4.7  |
| 19  | c7    | 3       | ARG  | 4.7  |
| 72  | o6    | 28      | TYR  | 4.7  |
| 1   | 2     | 1756[A] | A    | 4.7  |
| 16  | C4    | 14      | PHE  | 4.6  |
| 16  | C4    | 102     | LEU  | 4.6  |
| 65  | N9    | 54      | LEU  | 4.6  |
| 1   | 2     | 1370    | U    | 4.6  |
| 20  | c8    | 17      | LEU  | 4.6  |
| 1   | 2     | 1702    | A    | 4.6  |
| 61  | n5    | 23      | ALA  | 4.6  |
| 39  | l2    | 194     | ASN  | 4.6  |
| 19  | C7    | 102     | VAL  | 4.6  |
| 60  | N4    | 77      | LYS  | 4.6  |
| 1   | 2     | 1699    | G    | 4.6  |
| 34  | SR    | 136     | ILE  | 4.6  |
| 8   | S6    | 140     | ASN  | 4.6  |
| 2   | s0    | 19      | ALA  | 4.6  |
| 33  | e1    | 95      | HIS  | 4.6  |
| 19  | c7    | 10      | LYS  | 4.5  |
| 1   | 2     | 261     | U    | 4.5  |
| 55  | M9    | 5       | ARG  | 4.5  |
| 8   | S6    | 135     | PRO  | 4.5  |
| 19  | C7    | 124     | VAL  | 4.5  |
| 8   | S6    | 1       | MET  | 4.5  |
| 16  | C4    | 89      | THR  | 4.5  |
| 19  | c7    | 8       | THR  | 4.5  |
| 1   | 2     | 1625    | C    | 4.5  |
| 47  | m0    | 112     | GLN  | 4.5  |
| 2   | S0    | 41      | ARG  | 4.5  |
| 1   | 2     | 238     | U    | 4.5  |
| 60  | N4    | 90      | ILE  | 4.5  |
| 2   | S0    | 102     | PHE  | 4.5  |
| 2   | s0    | 2       | SER  | 4.4  |
| 8   | S6    | 175     | ILE  | 4.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 21  | c9    | 92   | LYS  | 4.4  |
| 8   | S6    | 186  | ARG  | 4.4  |
| 33  | e1    | 102  | VAL  | 4.4  |
| 2   | S0    | 162  | CYS  | 4.4  |
| 1   | 6     | 662  | U    | 4.4  |
| 1   | 6     | 651  | G    | 4.4  |
| 70  | o4    | 33   | GLN  | 4.4  |
| 18  | C6    | 21   | HIS  | 4.4  |
| 22  | D0    | 66   | SER  | 4.4  |
| 19  | c7    | 2    | GLY  | 4.4  |
| 1   | 2     | 715  | U    | 4.4  |
| 34  | sR    | 136  | ILE  | 4.4  |
| 3   | S1    | 94   | LYS  | 4.4  |
| 4   | S2    | 161  | LYS  | 4.4  |
| 26  | D4    | 117  | LYS  | 4.4  |
| 53  | M7    | 184  | ALA  | 4.4  |
| 63  | n7    | 2    | ALA  | 4.4  |
| 13  | c1    | 70   | ILE  | 4.4  |
| 47  | m0    | 111  | LEU  | 4.4  |
| 1   | 2     | 1704 | U    | 4.4  |
| 82  | p0    | 192  | ASP  | 4.4  |
| 80  | c0    | 27   | PHE  | 4.3  |
| 9   | S7    | 98   | ILE  | 4.3  |
| 60  | N4    | 82   | ILE  | 4.3  |
| 18  | c6    | 8    | GLN  | 4.3  |
| 3   | S1    | 201  | THR  | 4.3  |
| 39  | l2    | 16   | PHE  | 4.3  |
| 19  | c7    | 13   | SER  | 4.3  |
| 19  | C7    | 5    | ARG  | 4.3  |
| 4   | S2    | 90   | THR  | 4.3  |
| 28  | D6    | 14   | GLY  | 4.3  |
| 60  | N4    | 84   | GLY  | 4.3  |
| 8   | S6    | 179  | VAL  | 4.3  |
| 8   | S6    | 170  | THR  | 4.3  |
| 11  | s9    | 3    | ARG  | 4.3  |
| 34  | sR    | 253  | ALA  | 4.3  |
| 60  | n4    | 132  | GLY  | 4.3  |
| 1   | 2     | 218  | A    | 4.2  |
| 36  | 1     | 1234 | G    | 4.2  |
| 2   | S0    | 196  | SER  | 4.2  |
| 8   | S6    | 66   | GLY  | 4.2  |
| 1   | 6     | 679  | U    | 4.2  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 2          | S0           | 2          | SER         | 4.2         |
| 34         | sR           | 61         | PHE         | 4.2         |
| 36         | 1            | 1878       | G           | 4.2         |
| 33         | e1           | 78         | LYS         | 4.2         |
| 1          | 2            | 719        | U           | 4.2         |
| 19         | C7           | 41         | ILE         | 4.2         |
| 21         | C9           | 38         | LYS         | 4.2         |
| 8          | s6           | 88         | ARG         | 4.2         |
| 16         | C4           | 133        | ARG         | 4.2         |
| 2          | S0           | 207        | PRO         | 4.1         |
| 19         | c7           | 119        | LEU         | 4.1         |
| 18         | c6           | 125        | GLU         | 4.1         |
| 1          | 2            | 954        | G           | 4.1         |
| 2          | S0           | 187        | ALA         | 4.1         |
| 18         | c6           | 119        | ALA         | 4.1         |
| 60         | N4           | 85         | ALA         | 4.1         |
| 1          | 6            | 663        | U           | 4.1         |
| 12         | C0           | 40         | LEU         | 4.1         |
| 34         | SR           | 81         | LEU         | 4.1         |
| 8          | S6           | 158        | ILE         | 4.1         |
| 22         | D0           | 19         | ILE         | 4.1         |
| 7          | S5           | 36         | ALA         | 4.1         |
| 8          | S6           | 176        | GLN         | 4.1         |
| 31         | d9           | 27         | HIS         | 4.1         |
| 33         | e1           | 77         | GLY         | 4.1         |
| 8          | S6           | 68         | LEU         | 4.1         |
| 36         | 1            | 1237       | G           | 4.1         |
| 3          | S1           | 25         | THR         | 4.1         |
| 1          | 6            | 1708       | U           | 4.1         |
| 3          | S1           | 45         | LYS         | 4.1         |
| 8          | S6           | 5          | ILE         | 4.1         |
| 5          | S3           | 88         | ALA         | 4.1         |
| 5          | S3           | 179        | GLN         | 4.1         |
| 60         | N4           | 79         | GLN         | 4.1         |
| 38         | 8            | 80         | A           | 4.1         |
| 26         | d4           | 67         | GLY         | 4.1         |
| 14         | c2           | 45         | LEU         | 4.1         |
| 18         | C6           | 66         | ARG         | 4.1         |
| 18         | c6           | 68         | ARG         | 4.1         |
| 36         | 1            | 3079       | U           | 4.1         |
| 9          | s7           | 109        | VAL         | 4.0         |
| 19         | C7           | 120        | SER         | 4.0         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 5   | S3    | 148  | LYS  | 4.0  |
| 34  | sR    | 83   | ALA  | 4.0  |
| 21  | C9    | 79   | LEU  | 4.0  |
| 8   | S6    | 114  | VAL  | 4.0  |
| 60  | N4    | 63   | ILE  | 4.0  |
| 48  | M1    | 144  | CYS  | 4.0  |
| 60  | N4    | 81   | PRO  | 4.0  |
| 8   | S6    | 151  | ASP  | 4.0  |
| 1   | 6     | 1228 | G    | 4.0  |
| 6   | s4    | 26   | CYS  | 4.0  |
| 20  | C8    | 32   | LEU  | 4.0  |
| 18  | c6    | 29   | ILE  | 4.0  |
| 61  | N5    | 23   | ALA  | 4.0  |
| 36  | 1     | 2996 | U    | 4.0  |
| 19  | c7    | 100  | LEU  | 4.0  |
| 21  | c9    | 79   | LEU  | 4.0  |
| 8   | S6    | 157  | VAL  | 4.0  |
| 53  | M7    | 166  | VAL  | 4.0  |
| 1   | 2     | 1693 | A    | 4.0  |
| 45  | L8    | 113  | ALA  | 4.0  |
| 18  | c6    | 4    | VAL  | 3.9  |
| 1   | 6     | 1285 | U    | 3.9  |
| 72  | O6    | 56   | ARG  | 3.9  |
| 19  | c7    | 28   | PHE  | 3.9  |
| 28  | D6    | 4    | LYS  | 3.9  |
| 8   | S6    | 124  | LEU  | 3.9  |
| 21  | c9    | 91   | TYR  | 3.9  |
| 36  | 5     | 2874 | G    | 3.9  |
| 47  | M0    | 114  | GLY  | 3.9  |
| 2   | S0    | 23   | HIS  | 3.9  |
| 2   | s0    | 170  | ILE  | 3.9  |
| 23  | D1    | 34   | ILE  | 3.9  |
| 38  | 8     | 81   | U    | 3.9  |
| 63  | n7    | 56   | LYS  | 3.9  |
| 5   | S3    | 44   | THR  | 3.9  |
| 33  | e1    | 125  | THR  | 3.9  |
| 19  | C7    | 89   | SER  | 3.9  |
| 1   | 6     | 1707 | A    | 3.9  |
| 57  | n1    | 5    | HIS  | 3.9  |
| 1   | 2     | 320  | U    | 3.9  |
| 2   | S0    | 194  | PRO  | 3.9  |
| 30  | d8    | 24   | GLY  | 3.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | s0    | 40   | ALA  | 3.9  |
| 14  | C2    | 103  | LEU  | 3.9  |
| 36  | 1     | 1952 | G    | 3.9  |
| 36  | 5     | 620  | U    | 3.9  |
| 4   | S2    | 163  | GLY  | 3.9  |
| 16  | C4    | 27   | PHE  | 3.9  |
| 8   | S6    | 178  | LEU  | 3.9  |
| 9   | s7    | 93   | LEU  | 3.9  |
| 26  | d4    | 27   | VAL  | 3.8  |
| 53  | M7    | 165  | VAL  | 3.8  |
| 34  | sR    | 168  | THR  | 3.8  |
| 33  | e1    | 94   | LYS  | 3.8  |
| 18  | c6    | 139  | GLN  | 3.8  |
| 7   | S5    | 71   | ALA  | 3.8  |
| 71  | o5    | 2    | ALA  | 3.8  |
| 7   | s5    | 37   | GLN  | 3.8  |
| 8   | S6    | 190  | GLN  | 3.8  |
| 60  | N4    | 96   | LEU  | 3.8  |
| 17  | c5    | 136  | SER  | 3.8  |
| 20  | C8    | 22   | VAL  | 3.8  |
| 80  | c0    | 22   | VAL  | 3.8  |
| 36  | 1     | 1236 | G    | 3.8  |
| 71  | o5    | 107  | LYS  | 3.8  |
| 4   | s2    | 208  | GLU  | 3.8  |
| 34  | SR    | 160  | GLU  | 3.8  |
| 2   | S0    | 155  | PHE  | 3.8  |
| 2   | s0    | 146  | LEU  | 3.8  |
| 58  | N2    | 89   | LEU  | 3.8  |
| 21  | C9    | 37   | VAL  | 3.8  |
| 36  | 1     | 1025 | A    | 3.8  |
| 1   | 2     | 830  | U    | 3.8  |
| 1   | 2     | 1686 | C    | 3.8  |
| 8   | S6    | 144  | PHE  | 3.8  |
| 8   | S6    | 154  | ARG  | 3.8  |
| 34  | SR    | 23   | LEU  | 3.8  |
| 65  | N9    | 57   | ALA  | 3.8  |
| 14  | c2    | 64   | SER  | 3.8  |
| 60  | N4    | 72   | SER  | 3.8  |
| 60  | N4    | 98   | PRO  | 3.8  |
| 1   | 6     | 75   | U    | 3.8  |
| 36  | 5     | 1580 | A    | 3.8  |
| 39  | l2    | 252  | THR  | 3.8  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 19         | c7           | 35         | CYS         | 3.8         |
| 73         | o7           | 86         | ALA         | 3.7         |
| 42         | l5           | 270        | LYS         | 3.7         |
| 1          | 2            | 656        | G           | 3.7         |
| 24         | D2           | 85         | ASP         | 3.7         |
| 36         | 1            | 3289       | G           | 3.7         |
| 18         | C6           | 96         | TYR         | 3.7         |
| 18         | c6           | 142        | TYR         | 3.7         |
| 2          | s0           | 6          | THR         | 3.7         |
| 1          | 6            | 718        | U           | 3.7         |
| 1          | 6            | 794        | U           | 3.7         |
| 9          | S7           | 109        | VAL         | 3.7         |
| 17         | c5           | 6          | ASN         | 3.7         |
| 36         | 5            | 491        | C           | 3.7         |
| 3          | S1           | 164        | ILE         | 3.7         |
| 10         | s8           | 176        | SER         | 3.7         |
| 33         | E1           | 103        | LEU         | 3.7         |
| 45         | l8           | 120        | LYS         | 3.7         |
| 19         | C7           | 126        | ALA         | 3.7         |
| 36         | 1            | 3286       | G           | 3.7         |
| 5          | s3           | 175        | VAL         | 3.7         |
| 66         | o0           | 67         | VAL         | 3.7         |
| 42         | L5           | 151        | GLN         | 3.7         |
| 7          | S5           | 102        | ARG         | 3.7         |
| 8          | S6           | 142        | ARG         | 3.7         |
| 1          | 2            | 718        | U           | 3.7         |
| 1          | 2            | 1694       | A           | 3.7         |
| 48         | m1           | 135        | GLY         | 3.7         |
| 74         | O8           | 49         | SER         | 3.7         |
| 6          | S4           | 60         | GLU         | 3.7         |
| 8          | S6           | 153        | VAL         | 3.7         |
| 24         | D2           | 74         | VAL         | 3.7         |
| 61         | n5           | 33         | ARG         | 3.7         |
| 34         | SR           | 115        | ILE         | 3.7         |
| 54         | m8           | 11         | LYS         | 3.7         |
| 34         | sR           | 26         | SER         | 3.7         |
| 36         | 1            | 1028       | U           | 3.7         |
| 20         | C8           | 83         | ALA         | 3.7         |
| 11         | s9           | 148        | VAL         | 3.7         |
| 36         | 1            | 1238       | C           | 3.7         |
| 11         | s9           | 139        | GLN         | 3.7         |
| 28         | d6           | 17         | HIS         | 3.7         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 16         | C4           | 137        | LEU         | 3.7         |
| 8          | S6           | 146        | GLY         | 3.7         |
| 12         | C0           | 89         | GLY         | 3.7         |
| 21         | c9           | 80         | TYR         | 3.6         |
| 36         | 5            | 1349       | G           | 3.6         |
| 60         | N4           | 67         | VAL         | 3.6         |
| 1          | 2            | 74         | U           | 3.6         |
| 1          | 2            | 75         | U           | 3.6         |
| 19         | c7           | 11         | ARG         | 3.6         |
| 46         | L9           | 168        | ARG         | 3.6         |
| 1          | 2            | 1600       | A           | 3.6         |
| 6          | S4           | 134        | LYS         | 3.6         |
| 27         | D5           | 97         | LYS         | 3.6         |
| 31         | d9           | 7          | TRP         | 3.6         |
| 3          | S1           | 156        | ALA         | 3.6         |
| 73         | O7           | 87         | SER         | 3.6         |
| 80         | c0           | 65         | TYR         | 3.6         |
| 4          | S2           | 158        | THR         | 3.6         |
| 34         | SR           | 161        | LYS         | 3.6         |
| 38         | 4            | 82         | U           | 3.6         |
| 3          | S1           | 142        | PHE         | 3.6         |
| 1          | 2            | 740        | A           | 3.6         |
| 10         | S8           | 22         | ARG         | 3.6         |
| 55         | M9           | 74         | ARG         | 3.6         |
| 34         | sR           | 27         | ALA         | 3.6         |
| 39         | l2           | 235        | ALA         | 3.6         |
| 8          | S6           | 73         | ILE         | 3.6         |
| 20         | C8           | 66         | LEU         | 3.6         |
| 20         | c8           | 18         | LEU         | 3.6         |
| 29         | d7           | 33         | LEU         | 3.6         |
| 33         | e1           | 79         | LYS         | 3.6         |
| 53         | M7           | 179        | GLN         | 3.6         |
| 33         | E1           | 145        | HIS         | 3.6         |
| 4          | s2           | 93         | GLY         | 3.6         |
| 7          | s5           | 101        | GLY         | 3.6         |
| 36         | 1            | 1351       | U           | 3.6         |
| 19         | c7           | 4          | VAL         | 3.6         |
| 22         | d0           | 64         | LYS         | 3.6         |
| 80         | c0           | 2          | LEU         | 3.6         |
| 19         | c7           | 96         | SER         | 3.6         |
| 8          | S6           | 78         | THR         | 3.6         |
| 12         | C0           | 67         | THR         | 3.6         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 9   | S7    | 108  | GLN  | 3.6  |
| 14  | C2    | 117  | GLY  | 3.6  |
| 45  | L8    | 52   | TRP  | 3.6  |
| 9   | S7    | 100  | PRO  | 3.6  |
| 10  | S8    | 13   | ALA  | 3.6  |
| 34  | sR    | 244  | ALA  | 3.6  |
| 21  | C9    | 84   | LYS  | 3.6  |
| 59  | N3    | 2    | SER  | 3.6  |
| 62  | n6    | 62   | SER  | 3.6  |
| 45  | l8    | 124  | ASP  | 3.6  |
| 6   | s4    | 25   | GLY  | 3.5  |
| 36  | 5     | 1582 | C    | 3.5  |
| 2   | s0    | 194  | PRO  | 3.5  |
| 14  | c2    | 126  | TRP  | 3.5  |
| 40  | L3    | 51   | ALA  | 3.5  |
| 53  | M7    | 160  | ALA  | 3.5  |
| 68  | O2    | 61   | LYS  | 3.5  |
| 31  | D9    | 30   | LEU  | 3.5  |
| 67  | O1    | 69   | TYR  | 3.5  |
| 36  | 1     | 1955 | U    | 3.5  |
| 36  | 5     | 1820 | U    | 3.5  |
| 3   | S1    | 144  | ARG  | 3.5  |
| 8   | S6    | 99   | GLY  | 3.5  |
| 39  | l2    | 2    | GLY  | 3.5  |
| 21  | c9    | 84   | LYS  | 3.5  |
| 2   | s0    | 207  | PRO  | 3.5  |
| 19  | c7    | 118  | PRO  | 3.5  |
| 3   | S1    | 207  | LEU  | 3.5  |
| 8   | S6    | 184  | LEU  | 3.5  |
| 1   | 2     | 1703 | C    | 3.5  |
| 19  | C7    | 122  | ILE  | 3.5  |
| 21  | C9    | 141  | GLU  | 3.5  |
| 36  | 1     | 1016 | C    | 3.5  |
| 11  | s9    | 8    | TYR  | 3.5  |
| 1   | 6     | 657  | U    | 3.5  |
| 4   | S2    | 87   | GLN  | 3.5  |
| 33  | e1    | 147  | VAL  | 3.5  |
| 2   | S0    | 18   | LEU  | 3.5  |
| 7   | S5    | 164  | PRO  | 3.5  |
| 45  | L8    | 46   | LEU  | 3.5  |
| 34  | sR    | 121  | MET  | 3.5  |
| 19  | c7    | 5    | ARG  | 3.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 55  | M9    | 72   | GLU  | 3.5  |
| 1   | 2     | 1707 | A    | 3.5  |
| 80  | c0    | 28   | ASN  | 3.5  |
| 1   | 2     | 1692 | G    | 3.5  |
| 8   | S6    | 171  | LYS  | 3.5  |
| 60  | n4    | 75   | THR  | 3.5  |
| 2   | s0    | 106  | SER  | 3.5  |
| 7   | S5    | 70   | VAL  | 3.5  |
| 32  | e0    | 62   | VAL  | 3.5  |
| 16  | C4    | 110  | LEU  | 3.5  |
| 19  | C7    | 103  | ASP  | 3.5  |
| 10  | S8    | 37   | LYS  | 3.5  |
| 2   | S0    | 158  | VAL  | 3.5  |
| 36  | 1     | 1350 | A    | 3.5  |
| 36  | 5     | 1350 | A    | 3.5  |
| 2   | s0    | 57   | LEU  | 3.5  |
| 73  | o7    | 87   | SER  | 3.5  |
| 1   | 2     | 1624 | C    | 3.5  |
| 11  | s9    | 45   | ILE  | 3.5  |
| 22  | d0    | 99   | ILE  | 3.5  |
| 1   | 2     | 846  | G    | 3.5  |
| 1   | 2     | 260  | U    | 3.5  |
| 1   | 6     | 232  | U    | 3.5  |
| 36  | 1     | 3287 | U    | 3.5  |
| 36  | 5     | 2506 | U    | 3.5  |
| 60  | N4    | 97   | LYS  | 3.4  |
| 3   | S1    | 46   | THR  | 3.4  |
| 18  | C6    | 11   | GLY  | 3.4  |
| 2   | S0    | 131  | GLN  | 3.4  |
| 18  | c6    | 3    | ALA  | 3.4  |
| 19  | C7    | 100  | LEU  | 3.4  |
| 19  | c7    | 113  | LEU  | 3.4  |
| 10  | S8    | 92   | ARG  | 3.4  |
| 14  | c2    | 71   | ILE  | 3.4  |
| 21  | C9    | 94   | ILE  | 3.4  |
| 23  | D1    | 23   | ILE  | 3.4  |
| 80  | c0    | 25   | LYS  | 3.4  |
| 4   | S2    | 208  | GLU  | 3.4  |
| 34  | sR    | 79   | TYR  | 3.4  |
| 1   | 6     | 1710 | U    | 3.4  |
| 19  | c7    | 121  | VAL  | 3.4  |
| 2   | S0    | 24   | LEU  | 3.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 19  | c7    | 16   | LEU  | 3.4  |
| 21  | C9    | 82   | GLY  | 3.4  |
| 28  | D6    | 16   | GLY  | 3.4  |
| 60  | n4    | 131  | ALA  | 3.4  |
| 9   | s7    | 8    | ILE  | 3.4  |
| 19  | C7    | 118  | PRO  | 3.4  |
| 4   | S2    | 164  | SER  | 3.4  |
| 45  | L8    | 213  | LYS  | 3.4  |
| 60  | N4    | 74   | LYS  | 3.4  |
| 21  | c9    | 44   | GLU  | 3.4  |
| 38  | 4     | 80   | A    | 3.4  |
| 66  | o0    | 59   | TYR  | 3.4  |
| 2   | S0    | 189  | VAL  | 3.4  |
| 34  | sR    | 157  | VAL  | 3.4  |
| 7   | s5    | 58   | LEU  | 3.4  |
| 39  | L2    | 12   | ALA  | 3.4  |
| 74  | o8    | 2    | ALA  | 3.4  |
| 26  | D4    | 34   | ASN  | 3.4  |
| 7   | S5    | 137  | ILE  | 3.4  |
| 36  | 1     | 1356 | U    | 3.4  |
| 14  | c2    | 124  | LYS  | 3.4  |
| 19  | c7    | 7    | LYS  | 3.4  |
| 1   | 2     | 1698 | G    | 3.4  |
| 36  | 1     | 3361 | G    | 3.4  |
| 2   | S0    | 203  | PHE  | 3.4  |
| 4   | S2    | 57   | PHE  | 3.4  |
| 8   | S6    | 89   | ASP  | 3.4  |
| 17  | c5    | 106  | GLU  | 3.4  |
| 14  | C2    | 45   | LEU  | 3.4  |
| 26  | d4    | 12   | VAL  | 3.4  |
| 55  | m9    | 22   | VAL  | 3.4  |
| 4   | s2    | 91   | ARG  | 3.4  |
| 7   | S5    | 152  | GLY  | 3.4  |
| 18  | c6    | 18   | ALA  | 3.4  |
| 33  | e1    | 152  | ALA  | 3.4  |
| 56  | n0    | 1    | MET  | 3.4  |
| 18  | C6    | 17   | THR  | 3.4  |
| 28  | d6    | 19   | LYS  | 3.4  |
| 66  | o0    | 36   | GLN  | 3.4  |
| 70  | O4    | 69   | HIS  | 3.4  |
| 17  | c5    | 109  | PRO  | 3.4  |
| 36  | 1     | 1581 | C    | 3.4  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 36         | 5            | 252        | U           | 3.4         |
| 42         | L5           | 55         | PHE         | 3.4         |
| 65         | n9           | 4          | SER         | 3.4         |
| 3          | s1           | 91         | VAL         | 3.4         |
| 8          | S6           | 36         | VAL         | 3.4         |
| 8          | S6           | 150        | GLU         | 3.4         |
| 23         | D1           | 10         | GLU         | 3.4         |
| 70         | O4           | 53         | GLY         | 3.4         |
| 70         | o4           | 28         | GLY         | 3.4         |
| 20         | C8           | 69         | ILE         | 3.4         |
| 4          | s2           | 166        | THR         | 3.4         |
| 1          | 6            | 217        | A           | 3.3         |
| 13         | c1           | 4          | GLU         | 3.3         |
| 18         | C6           | 75         | VAL         | 3.3         |
| 19         | C7           | 113        | LEU         | 3.3         |
| 36         | 5            | 1764       | U           | 3.3         |
| 71         | o5           | 102        | GLU         | 3.3         |
| 2          | S0           | 129        | ASP         | 3.3         |
| 8          | S6           | 138        | ALA         | 3.3         |
| 19         | C7           | 7          | LYS         | 3.3         |
| 60         | n4           | 77         | LYS         | 3.3         |
| 3          | S1           | 140        | ILE         | 3.3         |
| 51         | M5           | 142        | ILE         | 3.3         |
| 1          | 2            | 1288       | G           | 3.3         |
| 3          | S1           | 95         | ASN         | 3.3         |
| 11         | S9           | 3          | ARG         | 3.3         |
| 60         | N4           | 73         | ARG         | 3.3         |
| 5          | s3           | 176        | LEU         | 3.3         |
| 4          | s2           | 84         | LYS         | 3.3         |
| 16         | c4           | 125        | SER         | 3.3         |
| 36         | 1            | 1352       | A           | 3.3         |
| 20         | c8           | 146        | ALA         | 3.3         |
| 65         | n9           | 27         | TYR         | 3.3         |
| 36         | 5            | 1567       | U           | 3.3         |
| 8          | S6           | 183        | ARG         | 3.3         |
| 19         | c7           | 26         | LEU         | 3.3         |
| 20         | C8           | 44         | ASN         | 3.3         |
| 34         | sR           | 294        | TRP         | 3.3         |
| 60         | n4           | 76         | VAL         | 3.3         |
| 8          | S6           | 223        | LYS         | 3.3         |
| 1          | 6            | 655        | G           | 3.3         |
| 1          | 6            | 677        | G           | 3.3         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | S0    | 144  | ILE  | 3.3  |
| 3   | S1    | 161  | ILE  | 3.3  |
| 6   | S4    | 203  | GLY  | 3.3  |
| 20  | C8    | 35   | ILE  | 3.3  |
| 36  | 5     | 1560 | G    | 3.3  |
| 36  | 5     | 3276 | G    | 3.3  |
| 65  | n9    | 2    | ALA  | 3.3  |
| 1   | 2     | 1346 | A    | 3.3  |
| 36  | 1     | 3375 | A    | 3.3  |
| 4   | S2    | 91   | ARG  | 3.3  |
| 31  | D9    | 20   | GLN  | 3.3  |
| 51  | m5    | 193  | ARG  | 3.3  |
| 1   | 2     | 1711 | C    | 3.3  |
| 8   | S6    | 156  | PHE  | 3.3  |
| 3   | S1    | 91   | VAL  | 3.3  |
| 21  | C9    | 6    | VAL  | 3.3  |
| 28  | D6    | 3    | LYS  | 3.3  |
| 30  | D8    | 15   | VAL  | 3.3  |
| 47  | M0    | 203  | LYS  | 3.3  |
| 45  | L8    | 114  | ALA  | 3.3  |
| 58  | N2    | 93   | ILE  | 3.3  |
| 70  | o4    | 29   | ILE  | 3.3  |
| 21  | C9    | 72   | GLY  | 3.3  |
| 24  | D2    | 73   | GLY  | 3.3  |
| 25  | D3    | 2    | GLY  | 3.3  |
| 35  | SM    | 67   | GLY  | 3.3  |
| 19  | c7    | 120  | SER  | 3.3  |
| 45  | l8    | 253  | SER  | 3.3  |
| 53  | M7    | 142  | SER  | 3.3  |
| 36  | 1     | 1261 | G    | 3.3  |
| 25  | D3    | 124  | VAL  | 3.3  |
| 33  | E1    | 97   | LYS  | 3.3  |
| 33  | e1    | 98   | VAL  | 3.3  |
| 15  | C3    | 14   | SER  | 3.2  |
| 8   | S6    | 109  | LEU  | 3.2  |
| 17  | C5    | 72   | LYS  | 3.2  |
| 77  | Q1    | 16   | LYS  | 3.2  |
| 2   | S0    | 143  | VAL  | 3.2  |
| 11  | S9    | 101  | VAL  | 3.2  |
| 28  | d6    | 86   | VAL  | 3.2  |
| 31  | d9    | 23   | VAL  | 3.2  |
| 8   | S6    | 226  | ILE  | 3.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 13  | c1    | 144  | ALA  | 3.2  |
| 65  | N9    | 55   | ALA  | 3.2  |
| 1   | 2     | 193  | U    | 3.2  |
| 7   | s5    | 152  | GLY  | 3.2  |
| 36  | 1     | 2714 | G    | 3.2  |
| 36  | 5     | 442  | G    | 3.2  |
| 2   | S0    | 152  | PRO  | 3.2  |
| 6   | S4    | 133  | LYS  | 3.2  |
| 8   | S6    | 148  | SER  | 3.2  |
| 29  | D7    | 41   | LEU  | 3.2  |
| 35  | SM    | 84   | LYS  | 3.2  |
| 36  | 1     | 2539 | C    | 3.2  |
| 18  | c6    | 126  | PRO  | 3.2  |
| 17  | c5    | 5    | VAL  | 3.2  |
| 28  | D6    | 86   | VAL  | 3.2  |
| 2   | S0    | 98   | ILE  | 3.2  |
| 7   | s5    | 74   | ALA  | 3.2  |
| 53  | M7    | 161  | ALA  | 3.2  |
| 19  | C7    | 101  | ASN  | 3.2  |
| 55  | M9    | 85   | ARG  | 3.2  |
| 33  | e1    | 85   | TYR  | 3.2  |
| 42  | L5    | 150  | LEU  | 3.2  |
| 53  | M7    | 164  | LYS  | 3.2  |
| 70  | O4    | 21   | LYS  | 3.2  |
| 36  | 1     | 2771 | U    | 3.2  |
| 8   | S6    | 181  | PRO  | 3.2  |
| 17  | c5    | 125  | PRO  | 3.2  |
| 1   | 2     | 228  | G    | 3.2  |
| 1   | 2     | 488  | G    | 3.2  |
| 2   | S0    | 139  | VAL  | 3.2  |
| 19  | c7    | 66   | VAL  | 3.2  |
| 19  | c7    | 89   | SER  | 3.2  |
| 21  | C9    | 88   | VAL  | 3.2  |
| 33  | e1    | 146  | SER  | 3.2  |
| 33  | e1    | 150  | VAL  | 3.2  |
| 36  | 1     | 3288 | G    | 3.2  |
| 36  | 5     | 1261 | G    | 3.2  |
| 61  | N5    | 26   | VAL  | 3.2  |
| 70  | O4    | 65   | VAL  | 3.2  |
| 1   | 6     | 1711 | C    | 3.2  |
| 60  | n4    | 78   | ALA  | 3.2  |
| 2   | s0    | 54   | TRP  | 3.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 34  | sR    | 28   | GLY  | 3.2  |
| 34  | sR    | 92   | TRP  | 3.2  |
| 8   | S6    | 136  | LYS  | 3.2  |
| 33  | e1    | 90   | LYS  | 3.2  |
| 18  | c6    | 89   | LEU  | 3.2  |
| 40  | l3    | 178  | LEU  | 3.2  |
| 11  | s9    | 67   | PRO  | 3.2  |
| 16  | C4    | 125  | SER  | 3.2  |
| 2   | S0    | 113  | ARG  | 3.2  |
| 18  | c6    | 118  | ILE  | 3.2  |
| 22  | d0    | 70   | THR  | 3.2  |
| 40  | l3    | 77   | THR  | 3.2  |
| 28  | D6    | 6    | ALA  | 3.2  |
| 47  | m0    | 195  | ALA  | 3.2  |
| 1   | 2     | 1011 | G    | 3.2  |
| 36  | 1     | 1525 | G    | 3.2  |
| 2   | s0    | 24   | LEU  | 3.2  |
| 8   | S6    | 147  | LEU  | 3.2  |
| 9   | S7    | 41   | LEU  | 3.2  |
| 34  | SR    | 91   | LEU  | 3.2  |
| 8   | S6    | 145  | PHE  | 3.2  |
| 58  | N2    | 108  | TYR  | 3.2  |
| 18  | c6    | 5    | PRO  | 3.2  |
| 33  | E1    | 88   | PRO  | 3.2  |
| 10  | S8    | 148  | ALA  | 3.2  |
| 17  | C5    | 39   | ALA  | 3.2  |
| 7   | s5    | 80   | LYS  | 3.1  |
| 8   | S6    | 174  | LYS  | 3.1  |
| 36  | 1     | 1815 | U    | 3.1  |
| 10  | s8    | 177  | GLY  | 3.1  |
| 13  | c1    | 147  | GLY  | 3.1  |
| 29  | D7    | 33   | LEU  | 3.1  |
| 33  | e1    | 103  | LEU  | 3.1  |
| 8   | S6    | 50   | PHE  | 3.1  |
| 45  | l8    | 252  | ASN  | 3.1  |
| 2   | S0    | 161  | PRO  | 3.1  |
| 17  | C5    | 53   | PRO  | 3.1  |
| 45  | L8    | 127  | PRO  | 3.1  |
| 1   | 2     | 490  | C    | 3.1  |
| 1   | 2     | 697  | C    | 3.1  |
| 1   | 2     | 1705 | C    | 3.1  |
| 36  | 5     | 1192 | C    | 3.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 15  | C3    | 62   | GLN  | 3.1  |
| 18  | C6    | 12   | LYS  | 3.1  |
| 21  | C9    | 50   | ALA  | 3.1  |
| 41  | L4    | 185  | LYS  | 3.1  |
| 34  | SR    | 96   | THR  | 3.1  |
| 8   | S6    | 77   | LEU  | 3.1  |
| 14  | C2    | 62   | LEU  | 3.1  |
| 34  | sR    | 141  | LEU  | 3.1  |
| 60  | N4    | 4    | GLU  | 3.1  |
| 80  | c0    | 84   | GLU  | 3.1  |
| 36  | 1     | 3275 | U    | 3.1  |
| 11  | s9    | 127  | VAL  | 3.1  |
| 14  | C2    | 115  | VAL  | 3.1  |
| 14  | c2    | 120  | VAL  | 3.1  |
| 27  | d5    | 62   | VAL  | 3.1  |
| 63  | n7    | 13   | VAL  | 3.1  |
| 2   | S0    | 28   | ASN  | 3.1  |
| 1   | 6     | 225  | A    | 3.1  |
| 7   | S5    | 54   | LYS  | 3.1  |
| 3   | S1    | 60   | ALA  | 3.1  |
| 39  | l2    | 250  | GLN  | 3.1  |
| 1   | 2     | 700  | C    | 3.1  |
| 35  | SM    | 87   | THR  | 3.1  |
| 36  | 5     | 1562 | C    | 3.1  |
| 36  | 5     | 2507 | C    | 3.1  |
| 71  | O5    | 101  | THR  | 3.1  |
| 39  | L2    | 228  | GLY  | 3.1  |
| 53  | m7    | 66   | SER  | 3.1  |
| 19  | c7    | 9    | VAL  | 3.1  |
| 24  | D2    | 33   | VAL  | 3.1  |
| 74  | o8    | 11   | PHE  | 3.1  |
| 1   | 2     | 493  | U    | 3.1  |
| 1   | 6     | 1370 | U    | 3.1  |
| 52  | M6    | 42   | ASN  | 3.1  |
| 67  | O1    | 102  | LYS  | 3.1  |
| 41  | l4    | 187  | LEU  | 3.1  |
| 36  | 1     | 1879 | A    | 3.1  |
| 43  | l6    | 67   | GLY  | 3.1  |
| 28  | D6    | 29   | SER  | 3.1  |
| 1   | 6     | 1447 | C    | 3.1  |
| 16  | C4    | 13   | VAL  | 3.1  |
| 17  | c5    | 126  | VAL  | 3.1  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 19         | c7           | 102        | VAL         | 3.1         |
| 63         | n7           | 74         | VAL         | 3.1         |
| 39         | L2           | 251        | LYS         | 3.1         |
| 1          | 2            | 234        | G           | 3.1         |
| 3          | S1           | 32         | ILE         | 3.1         |
| 6          | S4           | 57         | ASN         | 3.1         |
| 22         | D0           | 121        | ASN         | 3.1         |
| 9          | S7           | 12         | ALA         | 3.1         |
| 19         | c7           | 56         | HIS         | 3.1         |
| 19         | c7           | 90         | ALA         | 3.1         |
| 32         | E0           | 2          | ALA         | 3.1         |
| 19         | C7           | 24         | LEU         | 3.1         |
| 6          | S4           | 4          | GLY         | 3.1         |
| 31         | d9           | 43         | PHE         | 3.1         |
| 1          | 2            | 140        | A           | 3.1         |
| 1          | 2            | 992        | A           | 3.1         |
| 36         | 5            | 2971       | A           | 3.1         |
| 51         | m5           | 204        | LYS         | 3.1         |
| 58         | N2           | 77         | LYS         | 3.1         |
| 60         | n4           | 74         | LYS         | 3.1         |
| 4          | s2           | 85         | PRO         | 3.1         |
| 6          | S4           | 162        | ILE         | 3.1         |
| 11         | S9           | 2          | PRO         | 3.1         |
| 80         | c0           | 1          | MET         | 3.1         |
| 21         | C9           | 66         | TYR         | 3.1         |
| 55         | M9           | 78         | TYR         | 3.1         |
| 36         | 1            | 3360       | C           | 3.0         |
| 11         | s9           | 142        | ASN         | 3.0         |
| 41         | l4           | 101        | ALA         | 3.0         |
| 60         | n4           | 128        | ALA         | 3.0         |
| 68         | O2           | 127        | ALA         | 3.0         |
| 36         | 1            | 566        | G           | 3.0         |
| 42         | l5           | 56         | THR         | 3.0         |
| 1          | 6            | 1390       | U           | 3.0         |
| 36         | 5            | 1569       | U           | 3.0         |
| 13         | c1           | 43         | LYS         | 3.0         |
| 60         | n4           | 72         | SER         | 3.0         |
| 18         | c6           | 36         | ILE         | 3.0         |
| 21         | C9           | 31         | PRO         | 3.0         |
| 34         | SR           | 206        | PRO         | 3.0         |
| 24         | d2           | 9          | ASP         | 3.0         |
| 6          | S4           | 54         | TYR         | 3.0         |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 11  | s9    | 76  | LEU  | 3.0  |
| 34  | SR    | 32  | LEU  | 3.0  |
| 50  | M4    | 135 | LEU  | 3.0  |
| 4   | s2    | 87  | GLN  | 3.0  |
| 11  | S9    | 6   | ARG  | 3.0  |
| 18  | C6    | 70  | THR  | 3.0  |
| 34  | SR    | 72  | THR  | 3.0  |
| 34  | SR    | 156 | VAL  | 3.0  |
| 40  | L3    | 104 | THR  | 3.0  |
| 41  | l4    | 103 | THR  | 3.0  |
| 58  | n2    | 100 | THR  | 3.0  |
| 77  | q1    | 19  | LYS  | 3.0  |
| 82  | p0    | 105 | VAL  | 3.0  |
| 11  | s9    | 146 | PHE  | 3.0  |
| 25  | D3    | 107 | PHE  | 3.0  |
| 3   | S1    | 90  | GLU  | 3.0  |
| 29  | D7    | 75  | GLU  | 3.0  |
| 40  | L3    | 277 | SER  | 3.0  |
| 5   | s3    | 110 | LEU  | 3.0  |
| 8   | S6    | 75  | LEU  | 3.0  |
| 10  | S8    | 96  | LEU  | 3.0  |
| 19  | c7    | 103 | ASP  | 3.0  |
| 22  | D0    | 93  | LEU  | 3.0  |
| 48  | M1    | 167 | TYR  | 3.0  |
| 49  | M3    | 132 | ALA  | 3.0  |
| 5   | s3    | 178 | ARG  | 3.0  |
| 78  | q2    | 17  | CYS  | 3.0  |
| 16  | C4    | 75  | GLY  | 3.0  |
| 25  | D3    | 3   | LYS  | 3.0  |
| 42  | l5    | 57  | ASN  | 3.0  |
| 60  | n4    | 70  | LYS  | 3.0  |
| 62  | n6    | 26  | GLN  | 3.0  |
| 72  | O6    | 29  | LYS  | 3.0  |
| 72  | o6    | 25  | LYS  | 3.0  |
| 2   | S0    | 121 | VAL  | 3.0  |
| 5   | s3    | 41  | VAL  | 3.0  |
| 14  | c2    | 37  | VAL  | 3.0  |
| 4   | s2    | 90  | THR  | 3.0  |
| 13  | C1    | 3   | THR  | 3.0  |
| 42  | l5    | 55  | PHE  | 3.0  |
| 80  | c0    | 59  | PHE  | 3.0  |
| 60  | N4    | 92  | GLU  | 3.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 19  | C7    | 107  | SER  | 3.0  |
| 2   | s0    | 110  | TYR  | 3.0  |
| 9   | s7    | 97   | ARG  | 3.0  |
| 19  | C7    | 3    | ARG  | 3.0  |
| 34  | SR    | 114  | ASP  | 3.0  |
| 36  | 5     | 3275 | U    | 3.0  |
| 3   | S1    | 151  | LYS  | 3.0  |
| 14  | C2    | 50   | LYS  | 3.0  |
| 19  | C7    | 116  | LYS  | 3.0  |
| 28  | D6    | 13   | LYS  | 3.0  |
| 33  | e1    | 96   | LYS  | 3.0  |
| 2   | s0    | 82   | GLY  | 3.0  |
| 22  | D0    | 118  | VAL  | 3.0  |
| 70  | O4    | 7    | PHE  | 3.0  |
| 31  | D9    | 28   | THR  | 3.0  |
| 32  | E0    | 48   | THR  | 3.0  |
| 9   | s7    | 98   | ILE  | 3.0  |
| 30  | d8    | 13   | ILE  | 3.0  |
| 34  | SR    | 122  | ILE  | 3.0  |
| 32  | E0    | 49   | LEU  | 3.0  |
| 45  | L8    | 109  | LEU  | 3.0  |
| 56  | N0    | 128  | GLU  | 3.0  |
| 1   | 2     | 1217 | A    | 3.0  |
| 24  | d2    | 117  | ARG  | 3.0  |
| 7   | S5    | 96   | SER  | 3.0  |
| 22  | d0    | 66   | SER  | 3.0  |
| 33  | e1    | 101  | ALA  | 3.0  |
| 47  | M0    | 221  | ALA  | 3.0  |
| 52  | m6    | 180  | SER  | 3.0  |
| 60  | n4    | 50   | ALA  | 3.0  |
| 34  | SR    | 62   | LYS  | 3.0  |
| 37  | 7     | 73   | C    | 3.0  |
| 2   | s0    | 46   | HIS  | 3.0  |
| 1   | 2     | 1414 | U    | 3.0  |
| 36  | 1     | 1095 | U    | 3.0  |
| 38  | 4     | 81   | U    | 3.0  |
| 26  | D4    | 96   | LEU  | 2.9  |
| 33  | e1    | 100  | LEU  | 2.9  |
| 18  | C6    | 125  | GLU  | 2.9  |
| 60  | N4    | 71   | ARG  | 2.9  |
| 1   | 2     | 1690 | G    | 2.9  |
| 8   | S6    | 40   | ALA  | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 32  | e0    | 2    | ALA  | 2.9  |
| 34  | SR    | 162  | ALA  | 2.9  |
| 18  | c6    | 121  | SER  | 2.9  |
| 70  | O4    | 55   | SER  | 2.9  |
| 36  | 1     | 1274 | A    | 2.9  |
| 8   | S6    | 67   | VAL  | 2.9  |
| 16  | c4    | 74   | VAL  | 2.9  |
| 82  | p0    | 184  | GLY  | 2.9  |
| 70  | o4    | 61   | GLN  | 2.9  |
| 12  | C0    | 1    | MET  | 2.9  |
| 48  | m1    | 65   | ILE  | 2.9  |
| 6   | S4    | 26   | CYS  | 2.9  |
| 1   | 2     | 649  | U    | 2.9  |
| 9   | S7    | 99   | LEU  | 2.9  |
| 14  | c2    | 34   | THR  | 2.9  |
| 17  | C5    | 78   | THR  | 2.9  |
| 19  | c7    | 95   | ARG  | 2.9  |
| 36  | 5     | 249  | U    | 2.9  |
| 36  | 5     | 1763 | U    | 2.9  |
| 54  | M8    | 124  | LEU  | 2.9  |
| 58  | N2    | 94   | ARG  | 2.9  |
| 58  | n2    | 98   | THR  | 2.9  |
| 3   | S1    | 198  | GLU  | 2.9  |
| 3   | S1    | 206  | PRO  | 2.9  |
| 4   | S2    | 144  | TRP  | 2.9  |
| 5   | S3    | 141  | LYS  | 2.9  |
| 11  | S9    | 182  | GLU  | 2.9  |
| 13  | c1    | 69   | LYS  | 2.9  |
| 24  | d2    | 119  | LYS  | 2.9  |
| 28  | d6    | 4    | LYS  | 2.9  |
| 45  | l8    | 52   | TRP  | 2.9  |
| 72  | o6    | 29   | LYS  | 2.9  |
| 45  | L8    | 141  | ALA  | 2.9  |
| 3   | S1    | 155  | TYR  | 2.9  |
| 3   | S1    | 43   | VAL  | 2.9  |
| 21  | C9    | 117  | SER  | 2.9  |
| 35  | SM    | 85   | SER  | 2.9  |
| 57  | N1    | 126  | VAL  | 2.9  |
| 16  | C4    | 29   | HIS  | 2.9  |
| 3   | S1    | 157  | GLN  | 2.9  |
| 19  | C7    | 42   | GLN  | 2.9  |
| 40  | L3    | 317  | ILE  | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 60  | N4    | 32   | GLN  | 2.9  |
| 1   | 2     | 1712 | A    | 2.9  |
| 74  | o8    | 69   | LEU  | 2.9  |
| 2   | S0    | 56   | LYS  | 2.9  |
| 18  | c6    | 140  | LYS  | 2.9  |
| 25  | D3    | 10   | ASN  | 2.9  |
| 68  | o2    | 16   | LYS  | 2.9  |
| 1   | 6     | 1284 | C    | 2.9  |
| 2   | S0    | 65   | ALA  | 2.9  |
| 3   | S1    | 28   | GLU  | 2.9  |
| 36  | 1     | 1280 | C    | 2.9  |
| 36  | 5     | 1016 | C    | 2.9  |
| 36  | 1     | 981  | U    | 2.9  |
| 36  | 5     | 250  | U    | 2.9  |
| 12  | C0    | 64   | TYR  | 2.9  |
| 18  | c6    | 90   | VAL  | 2.9  |
| 71  | O5    | 100  | VAL  | 2.9  |
| 80  | c0    | 79   | TYR  | 2.9  |
| 3   | S1    | 93   | GLY  | 2.9  |
| 13  | C1    | 2    | SER  | 2.9  |
| 19  | C7    | 70   | SER  | 2.9  |
| 33  | E1    | 95   | HIS  | 2.9  |
| 34  | SR    | 61   | PHE  | 2.9  |
| 73  | o7    | 57   | HIS  | 2.9  |
| 22  | D0    | 20   | ILE  | 2.9  |
| 34  | SR    | 43   | ILE  | 2.9  |
| 2   | S0    | 182  | LEU  | 2.9  |
| 14  | C2    | 28   | LEU  | 2.9  |
| 34  | sR    | 202  | LEU  | 2.9  |
| 35  | SM    | 88   | ARG  | 2.9  |
| 43  | L6    | 154  | LEU  | 2.9  |
| 71  | o5    | 105  | ARG  | 2.9  |
| 15  | C3    | 109  | LYS  | 2.9  |
| 18  | C6    | 140  | LYS  | 2.9  |
| 31  | d9    | 54   | LYS  | 2.9  |
| 34  | sR    | 118  | LYS  | 2.9  |
| 11  | S9    | 61   | THR  | 2.9  |
| 22  | D0    | 67   | THR  | 2.9  |
| 27  | d5    | 99   | ALA  | 2.9  |
| 30  | D8    | 43   | ASN  | 2.9  |
| 51  | m5    | 85   | THR  | 2.9  |
| 11  | s9    | 2    | PRO  | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 18  | C6    | 5    | PRO  | 2.9  |
| 18  | C6    | 124  | PRO  | 2.9  |
| 74  | O8    | 28   | ASN  | 2.9  |
| 1   | 2     | 829  | A    | 2.9  |
| 77  | Q1    | 5    | TRP  | 2.9  |
| 2   | S0    | 204  | TYR  | 2.9  |
| 16  | c4    | 98   | GLY  | 2.9  |
| 31  | D9    | 29   | GLY  | 2.9  |
| 36  | 1     | 1820 | U    | 2.9  |
| 51  | m5    | 69   | GLY  | 2.9  |
| 24  | D2    | 3    | ARG  | 2.9  |
| 11  | S9    | 60   | LEU  | 2.9  |
| 14  | c2    | 29   | LYS  | 2.9  |
| 20  | c8    | 3    | LEU  | 2.9  |
| 26  | D4    | 118  | ILE  | 2.9  |
| 34  | SR    | 169  | ILE  | 2.9  |
| 42  | L5    | 27   | LYS  | 2.9  |
| 62  | n6    | 126  | LEU  | 2.9  |
| 26  | D4    | 107  | GLN  | 2.9  |
| 80  | c0    | 47   | GLN  | 2.9  |
| 2   | s0    | 206  | ASP  | 2.9  |
| 11  | s9    | 4    | ALA  | 2.9  |
| 18  | C6    | 3    | ALA  | 2.9  |
| 21  | C9    | 10   | ALA  | 2.9  |
| 21  | C9    | 39   | THR  | 2.9  |
| 22  | D0    | 60   | THR  | 2.9  |
| 34  | sR    | 30   | PRO  | 2.9  |
| 68  | O2    | 2    | ALA  | 2.9  |
| 54  | m8    | 145  | ASN  | 2.9  |
| 2   | S0    | 195  | TRP  | 2.9  |
| 9   | s7    | 90   | VAL  | 2.9  |
| 48  | M1    | 148  | VAL  | 2.9  |
| 8   | s6    | 50   | PHE  | 2.9  |
| 15  | c3    | 90   | TYR  | 2.9  |
| 19  | C7    | 11   | ARG  | 2.9  |
| 26  | D4    | 67   | GLY  | 2.9  |
| 33  | e1    | 106  | TYR  | 2.9  |
| 21  | C9    | 45   | MET  | 2.9  |
| 33  | E1    | 117  | LEU  | 2.9  |
| 33  | e1    | 82   | LYS  | 2.9  |
| 33  | e1    | 97   | LYS  | 2.9  |
| 34  | sR    | 67   | ILE  | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 35  | sM    | 84   | LYS  | 2.9  |
| 40  | l3    | 335  | ILE  | 2.9  |
| 46  | l9    | 118  | LEU  | 2.9  |
| 1   | 2     | 1688 | U    | 2.8  |
| 14  | C2    | 141  | SER  | 2.8  |
| 1   | 6     | 659  | C    | 2.8  |
| 34  | sR    | 69   | GLN  | 2.8  |
| 36  | 1     | 1574 | C    | 2.8  |
| 64  | N8    | 65   | GLN  | 2.8  |
| 15  | C3    | 110  | ASP  | 2.8  |
| 26  | D4    | 135  | ASP  | 2.8  |
| 9   | S7    | 4    | PRO  | 2.8  |
| 20  | c8    | 138  | THR  | 2.8  |
| 20  | c8    | 141  | THR  | 2.8  |
| 60  | n4    | 83   | THR  | 2.8  |
| 8   | S6    | 139  | ASN  | 2.8  |
| 19  | C7    | 121  | VAL  | 2.8  |
| 31  | D9    | 6    | VAL  | 2.8  |
| 67  | O1    | 23   | VAL  | 2.8  |
| 16  | C4    | 136  | ARG  | 2.8  |
| 49  | M3    | 174  | ARG  | 2.8  |
| 55  | M9    | 170  | ARG  | 2.8  |
| 8   | S6    | 149  | LYS  | 2.8  |
| 16  | C4    | 129  | LYS  | 2.8  |
| 20  | C8    | 142  | GLY  | 2.8  |
| 60  | N4    | 29   | PHE  | 2.8  |
| 77  | q1    | 25   | LYS  | 2.8  |
| 2   | s0    | 122  | ILE  | 2.8  |
| 3   | S1    | 120  | LEU  | 2.8  |
| 6   | S4    | 261  | LEU  | 2.8  |
| 1   | 2     | 492  | A    | 2.8  |
| 14  | c2    | 119  | SER  | 2.8  |
| 2   | s0    | 187  | ALA  | 2.8  |
| 11  | S9    | 4    | ALA  | 2.8  |
| 1   | 6     | 240  | U    | 2.8  |
| 1   | 6     | 320  | U    | 2.8  |
| 27  | d5    | 55   | PRO  | 2.8  |
| 34  | sR    | 206  | PRO  | 2.8  |
| 22  | D0    | 92   | ASP  | 2.8  |
| 1   | 6     | 1156 | C    | 2.8  |
| 2   | S0    | 101  | ARG  | 2.8  |
| 8   | S6    | 41   | VAL  | 2.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 14  | c2    | 31   | VAL  | 2.8  |
| 31  | D9    | 23   | VAL  | 2.8  |
| 36  | 1     | 1192 | C    | 2.8  |
| 40  | l3    | 146  | ARG  | 2.8  |
| 60  | n4    | 47   | ARG  | 2.8  |
| 62  | n6    | 127  | GLU  | 2.8  |
| 10  | s8    | 17   | LYS  | 2.8  |
| 22  | d0    | 121  | ASN  | 2.8  |
| 16  | C4    | 130  | GLY  | 2.8  |
| 18  | C6    | 129  | PHE  | 2.8  |
| 59  | N3    | 5    | GLY  | 2.8  |
| 80  | c0    | 76   | LEU  | 2.8  |
| 34  | sR    | 250  | TYR  | 2.8  |
| 78  | Q2    | 11   | TYR  | 2.8  |
| 29  | D7    | 19   | HIS  | 2.8  |
| 68  | O2    | 26   | HIS  | 2.8  |
| 55  | M9    | 92   | GLN  | 2.8  |
| 2   | S0    | 137  | SER  | 2.8  |
| 18  | C6    | 134  | ALA  | 2.8  |
| 45  | L8    | 126  | SER  | 2.8  |
| 60  | N4    | 50   | ALA  | 2.8  |
| 3   | S1    | 66   | VAL  | 2.8  |
| 4   | s2    | 96   | THR  | 2.8  |
| 16  | C4    | 48   | VAL  | 2.8  |
| 7   | S5    | 181  | GLU  | 2.8  |
| 18  | c6    | 17   | THR  | 2.8  |
| 22  | D0    | 31   | VAL  | 2.8  |
| 34  | SR    | 94   | VAL  | 2.8  |
| 39  | L2    | 230  | VAL  | 2.8  |
| 35  | sM    | 49   | LYS  | 2.8  |
| 51  | m5    | 176  | LYS  | 2.8  |
| 63  | n7    | 21   | LYS  | 2.8  |
| 36  | 1     | 3163 | A    | 2.8  |
| 36  | 5     | 1566 | A    | 2.8  |
| 10  | s8    | 67   | TRP  | 2.8  |
| 1   | 2     | 141  | U    | 2.8  |
| 1   | 2     | 170  | U    | 2.8  |
| 1   | 2     | 494  | U    | 2.8  |
| 14  | C2    | 32   | LEU  | 2.8  |
| 14  | c2    | 100  | TRP  | 2.8  |
| 39  | l2    | 186  | PHE  | 2.8  |
| 40  | L3    | 47   | LEU  | 2.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 19  | c7    | 97   | ASN  | 2.8  |
| 19  | c7    | 98   | GLY  | 2.8  |
| 51  | M5    | 177  | GLY  | 2.8  |
| 57  | n1    | 2    | GLY  | 2.8  |
| 1   | 2     | 696  | C    | 2.8  |
| 1   | 2     | 716  | C    | 2.8  |
| 1   | 2     | 913  | G    | 2.8  |
| 1   | 6     | 239  | C    | 2.8  |
| 45  | L8    | 49   | TYR  | 2.8  |
| 33  | E1    | 152  | ALA  | 2.8  |
| 47  | M0    | 112  | GLN  | 2.8  |
| 57  | N1    | 121  | ALA  | 2.8  |
| 62  | N6    | 26   | GLN  | 2.8  |
| 70  | O4    | 32   | ALA  | 2.8  |
| 9   | s7    | 4    | PRO  | 2.8  |
| 9   | s7    | 20   | VAL  | 2.8  |
| 11  | S9    | 180  | LYS  | 2.8  |
| 60  | n4    | 115  | LYS  | 2.8  |
| 63  | n7    | 75   | VAL  | 2.8  |
| 70  | o4    | 79   | SER  | 2.8  |
| 2   | s0    | 192  | THR  | 2.8  |
| 8   | S6    | 71   | THR  | 2.8  |
| 8   | S6    | 212  | LEU  | 2.8  |
| 13  | c1    | 3    | THR  | 2.8  |
| 62  | N6    | 127  | GLU  | 2.8  |
| 71  | O5    | 102  | GLU  | 2.8  |
| 8   | S6    | 28   | PHE  | 2.8  |
| 18  | c6    | 138  | PHE  | 2.8  |
| 41  | L4    | 106  | TRP  | 2.8  |
| 80  | c0    | 26   | ASP  | 2.8  |
| 3   | S1    | 44   | GLY  | 2.8  |
| 6   | S4    | 74   | GLY  | 2.8  |
| 28  | D6    | 11   | ASN  | 2.8  |
| 52  | m6    | 182  | ASN  | 2.8  |
| 1   | 2     | 106  | U    | 2.8  |
| 1   | 2     | 1314 | U    | 2.8  |
| 1   | 6     | 226  | A    | 2.8  |
| 1   | 6     | 1600 | A    | 2.8  |
| 1   | 2     | 491  | C    | 2.8  |
| 23  | d1    | 33   | GLN  | 2.8  |
| 36  | 1     | 2507 | C    | 2.8  |
| 1   | 6     | 214  | G    | 2.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | 6     | 1267 | G    | 2.8  |
| 33  | E1    | 102  | VAL  | 2.8  |
| 36  | 5     | 244  | G    | 2.8  |
| 36  | 5     | 2503 | G    | 2.8  |
| 9   | s7    | 2    | SER  | 2.8  |
| 7   | s5    | 184  | PHE  | 2.7  |
| 16  | C4    | 83   | ILE  | 2.8  |
| 20  | c8    | 85   | PHE  | 2.7  |
| 2   | s0    | 190  | ASP  | 2.7  |
| 45  | l8    | 227  | ASP  | 2.7  |
| 57  | n1    | 6    | GLY  | 2.7  |
| 59  | N3    | 3    | GLY  | 2.7  |
| 67  | o1    | 22   | GLY  | 2.7  |
| 18  | C6    | 92   | TYR  | 2.7  |
| 17  | C5    | 79   | HIS  | 2.7  |
| 13  | c1    | 146  | ALA  | 2.7  |
| 33  | e1    | 99   | LYS  | 2.7  |
| 47  | m0    | 219  | ALA  | 2.7  |
| 1   | 2     | 828  | U    | 2.7  |
| 1   | 2     | 1691 | A    | 2.7  |
| 1   | 6     | 675  | U    | 2.7  |
| 11  | S9    | 136  | VAL  | 2.7  |
| 19  | C7    | 105  | GLN  | 2.7  |
| 21  | C9    | 70   | GLN  | 2.7  |
| 71  | o5    | 104  | GLN  | 2.7  |
| 11  | s9    | 93   | LEU  | 2.7  |
| 19  | C7    | 46   | LEU  | 2.7  |
| 19  | c7    | 24   | LEU  | 2.7  |
| 33  | e1    | 117  | LEU  | 2.7  |
| 2   | S0    | 128  | SER  | 2.7  |
| 27  | D5    | 93   | SER  | 2.7  |
| 33  | e1    | 91   | ILE  | 2.7  |
| 34  | sR    | 44   | SER  | 2.7  |
| 36  | 5     | 1238 | C    | 2.7  |
| 36  | 5     | 1579 | C    | 2.7  |
| 72  | O6    | 79   | SER  | 2.7  |
| 17  | c5    | 135  | THR  | 2.7  |
| 2   | S0    | 174  | TRP  | 2.7  |
| 14  | C2    | 100  | TRP  | 2.7  |
| 21  | C9    | 87   | GLY  | 2.7  |
| 1   | 2     | 723  | G    | 2.7  |
| 1   | 2     | 1241 | G    | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 33  | E1    | 137  | ASP  | 2.7  |
| 36  | 5     | 2549 | G    | 2.7  |
| 48  | M1    | 126  | ASP  | 2.7  |
| 2   | s0    | 127  | ARG  | 2.7  |
| 35  | SM    | 89   | ARG  | 2.7  |
| 4   | S2    | 84   | LYS  | 2.7  |
| 24  | D2    | 60   | LYS  | 2.7  |
| 25  | D3    | 123  | LYS  | 2.7  |
| 30  | D8    | 45   | LYS  | 2.7  |
| 34  | SR    | 117  | LYS  | 2.7  |
| 51  | M5    | 148  | TYR  | 2.7  |
| 67  | O1    | 26   | LYS  | 2.7  |
| 68  | o2    | 31   | ASN  | 2.7  |
| 51  | M5    | 100  | ALA  | 2.7  |
| 22  | D0    | 51   | VAL  | 2.7  |
| 18  | c6    | 44   | LEU  | 2.7  |
| 62  | N6    | 111  | LEU  | 2.7  |
| 1   | 6     | 194  | U    | 2.7  |
| 1   | 6     | 261  | U    | 2.7  |
| 1   | 6     | 664  | U    | 2.7  |
| 8   | S6    | 113  | ILE  | 2.7  |
| 11  | s9    | 156  | ILE  | 2.7  |
| 36  | 1     | 1555 | U    | 2.7  |
| 36  | 5     | 981  | U    | 2.7  |
| 51  | m5    | 180  | PHE  | 2.7  |
| 45  | l8    | 107  | GLU  | 2.7  |
| 54  | M8    | 74   | GLU  | 2.7  |
| 3   | S1    | 63   | GLY  | 2.7  |
| 36  | 1     | 398  | A    | 2.7  |
| 58  | N2    | 98   | THR  | 2.7  |
| 62  | n6    | 72   | SER  | 2.7  |
| 77  | Q1    | 10   | THR  | 2.7  |
| 15  | c3    | 114  | ARG  | 2.7  |
| 35  | SM    | 68   | ARG  | 2.7  |
| 19  | c7    | 116  | LYS  | 2.7  |
| 42  | l5    | 58   | LYS  | 2.7  |
| 50  | m4    | 8    | LYS  | 2.7  |
| 8   | s6    | 140  | ASN  | 2.7  |
| 13  | C1    | 146  | ALA  | 2.7  |
| 14  | C2    | 104  | ALA  | 2.7  |
| 24  | D2    | 70   | ASN  | 2.7  |
| 31  | d9    | 5    | ASN  | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 42  | L5    | 7    | ALA  | 2.7  |
| 65  | n9    | 53   | ALA  | 2.7  |
| 7   | S5    | 53   | VAL  | 2.7  |
| 5   | S3    | 142  | LEU  | 2.7  |
| 16  | C4    | 57   | PRO  | 2.7  |
| 28  | D6    | 20   | PRO  | 2.7  |
| 24  | d2    | 83   | ILE  | 2.7  |
| 42  | L5    | 148  | ILE  | 2.7  |
| 4   | S2    | 88   | LYS  | 2.7  |
| 34  | sR    | 117  | LYS  | 2.7  |
| 1   | 2     | 1520 | U    | 2.7  |
| 1   | 2     | 1626 | U    | 2.7  |
| 1   | 2     | 506  | A    | 2.7  |
| 2   | S0    | 36   | TYR  | 2.7  |
| 17  | c5    | 133  | ALA  | 2.7  |
| 21  | C9    | 35   | ASP  | 2.7  |
| 32  | E0    | 35   | TYR  | 2.7  |
| 63  | n7    | 59   | ALA  | 2.7  |
| 3   | S1    | 47   | LEU  | 2.7  |
| 3   | S1    | 160  | HIS  | 2.7  |
| 4   | s2    | 240  | LEU  | 2.7  |
| 14  | C2    | 41   | LEU  | 2.7  |
| 27  | D5    | 62   | VAL  | 2.7  |
| 30  | D8    | 48   | VAL  | 2.7  |
| 34  | sR    | 252  | LEU  | 2.7  |
| 41  | L4    | 182  | LEU  | 2.7  |
| 42  | l5    | 236  | LEU  | 2.7  |
| 45  | l8    | 40   | VAL  | 2.7  |
| 45  | L8    | 240  | ASN  | 2.7  |
| 29  | D7    | 38   | PRO  | 2.7  |
| 31  | d9    | 38   | ILE  | 2.7  |
| 34  | SR    | 69   | GLN  | 2.7  |
| 36  | 1     | 1017 | C    | 2.7  |
| 36  | 1     | 3154 | C    | 2.7  |
| 36  | 5     | 1581 | C    | 2.7  |
| 38  | 4     | 84   | C    | 2.7  |
| 15  | C3    | 16   | ILE  | 2.7  |
| 45  | l8    | 237  | ILE  | 2.7  |
| 8   | S6    | 63   | MET  | 2.7  |
| 32  | E0    | 54   | ARG  | 2.7  |
| 39  | l2    | 247  | ARG  | 2.7  |
| 52  | m6    | 172  | ARG  | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 70  | O4    | 16   | ARG  | 2.7  |
| 54  | m8    | 2    | GLY  | 2.7  |
| 58  | n2    | 44   | GLU  | 2.7  |
| 60  | n4    | 69   | LYS  | 2.7  |
| 71  | o5    | 106  | LYS  | 2.7  |
| 22  | d0    | 104  | THR  | 2.7  |
| 69  | O3    | 72   | THR  | 2.7  |
| 80  | c0    | 50   | THR  | 2.7  |
| 1   | 2     | 1201 | G    | 2.7  |
| 1   | 6     | 834  | G    | 2.7  |
| 34  | SR    | 44   | SER  | 2.7  |
| 34  | SR    | 65   | SER  | 2.7  |
| 8   | S6    | 100  | ALA  | 2.7  |
| 8   | S6    | 172  | ALA  | 2.7  |
| 17  | c5    | 7    | ALA  | 2.7  |
| 34  | sR    | 204  | ALA  | 2.7  |
| 1   | 2     | 1286 | U    | 2.7  |
| 1   | 6     | 241  | U    | 2.7  |
| 21  | C9    | 80   | TYR  | 2.7  |
| 23  | D1    | 39   | VAL  | 2.7  |
| 26  | D4    | 70   | VAL  | 2.7  |
| 36  | 5     | 1356 | U    | 2.7  |
| 47  | M0    | 200  | LEU  | 2.7  |
| 63  | N7    | 14   | VAL  | 2.7  |
| 42  | L5    | 59   | ASP  | 2.7  |
| 1   | 6     | 1081 | A    | 2.6  |
| 2   | s0    | 199  | PRO  | 2.6  |
| 9   | s7    | 49   | ILE  | 2.6  |
| 26  | d4    | 106  | GLN  | 2.6  |
| 36  | 1     | 2207 | A    | 2.6  |
| 45  | l8    | 36   | ILE  | 2.6  |
| 74  | O8    | 27   | ILE  | 2.6  |
| 61  | n5    | 88   | MET  | 2.6  |
| 8   | s6    | 177  | ARG  | 2.6  |
| 26  | D4    | 128  | LYS  | 2.6  |
| 32  | E0    | 36   | LYS  | 2.6  |
| 1   | 6     | 654  | C    | 2.6  |
| 14  | c2    | 132  | GLU  | 2.6  |
| 72  | o6    | 78   | GLY  | 2.6  |
| 7   | S5    | 73   | THR  | 2.6  |
| 7   | S5    | 125  | THR  | 2.6  |
| 39  | L2    | 252  | THR  | 2.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 52  | M6    | 184  | THR  | 2.6  |
| 60  | n4    | 133  | THR  | 2.6  |
| 2   | S0    | 14   | ALA  | 2.6  |
| 7   | S5    | 194  | LEU  | 2.6  |
| 14  | C2    | 116  | VAL  | 2.6  |
| 22  | D0    | 45   | ALA  | 2.6  |
| 28  | D6    | 18   | VAL  | 2.6  |
| 28  | D6    | 84   | VAL  | 2.6  |
| 1   | 2     | 1486 | G    | 2.6  |
| 21  | C9    | 36   | ILE  | 2.6  |
| 24  | d2    | 41   | MET  | 2.6  |
| 31  | D9    | 8    | PHE  | 2.6  |
| 31  | d9    | 40   | ARG  | 2.6  |
| 36  | 1     | 1242 | G    | 2.6  |
| 45  | l8    | 254  | ASP  | 2.6  |
| 49  | M3    | 98   | ASP  | 2.6  |
| 2   | S0    | 4    | PRO  | 2.6  |
| 1   | 6     | 719  | U    | 2.6  |
| 5   | s3    | 148  | LYS  | 2.6  |
| 7   | s5    | 102  | ARG  | 2.6  |
| 60  | n4    | 73   | ARG  | 2.6  |
| 67  | o1    | 31   | ARG  | 2.6  |
| 71  | O5    | 48   | ARG  | 2.6  |
| 22  | D0    | 73   | GLY  | 2.6  |
| 1   | 2     | 1065 | A    | 2.6  |
| 1   | 6     | 1157 | A    | 2.6  |
| 45  | L8    | 118  | GLU  | 2.6  |
| 54  | m8    | 95   | GLU  | 2.6  |
| 3   | S1    | 37   | THR  | 2.6  |
| 5   | s3    | 42   | THR  | 2.6  |
| 13  | C1    | 72   | THR  | 2.6  |
| 45  | L8    | 194  | THR  | 2.6  |
| 52  | m6    | 184  | THR  | 2.6  |
| 7   | S5    | 154  | ALA  | 2.6  |
| 41  | l4    | 62   | ALA  | 2.6  |
| 45  | l8    | 117  | ALA  | 2.6  |
| 10  | s8    | 66   | SER  | 2.6  |
| 36  | 5     | 1759 | C    | 2.6  |
| 18  | c6    | 49   | TYR  | 2.6  |
| 4   | s2    | 203  | LYS  | 2.6  |
| 27  | D5    | 50   | ILE  | 2.6  |
| 34  | sR    | 122  | ILE  | 2.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 45  | L8    | 245  | LYS  | 2.6  |
| 55  | m9    | 21   | LYS  | 2.6  |
| 70  | o4    | 8    | ARG  | 2.6  |
| 3   | S1    | 100  | PHE  | 2.6  |
| 5   | s3    | 43   | PRO  | 2.6  |
| 15  | C3    | 113  | PHE  | 2.6  |
| 21  | C9    | 2    | PRO  | 2.6  |
| 28  | d6    | 2    | PRO  | 2.6  |
| 12  | C0    | 13   | GLN  | 2.6  |
| 40  | l3    | 140  | ASP  | 2.6  |
| 12  | C0    | 96   | ASN  | 2.6  |
| 45  | l8    | 192  | GLN  | 2.6  |
| 16  | C4    | 109  | GLY  | 2.6  |
| 31  | d9    | 29   | GLY  | 2.6  |
| 39  | l2    | 248  | GLY  | 2.6  |
| 1   | 2     | 1710 | U    | 2.6  |
| 36  | 1     | 2975 | U    | 2.6  |
| 1   | 2     | 279  | G    | 2.6  |
| 1   | 2     | 540  | G    | 2.6  |
| 1   | 6     | 1268 | G    | 2.6  |
| 36  | 1     | 2522 | G    | 2.6  |
| 4   | S2    | 240  | LEU  | 2.6  |
| 2   | s0    | 195  | TRP  | 2.6  |
| 6   | s4    | 105  | VAL  | 2.6  |
| 7   | s5    | 73   | THR  | 2.6  |
| 10  | S8    | 167  | ALA  | 2.6  |
| 15  | C3    | 61   | THR  | 2.6  |
| 33  | E1    | 100  | LEU  | 2.6  |
| 16  | C4    | 121  | VAL  | 2.6  |
| 17  | C5    | 101  | ALA  | 2.6  |
| 26  | D4    | 75   | VAL  | 2.6  |
| 72  | o6    | 2    | THR  | 2.6  |
| 1   | 2     | 197  | A    | 2.6  |
| 1   | 6     | 1371 | A    | 2.6  |
| 1   | 6     | 1516 | A    | 2.6  |
| 2   | S0    | 185  | ARG  | 2.6  |
| 4   | s2    | 64   | LYS  | 2.6  |
| 6   | S4    | 22   | LYS  | 2.6  |
| 8   | S6    | 88   | ARG  | 2.6  |
| 7   | S5    | 172  | ILE  | 2.6  |
| 10  | S8    | 200  | LYS  | 2.6  |
| 34  | SR    | 90   | ARG  | 2.6  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 34         | SR           | 102        | ARG         | 2.6         |
| 35         | sM           | 83         | LYS         | 2.6         |
| 36         | 1            | 1859       | A           | 2.6         |
| 36         | 1            | 2995       | A           | 2.6         |
| 48         | M1           | 140        | ARG         | 2.6         |
| 11         | S9           | 129        | ILE         | 2.6         |
| 40         | l3           | 363        | SER         | 2.6         |
| 60         | n4           | 63         | ILE         | 2.6         |
| 17         | c5           | 80         | MET         | 2.6         |
| 33         | e1           | 124        | PRO         | 2.6         |
| 61         | n5           | 32         | PHE         | 2.6         |
| 1          | 2            | 233        | C           | 2.6         |
| 1          | 2            | 848        | C           | 2.6         |
| 1          | 6            | 658        | C           | 2.6         |
| 8          | S6           | 199        | GLN         | 2.6         |
| 14         | c2           | 131        | ASP         | 2.6         |
| 19         | c7           | 105        | GLN         | 2.6         |
| 36         | 1            | 1255       | C           | 2.6         |
| 36         | 1            | 3001       | C           | 2.6         |
| 36         | 5            | 3154       | C           | 2.6         |
| 35         | SM           | 11         | ASP         | 2.6         |
| 50         | M4           | 119        | GLN         | 2.6         |
| 19         | C7           | 123        | ASN         | 2.6         |
| 20         | c8           | 19         | ASN         | 2.6         |
| 53         | M7           | 174        | GLY         | 2.6         |
| 5          | S3           | 69         | LEU         | 2.6         |
| 8          | S6           | 211        | LEU         | 2.6         |
| 9          | S7           | 126        | LEU         | 2.6         |
| 17         | c5           | 105        | VAL         | 2.6         |
| 27         | D5           | 40         | VAL         | 2.6         |
| 1          | 2            | 1056       | U           | 2.6         |
| 1          | 6            | 1398       | U           | 2.6         |
| 1          | 6            | 1414       | U           | 2.6         |
| 2          | s0           | 41         | ARG         | 2.6         |
| 3          | S1           | 185        | THR         | 2.6         |
| 5          | S3           | 143        | ARG         | 2.6         |
| 17         | c5           | 134        | THR         | 2.6         |
| 52         | M6           | 185        | ALA         | 2.6         |
| 55         | M9           | 54         | ALA         | 2.6         |
| 8          | s6           | 143        | LYS         | 2.6         |
| 22         | D0           | 61         | LYS         | 2.6         |
| 31         | D9           | 7          | TRP         | 2.6         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 34  | sR    | 46   | LYS  | 2.6  |
| 36  | 1     | 1764 | U    | 2.6  |
| 36  | 5     | 2505 | U    | 2.6  |
| 72  | o6    | 68   | ARG  | 2.6  |
| 80  | c0    | 44   | LYS  | 2.6  |
| 7   | S5    | 68   | ILE  | 2.6  |
| 34  | sR    | 123  | ILE  | 2.6  |
| 74  | O8    | 5    | ILE  | 2.6  |
| 1   | 2     | 143  | G    | 2.6  |
| 1   | 2     | 195  | G    | 2.6  |
| 1   | 2     | 1594 | G    | 2.6  |
| 1   | 6     | 720  | G    | 2.6  |
| 1   | 6     | 1695 | G    | 2.6  |
| 3   | s1    | 30   | PHE  | 2.6  |
| 18  | C6    | 74   | HIS  | 2.6  |
| 31  | D9    | 27   | HIS  | 2.6  |
| 33  | E1    | 105  | TYR  | 2.6  |
| 36  | 1     | 547  | G    | 2.6  |
| 36  | 5     | 1262 | G    | 2.6  |
| 17  | C5    | 125  | PRO  | 2.6  |
| 26  | D4    | 30   | PRO  | 2.6  |
| 45  | l8    | 127  | PRO  | 2.6  |
| 58  | n2    | 97   | SER  | 2.6  |
| 2   | S0    | 33   | GLN  | 2.6  |
| 36  | 1     | 1278 | A    | 2.6  |
| 78  | Q2    | 99   | GLN  | 2.6  |
| 10  | s8    | 80   | GLY  | 2.6  |
| 12  | C0    | 39   | ASN  | 2.6  |
| 20  | C8    | 23   | ASP  | 2.6  |
| 45  | L8    | 207  | ASP  | 2.6  |
| 65  | N9    | 6    | ASN  | 2.6  |
| 9   | S7    | 154  | LEU  | 2.6  |
| 34  | SR    | 73   | LEU  | 2.6  |
| 1   | 6     | 1624 | C    | 2.6  |
| 71  | o5    | 27   | GLU  | 2.6  |
| 3   | S1    | 147  | ALA  | 2.6  |
| 8   | S6    | 164  | LYS  | 2.6  |
| 24  | D2    | 108  | ALA  | 2.6  |
| 30  | d8    | 63   | ALA  | 2.6  |
| 39  | l2    | 251  | LYS  | 2.6  |
| 42  | l5    | 27   | LYS  | 2.6  |
| 45  | l8    | 125  | ALA  | 2.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 74  | O8    | 26   | LYS  | 2.6  |
| 19  | C7    | 6    | THR  | 2.6  |
| 60  | N4    | 51   | TRP  | 2.5  |
| 70  | O4    | 71   | THR  | 2.6  |
| 2   | S0    | 141  | ILE  | 2.5  |
| 15  | c3    | 16   | ILE  | 2.5  |
| 2   | S0    | 115  | PHE  | 2.5  |
| 1   | 2     | 267  | U    | 2.5  |
| 3   | s1    | 153  | HIS  | 2.5  |
| 51  | M5    | 62   | TYR  | 2.5  |
| 18  | c6    | 2    | SER  | 2.5  |
| 16  | C4    | 12   | GLN  | 2.5  |
| 27  | d5    | 37   | GLN  | 2.5  |
| 45  | L8    | 123  | GLN  | 2.5  |
| 70  | O4    | 61   | GLN  | 2.5  |
| 8   | S6    | 216  | LEU  | 2.5  |
| 14  | c2    | 59   | LEU  | 2.5  |
| 40  | L3    | 387  | LEU  | 2.5  |
| 61  | n5    | 34   | LEU  | 2.5  |
| 63  | N7    | 42   | LEU  | 2.5  |
| 1   | 2     | 235  | G    | 2.5  |
| 1   | 6     | 1047 | G    | 2.5  |
| 2   | s0    | 185  | ARG  | 2.5  |
| 3   | S1    | 89   | ASP  | 2.5  |
| 3   | S1    | 199  | ASN  | 2.5  |
| 7   | S5    | 41   | LYS  | 2.5  |
| 11  | s9    | 132  | ARG  | 2.5  |
| 1   | 2     | 1371 | A    | 2.5  |
| 1   | 6     | 1694 | A    | 2.5  |
| 3   | S1    | 123  | ALA  | 2.5  |
| 10  | S8    | 28   | GLU  | 2.5  |
| 14  | c2    | 56   | GLU  | 2.5  |
| 15  | c3    | 7    | ALA  | 2.5  |
| 16  | C4    | 37   | GLU  | 2.5  |
| 17  | c5    | 9    | LYS  | 2.5  |
| 21  | C9    | 43   | ASN  | 2.5  |
| 39  | L2    | 161  | ASP  | 2.5  |
| 49  | M3    | 129  | ASN  | 2.5  |
| 52  | M6    | 182  | ASN  | 2.5  |
| 74  | O8    | 55   | VAL  | 2.5  |
| 76  | Q0    | 106  | ARG  | 2.5  |
| 17  | C5    | 74   | ALA  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 20  | C8    | 146  | ALA  | 2.5  |
| 2   | S0    | 22   | THR  | 2.5  |
| 16  | C4    | 39   | ILE  | 2.5  |
| 22  | D0    | 86   | ILE  | 2.5  |
| 45  | L8    | 74   | THR  | 2.5  |
| 46  | L9    | 10   | ILE  | 2.5  |
| 60  | n4    | 82   | ILE  | 2.5  |
| 1   | 6     | 674  | C    | 2.5  |
| 1   | 6     | 741  | C    | 2.5  |
| 38  | 8     | 84   | C    | 2.5  |
| 3   | S1    | 153  | HIS  | 2.5  |
| 28  | D6    | 2    | PRO  | 2.5  |
| 32  | e0    | 30   | PRO  | 2.5  |
| 33  | e1    | 93   | HIS  | 2.5  |
| 80  | c0    | 64   | TYR  | 2.5  |
| 3   | S1    | 130  | SER  | 2.5  |
| 1   | 6     | 665  | U    | 2.5  |
| 1   | 6     | 705  | U    | 2.5  |
| 1   | 6     | 1657 | U    | 2.5  |
| 3   | S1    | 226  | GLY  | 2.5  |
| 14  | c2    | 88   | LEU  | 2.5  |
| 16  | C4    | 65   | GLN  | 2.5  |
| 19  | c7    | 117  | LEU  | 2.5  |
| 45  | L8    | 47   | SER  | 2.5  |
| 60  | N4    | 62   | GLY  | 2.5  |
| 60  | N4    | 86   | SER  | 2.5  |
| 4   | S2    | 116  | LYS  | 2.5  |
| 8   | S6    | 194  | LYS  | 2.5  |
| 21  | c9    | 86   | ARG  | 2.5  |
| 25  | D3    | 114  | LYS  | 2.5  |
| 40  | l3    | 240  | ARG  | 2.5  |
| 43  | l6    | 128  | LYS  | 2.5  |
| 2   | S0    | 123  | VAL  | 2.5  |
| 18  | c6    | 39   | VAL  | 2.5  |
| 27  | d5    | 64   | VAL  | 2.5  |
| 4   | S2    | 92   | ALA  | 2.5  |
| 10  | S8    | 89   | GLU  | 2.5  |
| 21  | c9    | 43   | ASN  | 2.5  |
| 23  | d1    | 42   | GLU  | 2.5  |
| 24  | D2    | 55   | ASP  | 2.5  |
| 24  | d2    | 114  | GLU  | 2.5  |
| 28  | d6    | 81   | ALA  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 45  | l8    | 113  | ALA  | 2.5  |
| 53  | M7    | 2    | ALA  | 2.5  |
| 53  | M7    | 57   | ALA  | 2.5  |
| 53  | M7    | 177  | ALA  | 2.5  |
| 5   | s3    | 217  | ILE  | 2.5  |
| 6   | s4    | 64   | ILE  | 2.5  |
| 2   | S0    | 124  | THR  | 2.5  |
| 9   | S7    | 119  | THR  | 2.5  |
| 34  | SR    | 92   | TRP  | 2.5  |
| 58  | N2    | 100  | THR  | 2.5  |
| 25  | d3    | 122  | PHE  | 2.5  |
| 1   | 2     | 359  | A    | 2.5  |
| 1   | 2     | 847  | A    | 2.5  |
| 1   | 6     | 1329 | A    | 2.5  |
| 36  | 1     | 1259 | A    | 2.5  |
| 36  | 1     | 1571 | A    | 2.5  |
| 36  | 5     | 1093 | A    | 2.5  |
| 1   | 6     | 1201 | G    | 2.5  |
| 36  | 5     | 171  | G    | 2.5  |
| 34  | SR    | 66   | HIS  | 2.5  |
| 42  | l5    | 86   | TYR  | 2.5  |
| 52  | M6    | 135  | TYR  | 2.5  |
| 80  | c0    | 66   | TYR  | 2.5  |
| 8   | S6    | 193  | LEU  | 2.5  |
| 1   | 2     | 573  | C    | 2.5  |
| 1   | 2     | 1215 | C    | 2.5  |
| 1   | 2     | 1373 | C    | 2.5  |
| 3   | S1    | 55   | LYS  | 2.5  |
| 3   | S1    | 181  | LEU  | 2.5  |
| 19  | C7    | 95   | ARG  | 2.5  |
| 20  | C8    | 101  | LEU  | 2.5  |
| 25  | D3    | 4    | GLY  | 2.5  |
| 26  | D4    | 61   | ARG  | 2.5  |
| 40  | L3    | 178  | LEU  | 2.5  |
| 51  | m5    | 179  | LYS  | 2.5  |
| 60  | n4    | 110  | LYS  | 2.5  |
| 61  | N5    | 24   | LEU  | 2.5  |
| 72  | o6    | 30   | LYS  | 2.5  |
| 78  | q2    | 13   | LYS  | 2.5  |
| 5   | S3    | 206  | VAL  | 2.5  |
| 22  | d0    | 114  | VAL  | 2.5  |
| 54  | M8    | 186  | VAL  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | 2     | 721  | U    | 2.5  |
| 36  | 1     | 1568 | U    | 2.5  |
| 6   | S4    | 45   | ILE  | 2.5  |
| 7   | S5    | 130  | ILE  | 2.5  |
| 39  | l2    | 238  | ILE  | 2.5  |
| 46  | l9    | 107  | ASP  | 2.5  |
| 62  | N6    | 112  | ASP  | 2.5  |
| 64  | N8    | 76   | ASP  | 2.5  |
| 65  | n9    | 26   | THR  | 2.5  |
| 74  | o8    | 72   | THR  | 2.5  |
| 2   | S0    | 146  | LEU  | 2.5  |
| 11  | S9    | 138  | LYS  | 2.5  |
| 14  | C2    | 88   | LEU  | 2.5  |
| 20  | C8    | 55   | HIS  | 2.5  |
| 20  | c8    | 32   | LEU  | 2.5  |
| 31  | d9    | 34   | TYR  | 2.5  |
| 33  | E1    | 96   | LYS  | 2.5  |
| 60  | N4    | 93   | ARG  | 2.5  |
| 68  | o2    | 54   | LYS  | 2.5  |
| 17  | c5    | 91   | GLY  | 2.5  |
| 2   | s0    | 47   | VAL  | 2.5  |
| 4   | s2    | 89   | GLN  | 2.5  |
| 8   | S6    | 112  | VAL  | 2.5  |
| 9   | S7    | 170  | GLN  | 2.5  |
| 9   | s7    | 108  | GLN  | 2.5  |
| 14  | C2    | 31   | VAL  | 2.5  |
| 16  | C4    | 118  | VAL  | 2.5  |
| 53  | M7    | 157  | VAL  | 2.5  |
| 1   | 2     | 720  | G    | 2.5  |
| 1   | 2     | 1199 | G    | 2.5  |
| 1   | 2     | 1297 | G    | 2.5  |
| 1   | 2     | 1697 | G    | 2.5  |
| 28  | d6    | 29   | SER  | 2.5  |
| 31  | D9    | 25   | SER  | 2.5  |
| 36  | 5     | 3158 | G    | 2.5  |
| 60  | n4    | 68   | ALA  | 2.5  |
| 68  | o2    | 127  | ALA  | 2.5  |
| 72  | O6    | 27   | SER  | 2.5  |
| 5   | S3    | 208  | ILE  | 2.5  |
| 1   | 2     | 361  | C    | 2.5  |
| 1   | 2     | 1082 | C    | 2.5  |
| 1   | 2     | 1591 | C    | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | 2     | 1599 | C    | 2.5  |
| 1   | 6     | 38   | C    | 2.5  |
| 1   | 6     | 1209 | C    | 2.5  |
| 11  | S9    | 64   | GLU  | 2.5  |
| 16  | C4    | 19   | ILE  | 2.5  |
| 36  | 1     | 1563 | C    | 2.5  |
| 60  | n4    | 66   | GLU  | 2.5  |
| 2   | s0    | 107  | PHE  | 2.5  |
| 6   | s4    | 79   | ASP  | 2.5  |
| 16  | C4    | 66   | ASP  | 2.5  |
| 1   | 6     | 667  | U    | 2.5  |
| 19  | C7    | 8    | THR  | 2.5  |
| 19  | c7    | 54   | THR  | 2.5  |
| 22  | d0    | 60   | THR  | 2.5  |
| 36  | 5     | 2996 | U    | 2.5  |
| 6   | S4    | 127  | LYS  | 2.5  |
| 9   | S7    | 101  | LYS  | 2.5  |
| 13  | c1    | 29   | LYS  | 2.5  |
| 53  | M7    | 159  | LYS  | 2.5  |
| 2   | S0    | 57   | LEU  | 2.5  |
| 2   | s0    | 4    | PRO  | 2.5  |
| 11  | S9    | 70   | LEU  | 2.5  |
| 18  | c6    | 124  | PRO  | 2.5  |
| 20  | C8    | 3    | LEU  | 2.5  |
| 29  | d7    | 21   | LEU  | 2.5  |
| 46  | l9    | 191  | LEU  | 2.5  |
| 75  | O9    | 46   | ARG  | 2.5  |
| 80  | c0    | 49   | LEU  | 2.5  |
| 80  | c0    | 83   | PRO  | 2.5  |
| 42  | l5    | 272  | TYR  | 2.5  |
| 51  | m5    | 62   | TYR  | 2.5  |
| 7   | s5    | 151  | GLY  | 2.5  |
| 11  | S9    | 32   | GLY  | 2.5  |
| 19  | C7    | 98   | GLY  | 2.5  |
| 78  | q2    | 49   | GLY  | 2.5  |
| 13  | c1    | 142  | VAL  | 2.5  |
| 22  | d0    | 100  | VAL  | 2.5  |
| 24  | D2    | 6    | VAL  | 2.5  |
| 67  | O1    | 108  | VAL  | 2.5  |
| 7   | s5    | 127  | GLN  | 2.5  |
| 8   | s6    | 176  | GLN  | 2.5  |
| 41  | L4    | 304  | GLN  | 2.5  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 51         | m5           | 23         | GLN         | 2.5         |
| 80         | c0           | 62         | GLN         | 2.5         |
| 2          | s0           | 5          | ALA         | 2.4         |
| 24         | d2           | 108        | ALA         | 2.4         |
| 18         | C6           | 141        | SER         | 2.4         |
| 19         | C7           | 69         | ILE         | 2.4         |
| 31         | D9           | 31         | ILE         | 2.4         |
| 34         | sR           | 205        | SER         | 2.4         |
| 61         | n5           | 29         | SER         | 2.4         |
| 1          | 2            | 105        | A           | 2.4         |
| 1          | 2            | 265        | A           | 2.4         |
| 1          | 2            | 1287       | A           | 2.4         |
| 1          | 2            | 1592       | A           | 2.4         |
| 13         | c1           | 101        | GLU         | 2.4         |
| 36         | 1            | 3362       | A           | 2.4         |
| 12         | C0           | 27         | PHE         | 2.4         |
| 16         | C4           | 23         | PHE         | 2.4         |
| 48         | M1           | 96         | PHE         | 2.4         |
| 74         | o8           | 43         | PHE         | 2.4         |
| 39         | L2           | 196        | TRP         | 2.4         |
| 48         | M1           | 143        | ARG         | 2.4         |
| 60         | N4           | 47         | ARG         | 2.4         |
| 60         | N4           | 94         | ARG         | 2.4         |
| 2          | S0           | 176        | LEU         | 2.4         |
| 2          | S0           | 184        | LEU         | 2.4         |
| 3          | s1           | 73         | LEU         | 2.4         |
| 14         | C2           | 67         | THR         | 2.4         |
| 14         | c2           | 49         | THR         | 2.4         |
| 14         | c2           | 97         | LEU         | 2.4         |
| 16         | C4           | 43         | THR         | 2.4         |
| 18         | C6           | 9          | THR         | 2.4         |
| 68         | o2           | 23         | ASP         | 2.4         |
| 36         | 1            | 1573       | G           | 2.4         |
| 36         | 5            | 176        | G           | 2.4         |
| 36         | 5            | 1201       | C           | 2.4         |
| 36         | 5            | 1354       | G           | 2.4         |
| 45         | L8           | 189        | LEU         | 2.4         |
| 1          | 2            | 66         | U           | 2.4         |
| 1          | 6            | 229        | U           | 2.4         |
| 2          | s0           | 204        | TYR         | 2.4         |
| 8          | s6           | 169        | TYR         | 2.4         |
| 25         | d3           | 18         | HIS         | 2.4         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 36  | 1     | 1572 | U    | 2.4  |
| 36  | 1     | 2205 | U    | 2.4  |
| 36  | 5     | 1028 | U    | 2.4  |
| 11  | S9    | 141  | VAL  | 2.4  |
| 39  | L2    | 201  | GLY  | 2.4  |
| 55  | M9    | 51   | VAL  | 2.4  |
| 60  | n4    | 67   | VAL  | 2.4  |
| 67  | O1    | 107  | VAL  | 2.4  |
| 66  | O0    | 95   | ALA  | 2.4  |
| 70  | o4    | 2    | ALA  | 2.4  |
| 8   | S6    | 101  | ILE  | 2.4  |
| 63  | N7    | 72   | ILE  | 2.4  |
| 20  | C8    | 73   | MET  | 2.4  |
| 2   | S0    | 106  | SER  | 2.4  |
| 11  | s9    | 46   | SER  | 2.4  |
| 24  | d2    | 58   | SER  | 2.4  |
| 45  | L8    | 89   | GLU  | 2.4  |
| 13  | c1    | 115  | PHE  | 2.4  |
| 33  | E1    | 92   | LYS  | 2.4  |
| 51  | m5    | 59   | PHE  | 2.4  |
| 8   | S6    | 87   | ARG  | 2.4  |
| 53  | M7    | 163  | LYS  | 2.4  |
| 61  | N5    | 25   | LYS  | 2.4  |
| 2   | s0    | 17   | LEU  | 2.4  |
| 16  | C4    | 33   | LEU  | 2.4  |
| 16  | C4    | 105  | LEU  | 2.4  |
| 30  | D8    | 54   | LEU  | 2.4  |
| 42  | L5    | 92   | LEU  | 2.4  |
| 55  | M9    | 89   | LEU  | 2.4  |
| 62  | n6    | 98   | ASN  | 2.4  |
| 1   | 2     | 844  | A    | 2.4  |
| 38  | 8     | 79   | A    | 2.4  |
| 39  | L2    | 208  | ASP  | 2.4  |
| 7   | s5    | 129  | PRO  | 2.4  |
| 2   | S0    | 73   | VAL  | 2.4  |
| 3   | S1    | 65   | VAL  | 2.4  |
| 13  | c1    | 139  | VAL  | 2.4  |
| 26  | D4    | 24   | VAL  | 2.4  |
| 35  | sM    | 67   | GLY  | 2.4  |
| 51  | m5    | 58   | GLY  | 2.4  |
| 73  | o7    | 9    | GLY  | 2.4  |
| 4   | S2    | 47   | ALA  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 7   | S5    | 78   | ALA  | 2.4  |
| 1   | 2     | 1657 | U    | 2.4  |
| 7   | S5    | 187  | ILE  | 2.4  |
| 9   | S7    | 42   | GLN  | 2.4  |
| 14  | c2    | 89   | ILE  | 2.4  |
| 15  | C3    | 66   | ILE  | 2.4  |
| 34  | SR    | 253  | ALA  | 2.4  |
| 35  | sM    | 60   | ALA  | 2.4  |
| 36  | 1     | 1279 | C    | 2.4  |
| 36  | 5     | 1017 | C    | 2.4  |
| 36  | 5     | 2772 | C    | 2.4  |
| 36  | 1     | 1786 | G    | 2.4  |
| 15  | C3    | 4    | MET  | 2.4  |
| 32  | e0    | 56   | MET  | 2.4  |
| 14  | c2    | 33   | ARG  | 2.4  |
| 26  | d4    | 8    | ARG  | 2.4  |
| 34  | SR    | 137  | LYS  | 2.4  |
| 51  | m5    | 184  | LYS  | 2.4  |
| 66  | o0    | 32   | LYS  | 2.4  |
| 71  | O5    | 8    | GLU  | 2.4  |
| 35  | sM    | 28   | SER  | 2.4  |
| 8   | s6    | 111  | LEU  | 2.4  |
| 27  | D5    | 75   | LEU  | 2.4  |
| 32  | e0    | 49   | LEU  | 2.4  |
| 80  | c0    | 40   | LEU  | 2.4  |
| 2   | S0    | 192  | THR  | 2.4  |
| 20  | C8    | 84   | TRP  | 2.4  |
| 9   | S7    | 13   | PRO  | 2.4  |
| 9   | S7    | 105  | THR  | 2.4  |
| 11  | S9    | 5    | PRO  | 2.4  |
| 25  | D3    | 6    | PRO  | 2.4  |
| 70  | o4    | 71   | THR  | 2.4  |
| 74  | o8    | 24   | THR  | 2.4  |
| 5   | S3    | 41   | VAL  | 2.4  |
| 16  | C4    | 124  | ASP  | 2.4  |
| 58  | N2    | 27   | VAL  | 2.4  |
| 28  | D6    | 9    | GLY  | 2.4  |
| 33  | e1    | 105  | TYR  | 2.4  |
| 45  | L8    | 119  | GLY  | 2.4  |
| 80  | c0    | 41   | TYR  | 2.4  |
| 80  | c0    | 75   | TYR  | 2.4  |
| 1   | 2     | 80   | A    | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 9   | S7    | 8    | ILE  | 2.4  |
| 13  | C1    | 38   | ALA  | 2.4  |
| 19  | C7    | 12   | ALA  | 2.4  |
| 19  | c7    | 69   | ILE  | 2.4  |
| 19  | c7    | 122  | ILE  | 2.4  |
| 24  | D2    | 53   | ILE  | 2.4  |
| 34  | sR    | 115  | ILE  | 2.4  |
| 70  | o4    | 32   | ALA  | 2.4  |
| 36  | 1     | 1093 | A    | 2.4  |
| 12  | C0    | 3    | MET  | 2.4  |
| 17  | c5    | 111  | MET  | 2.4  |
| 31  | d9    | 20   | GLN  | 2.4  |
| 32  | E0    | 29   | LYS  | 2.4  |
| 47  | M0    | 202  | LYS  | 2.4  |
| 60  | n4    | 79   | GLN  | 2.4  |
| 6   | S4    | 11   | ARG  | 2.4  |
| 60  | n4    | 129  | LYS  | 2.4  |
| 61  | n5    | 100  | LYS  | 2.4  |
| 73  | O7    | 10   | LYS  | 2.4  |
| 53  | M7    | 90   | PHE  | 2.4  |
| 1   | 2     | 717  | C    | 2.4  |
| 1   | 2     | 1156 | C    | 2.4  |
| 1   | 2     | 1518 | C    | 2.4  |
| 1   | 6     | 1426 | C    | 2.4  |
| 5   | s3    | 21   | LEU  | 2.4  |
| 15  | c3    | 125  | LEU  | 2.4  |
| 27  | D5    | 51   | LEU  | 2.4  |
| 36  | 5     | 1821 | U    | 2.4  |
| 37  | 7     | 90   | U    | 2.4  |
| 60  | N4    | 66   | GLU  | 2.4  |
| 68  | O2    | 126  | LEU  | 2.4  |
| 16  | C4    | 56   | SER  | 2.4  |
| 33  | E1    | 146  | SER  | 2.4  |
| 34  | SR    | 120  | SER  | 2.4  |
| 1   | 2     | 722  | G    | 2.4  |
| 1   | 2     | 1008 | G    | 2.4  |
| 1   | 6     | 810  | G    | 2.4  |
| 36  | 5     | 1576 | G    | 2.4  |
| 36  | 5     | 2972 | G    | 2.4  |
| 10  | S8    | 67   | TRP  | 2.4  |
| 2   | s0    | 189  | VAL  | 2.4  |
| 4   | s2    | 63   | VAL  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4   | s2    | 86  | VAL  | 2.4  |
| 14  | c2    | 63  | VAL  | 2.4  |
| 19  | C7    | 86  | PRO  | 2.4  |
| 34  | sR    | 19  | TRP  | 2.4  |
| 19  | C7    | 106 | THR  | 2.4  |
| 21  | C9    | 114 | VAL  | 2.4  |
| 34  | SR    | 6   | VAL  | 2.4  |
| 34  | SR    | 99  | THR  | 2.4  |
| 45  | L8    | 99  | PRO  | 2.4  |
| 61  | n5    | 110 | VAL  | 2.4  |
| 70  | O4    | 68  | THR  | 2.4  |
| 74  | o8    | 53  | THR  | 2.4  |
| 2   | s0    | 186 | GLY  | 2.4  |
| 7   | s5    | 95  | ASN  | 2.4  |
| 21  | c9    | 93  | HIS  | 2.4  |
| 5   | S3    | 87  | TYR  | 2.4  |
| 6   | S4    | 202 | ASP  | 2.4  |
| 7   | S5    | 199 | ILE  | 2.4  |
| 26  | d4    | 126 | ALA  | 2.4  |
| 27  | D5    | 41  | ILE  | 2.4  |
| 39  | l2    | 15  | ILE  | 2.4  |
| 41  | L4    | 74  | ILE  | 2.4  |
| 45  | l8    | 114 | ALA  | 2.4  |
| 72  | o6    | 26  | ILE  | 2.4  |
| 73  | O7    | 88  | ALA  | 2.4  |
| 76  | q0    | 77  | ILE  | 2.4  |
| 33  | e1    | 89  | LYS  | 2.4  |
| 82  | p0    | 81  | LYS  | 2.4  |
| 2   | s0    | 27  | ARG  | 2.4  |
| 18  | c6    | 123 | ARG  | 2.4  |
| 26  | d4    | 61  | ARG  | 2.4  |
| 34  | SR    | 121 | MET  | 2.4  |
| 48  | M1    | 125 | MET  | 2.4  |
| 3   | S1    | 146 | GLN  | 2.4  |
| 8   | S6    | 65  | GLN  | 2.4  |
| 47  | m0    | 133 | GLN  | 2.4  |
| 56  | N0    | 138 | GLN  | 2.4  |
| 8   | S6    | 27  | PHE  | 2.4  |
| 2   | S0    | 188 | LEU  | 2.4  |
| 12  | C0    | 2   | LEU  | 2.4  |
| 20  | C8    | 17  | LEU  | 2.4  |
| 26  | D4    | 125 | LEU  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 30  | D8    | 16   | LEU  | 2.4  |
| 39  | L2    | 71   | LEU  | 2.4  |
| 1   | 2     | 707  | A    | 2.4  |
| 1   | 2     | 1526 | A    | 2.4  |
| 1   | 2     | 1543 | A    | 2.4  |
| 8   | S6    | 222  | GLU  | 2.4  |
| 60  | N4    | 38   | SER  | 2.4  |
| 72  | o6    | 27   | SER  | 2.4  |
| 1   | 2     | 132  | U    | 2.4  |
| 1   | 2     | 134  | U    | 2.4  |
| 3   | S1    | 23   | PRO  | 2.4  |
| 3   | S1    | 29   | TRP  | 2.4  |
| 3   | S1    | 225  | VAL  | 2.4  |
| 4   | S2    | 111  | VAL  | 2.4  |
| 7   | s5    | 164  | PRO  | 2.4  |
| 9   | S7    | 62   | VAL  | 2.4  |
| 10  | s8    | 179  | CYS  | 2.4  |
| 18  | C6    | 126  | PRO  | 2.4  |
| 18  | c6    | 31   | VAL  | 2.4  |
| 25  | D3    | 42   | PRO  | 2.4  |
| 38  | 4     | 158  | U    | 2.4  |
| 45  | L8    | 40   | VAL  | 2.4  |
| 55  | M9    | 94   | VAL  | 2.4  |
| 80  | c0    | 61   | TRP  | 2.4  |
| 7   | S5    | 151  | GLY  | 2.3  |
| 14  | C2    | 130  | THR  | 2.3  |
| 14  | c2    | 102  | GLY  | 2.3  |
| 17  | c5    | 50   | THR  | 2.3  |
| 27  | D5    | 105  | THR  | 2.3  |
| 34  | SR    | 12   | THR  | 2.3  |
| 42  | l5    | 295  | GLY  | 2.3  |
| 73  | O7    | 59   | THR  | 2.3  |
| 2   | S0    | 170  | ILE  | 2.3  |
| 3   | S1    | 182  | ALA  | 2.3  |
| 8   | s6    | 80   | ASN  | 2.3  |
| 10  | S8    | 23   | LYS  | 2.3  |
| 13  | c1    | 32   | LYS  | 2.3  |
| 4   | S2    | 95   | ARG  | 2.3  |
| 7   | S5    | 61   | TYR  | 2.3  |
| 16  | C4    | 17   | ALA  | 2.3  |
| 16  | C4    | 76   | ILE  | 2.3  |
| 21  | C9    | 62   | ALA  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 21  | c9    | 64   | HIS  | 2.3  |
| 25  | D3    | 27   | ASN  | 2.3  |
| 26  | d4    | 34   | ASN  | 2.3  |
| 27  | d5    | 50   | ILE  | 2.3  |
| 33  | E1    | 151  | ASN  | 2.3  |
| 33  | e1    | 123  | ASN  | 2.3  |
| 41  | l4    | 104  | LYS  | 2.3  |
| 63  | N7    | 52   | LYS  | 2.3  |
| 69  | O3    | 91   | ALA  | 2.3  |
| 70  | O4    | 24   | LYS  | 2.3  |
| 42  | L5    | 213  | ASP  | 2.3  |
| 45  | L8    | 44   | ARG  | 2.3  |
| 54  | m8    | 180  | ARG  | 2.3  |
| 1   | 2     | 730  | G    | 2.3  |
| 1   | 2     | 1523 | G    | 2.3  |
| 36  | 1     | 568  | G    | 2.3  |
| 36  | 1     | 3290 | G    | 2.3  |
| 3   | s1    | 217  | LEU  | 2.3  |
| 5   | S3    | 72   | LEU  | 2.3  |
| 6   | S4    | 259  | GLN  | 2.3  |
| 6   | s4    | 261  | LEU  | 2.3  |
| 9   | S7    | 183  | PHE  | 2.3  |
| 10  | s8    | 20   | GLN  | 2.3  |
| 12  | C0    | 62   | GLN  | 2.3  |
| 23  | D1    | 55   | LEU  | 2.3  |
| 51  | M5    | 199  | LEU  | 2.3  |
| 80  | c0    | 15   | LEU  | 2.3  |
| 18  | C6    | 19   | VAL  | 2.3  |
| 26  | d4    | 25   | VAL  | 2.3  |
| 45  | L8    | 116  | VAL  | 2.3  |
| 1   | 6     | 506  | A    | 2.3  |
| 13  | c1    | 143  | SER  | 2.3  |
| 19  | C7    | 96   | SER  | 2.3  |
| 24  | D2    | 109  | GLY  | 2.3  |
| 28  | D6    | 12   | LYS  | 2.3  |
| 33  | e1    | 116  | LYS  | 2.3  |
| 34  | SR    | 15   | GLY  | 2.3  |
| 36  | 1     | 621  | A    | 2.3  |
| 42  | l5    | 220  | SER  | 2.3  |
| 59  | N3    | 84   | SER  | 2.3  |
| 4   | S2    | 96   | THR  | 2.3  |
| 4   | s2    | 223  | GLY  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 6   | S4    | 78   | THR  | 2.3  |
| 8   | S6    | 79   | LYS  | 2.3  |
| 6   | S4    | 254  | ARG  | 2.3  |
| 8   | S6    | 134  | GLY  | 2.3  |
| 9   | S7    | 181  | ILE  | 2.3  |
| 9   | s7    | 105  | THR  | 2.3  |
| 14  | C2    | 72   | ILE  | 2.3  |
| 14  | C2    | 136  | ILE  | 2.3  |
| 14  | c2    | 67   | THR  | 2.3  |
| 44  | l7    | 238  | LYS  | 2.3  |
| 51  | M5    | 52   | GLY  | 2.3  |
| 52  | m6    | 66   | LYS  | 2.3  |
| 53  | m7    | 79   | THR  | 2.3  |
| 54  | M8    | 182  | LYS  | 2.3  |
| 60  | N4    | 69   | LYS  | 2.3  |
| 63  | N7    | 55   | LYS  | 2.3  |
| 14  | c2    | 118  | ALA  | 2.3  |
| 16  | C4    | 78   | ALA  | 2.3  |
| 16  | C4    | 112  | ILE  | 2.3  |
| 20  | c8    | 92   | ILE  | 2.3  |
| 28  | d6    | 44   | ILE  | 2.3  |
| 34  | SR    | 212  | ALA  | 2.3  |
| 34  | SR    | 220  | ILE  | 2.3  |
| 49  | M3    | 87   | ALA  | 2.3  |
| 51  | m5    | 146  | ALA  | 2.3  |
| 55  | M9    | 50   | ILE  | 2.3  |
| 63  | n7    | 86   | THR  | 2.3  |
| 64  | n8    | 149  | ALA  | 2.3  |
| 70  | o4    | 50   | ALA  | 2.3  |
| 11  | S9    | 38   | ASN  | 2.3  |
| 60  | n4    | 1    | MET  | 2.3  |
| 63  | n7    | 18   | TYR  | 2.3  |
| 16  | c4    | 124  | ASP  | 2.3  |
| 34  | SR    | 34   | LEU  | 2.3  |
| 36  | 1     | 1196 | C    | 2.3  |
| 36  | 5     | 1574 | C    | 2.3  |
| 67  | o1    | 6    | ASP  | 2.3  |
| 6   | S4    | 23   | LEU  | 2.3  |
| 7   | s5    | 165  | LEU  | 2.3  |
| 48  | M1    | 17   | LEU  | 2.3  |
| 67  | o1    | 16   | LEU  | 2.3  |
| 78  | q2    | 35   | LEU  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 82  | p0    | 197  | PHE  | 2.3  |
| 15  | c3    | 86   | GLU  | 2.3  |
| 52  | M6    | 166  | GLU  | 2.3  |
| 1   | 2     | 1243 | G    | 2.3  |
| 1   | 2     | 1616 | G    | 2.3  |
| 1   | 6     | 1270 | G    | 2.3  |
| 1   | 6     | 1699 | G    | 2.3  |
| 2   | S0    | 47   | VAL  | 2.3  |
| 2   | s0    | 158  | VAL  | 2.3  |
| 3   | S1    | 114  | VAL  | 2.3  |
| 7   | s5    | 62   | VAL  | 2.3  |
| 8   | S6    | 9    | VAL  | 2.3  |
| 19  | c7    | 110  | VAL  | 2.3  |
| 33  | E1    | 147  | VAL  | 2.3  |
| 34  | sR    | 167  | VAL  | 2.3  |
| 36  | 1     | 2311 | G    | 2.3  |
| 36  | 5     | 1561 | G    | 2.3  |
| 70  | O4    | 105  | VAL  | 2.3  |
| 6   | S4    | 3    | ARG  | 2.3  |
| 8   | S6    | 177  | ARG  | 2.3  |
| 68  | O2    | 24   | ARG  | 2.3  |
| 6   | s4    | 90   | ILE  | 2.3  |
| 8   | S6    | 55   | GLY  | 2.3  |
| 11  | S9    | 140  | ILE  | 2.3  |
| 25  | D3    | 119  | GLY  | 2.3  |
| 34  | sR    | 170  | ILE  | 2.3  |
| 39  | l2    | 225  | ILE  | 2.3  |
| 40  | l3    | 245  | GLY  | 2.3  |
| 45  | l8    | 121  | SER  | 2.3  |
| 48  | M1    | 100  | GLY  | 2.3  |
| 63  | n7    | 72   | ILE  | 2.3  |
| 2   | S0    | 93   | THR  | 2.3  |
| 3   | s1    | 147  | ALA  | 2.3  |
| 8   | s6    | 128  | THR  | 2.3  |
| 15  | C3    | 67   | THR  | 2.3  |
| 26  | d4    | 134  | ALA  | 2.3  |
| 34  | SR    | 296  | ALA  | 2.3  |
| 40  | l3    | 179  | ALA  | 2.3  |
| 10  | s8    | 116  | HIS  | 2.3  |
| 15  | C3    | 5    | HIS  | 2.3  |
| 33  | E1    | 93   | HIS  | 2.3  |
| 80  | c0    | 3    | MET  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 19  | C7    | 84   | TYR  | 2.3  |
| 42  | L5    | 207  | TYR  | 2.3  |
| 2   | S0    | 17   | LEU  | 2.3  |
| 2   | s0    | 49   | ASN  | 2.3  |
| 3   | S1    | 135  | LEU  | 2.3  |
| 4   | S2    | 134  | LEU  | 2.3  |
| 19  | C7    | 16   | LEU  | 2.3  |
| 22  | D0    | 58   | LEU  | 2.3  |
| 27  | D5    | 69   | LEU  | 2.3  |
| 47  | M0    | 209  | ASN  | 2.3  |
| 63  | N7    | 51   | LEU  | 2.3  |
| 80  | c0    | 46   | LEU  | 2.3  |
| 1   | 2     | 538  | A    | 2.3  |
| 1   | 6     | 1702 | A    | 2.3  |
| 3   | S1    | 30   | PHE  | 2.3  |
| 36  | 1     | 1270 | A    | 2.3  |
| 34  | sR    | 266  | ASP  | 2.3  |
| 52  | m6    | 56   | ASP  | 2.3  |
| 1   | 2     | 504  | U    | 2.3  |
| 1   | 2     | 1362 | U    | 2.3  |
| 1   | 6     | 501  | U    | 2.3  |
| 36  | 1     | 2506 | U    | 2.3  |
| 70  | O4    | 3    | GLN  | 2.3  |
| 31  | d9    | 4    | GLU  | 2.3  |
| 42  | l5    | 268  | GLU  | 2.3  |
| 53  | M7    | 162  | GLU  | 2.3  |
| 1   | 2     | 1205 | C    | 2.3  |
| 8   | s6    | 187  | LYS  | 2.3  |
| 10  | S8    | 17   | LYS  | 2.3  |
| 22  | D0    | 117  | VAL  | 2.3  |
| 22  | d0    | 118  | VAL  | 2.3  |
| 25  | d3    | 31   | LYS  | 2.3  |
| 28  | d6    | 18   | VAL  | 2.3  |
| 34  | sR    | 154  | VAL  | 2.3  |
| 36  | 1     | 1277 | C    | 2.3  |
| 36  | 5     | 893  | C    | 2.3  |
| 51  | M5    | 60   | VAL  | 2.3  |
| 55  | M9    | 93   | VAL  | 2.3  |
| 60  | N4    | 91   | LYS  | 2.3  |
| 8   | S6    | 85   | ARG  | 2.3  |
| 18  | C6    | 137  | ARG  | 2.3  |
| 51  | m5    | 188  | ARG  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 63  | n7    | 17   | ARG  | 2.3  |
| 71  | O5    | 105  | ARG  | 2.3  |
| 77  | q1    | 18   | ARG  | 2.3  |
| 9   | S7    | 91   | ILE  | 2.3  |
| 14  | C2    | 89   | ILE  | 2.3  |
| 15  | c3    | 66   | ILE  | 2.3  |
| 22  | D0    | 24   | ILE  | 2.3  |
| 31  | D9    | 50   | ILE  | 2.3  |
| 61  | n5    | 63   | ILE  | 2.3  |
| 63  | N7    | 50   | PRO  | 2.3  |
| 51  | m5    | 2    | GLY  | 2.3  |
| 14  | c2    | 128  | ALA  | 2.3  |
| 34  | sR    | 119  | ALA  | 2.3  |
| 53  | M7    | 178  | ALA  | 2.3  |
| 5   | s3    | 172  | THR  | 2.3  |
| 8   | S6    | 12   | SER  | 2.3  |
| 24  | D2    | 107  | SER  | 2.3  |
| 59  | n3    | 133  | SER  | 2.3  |
| 72  | O6    | 2    | THR  | 2.3  |
| 80  | c0    | 57   | THR  | 2.3  |
| 3   | S1    | 217  | LEU  | 2.3  |
| 17  | c5    | 36   | LEU  | 2.3  |
| 20  | C8    | 137  | HIS  | 2.3  |
| 34  | SR    | 9    | LEU  | 2.3  |
| 62  | n6    | 35   | LEU  | 2.3  |
| 1   | 2     | 872  | G    | 2.3  |
| 1   | 2     | 875  | G    | 2.3  |
| 1   | 2     | 957  | G    | 2.3  |
| 1   | 6     | 1051 | G    | 2.3  |
| 1   | 6     | 1330 | G    | 2.3  |
| 11  | S9    | 95   | TYR  | 2.3  |
| 20  | C8    | 42   | TYR  | 2.3  |
| 36  | 5     | 236  | G    | 2.3  |
| 40  | L3    | 118  | PHE  | 2.3  |
| 47  | M0    | 213  | PHE  | 2.3  |
| 70  | o4    | 7    | PHE  | 2.3  |
| 7   | S5    | 100  | ASN  | 2.3  |
| 7   | S5    | 104  | ASN  | 2.3  |
| 50  | M4    | 47   | ASP  | 2.3  |
| 28  | D6    | 19   | LYS  | 2.3  |
| 34  | SR    | 118  | LYS  | 2.3  |
| 55  | M9    | 80   | LYS  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | 2     | 929  | A    | 2.3  |
| 2   | s0    | 123  | VAL  | 2.3  |
| 8   | S6    | 219  | ARG  | 2.3  |
| 11  | s9    | 179  | ARG  | 2.3  |
| 17  | C5    | 105  | VAL  | 2.3  |
| 22  | D0    | 56   | VAL  | 2.3  |
| 39  | l2    | 168  | VAL  | 2.3  |
| 59  | N3    | 135  | VAL  | 2.3  |
| 1   | 2     | 380  | U    | 2.3  |
| 1   | 6     | 699  | U    | 2.3  |
| 36  | 1     | 979  | U    | 2.3  |
| 36  | 1     | 1569 | U    | 2.3  |
| 36  | 5     | 83   | U    | 2.3  |
| 36  | 5     | 1555 | U    | 2.3  |
| 8   | S6    | 173  | PRO  | 2.3  |
| 27  | D5    | 89   | ILE  | 2.3  |
| 3   | S1    | 178  | GLY  | 2.3  |
| 8   | S6    | 224  | ALA  | 2.3  |
| 10  | S8    | 147  | ALA  | 2.3  |
| 10  | s8    | 198  | ALA  | 2.3  |
| 25  | D3    | 35   | GLY  | 2.3  |
| 26  | D4    | 33   | ALA  | 2.3  |
| 49  | m3    | 60   | ALA  | 2.3  |
| 1   | 6     | 489  | C    | 2.3  |
| 36  | 5     | 1563 | C    | 2.3  |
| 36  | 5     | 1631 | C    | 2.3  |
| 2   | S0    | 53   | THR  | 2.3  |
| 17  | c5    | 112  | LEU  | 2.3  |
| 15  | c3    | 5    | HIS  | 2.3  |
| 34  | SR    | 41   | THR  | 2.3  |
| 70  | O4    | 34   | HIS  | 2.3  |
| 70  | o4    | 68   | THR  | 2.3  |
| 2   | S0    | 7    | PHE  | 2.3  |
| 2   | S0    | 38   | PHE  | 2.3  |
| 3   | S1    | 205  | PHE  | 2.3  |
| 8   | S6    | 16   | PHE  | 2.3  |
| 11  | S9    | 104  | PHE  | 2.3  |
| 17  | c5    | 138  | PHE  | 2.3  |
| 34  | SR    | 295  | SER  | 2.3  |
| 46  | L9    | 22   | SER  | 2.3  |
| 54  | M8    | 181  | SER  | 2.3  |
| 45  | l8    | 49   | TYR  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 61  | n5    | 60  | TYR  | 2.3  |
| 62  | n6    | 78  | PHE  | 2.3  |
| 2   | S0    | 39  | ASN  | 2.3  |
| 2   | s0    | 162 | CYS  | 2.3  |
| 6   | s4    | 7   | LYS  | 2.3  |
| 9   | S7    | 5   | GLN  | 2.3  |
| 18  | C6    | 13  | LYS  | 2.3  |
| 18  | c6    | 83  | GLN  | 2.3  |
| 19  | C7    | 14  | LYS  | 2.3  |
| 44  | l7    | 121 | LYS  | 2.3  |
| 48  | M1    | 49  | LYS  | 2.3  |
| 16  | C4    | 84  | ARG  | 2.3  |
| 60  | N4    | 80  | ARG  | 2.3  |
| 14  | c2    | 116 | VAL  | 2.3  |
| 22  | D0    | 62  | VAL  | 2.3  |
| 23  | d1    | 82  | VAL  | 2.3  |
| 8   | S6    | 161 | GLU  | 2.2  |
| 52  | M6    | 40  | GLU  | 2.2  |
| 36  | 5     | 170 | G    | 2.2  |
| 2   | S0    | 76  | ILE  | 2.2  |
| 22  | d0    | 65  | ILE  | 2.2  |
| 75  | O9    | 27  | ILE  | 2.2  |
| 2   | s0    | 161 | PRO  | 2.2  |
| 6   | S4    | 260 | GLY  | 2.2  |
| 14  | c2    | 27  | ALA  | 2.2  |
| 22  | D0    | 75  | GLY  | 2.2  |
| 26  | D4    | 134 | ALA  | 2.2  |
| 28  | d6    | 14  | GLY  | 2.2  |
| 29  | D7    | 68  | GLY  | 2.2  |
| 31  | d9    | 17  | GLY  | 2.2  |
| 34  | sR    | 214 | ALA  | 2.2  |
| 53  | M7    | 156 | ALA  | 2.2  |
| 57  | n1    | 44  | ALA  | 2.2  |
| 63  | n7    | 124 | ALA  | 2.2  |
| 65  | N9    | 56  | ALA  | 2.2  |
| 67  | O1    | 45  | GLY  | 2.2  |
| 70  | O4    | 63  | ALA  | 2.2  |
| 70  | O4    | 78  | GLY  | 2.2  |
| 1   | 2     | 678 | A    | 2.2  |
| 1   | 6     | 260 | U    | 2.2  |
| 1   | 6     | 493 | U    | 2.2  |
| 1   | 6     | 684 | A    | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | 6     | 1060 | U    | 2.2  |
| 1   | 6     | 1397 | U    | 2.2  |
| 2   | S0    | 120  | LEU  | 2.2  |
| 6   | S4    | 44   | LEU  | 2.2  |
| 9   | S7    | 118  | LEU  | 2.2  |
| 38  | 8     | 158  | U    | 2.2  |
| 51  | M5    | 116  | LEU  | 2.2  |
| 63  | N7    | 80   | LEU  | 2.2  |
| 2   | S0    | 96   | THR  | 2.2  |
| 11  | s9    | 130  | THR  | 2.2  |
| 16  | C4    | 86   | THR  | 2.2  |
| 17  | c5    | 56   | PHE  | 2.2  |
| 33  | E1    | 87   | THR  | 2.2  |
| 75  | O9    | 34   | THR  | 2.2  |
| 3   | s1    | 151  | LYS  | 2.2  |
| 11  | S9    | 16   | LYS  | 2.2  |
| 11  | s9    | 51   | LYS  | 2.2  |
| 22  | D0    | 30   | LYS  | 2.2  |
| 31  | D9    | 9    | SER  | 2.2  |
| 31  | d9    | 14   | TYR  | 2.2  |
| 45  | L8    | 216  | SER  | 2.2  |
| 59  | n3    | 2    | SER  | 2.2  |
| 68  | O2    | 62   | LYS  | 2.2  |
| 1   | 2     | 736  | C    | 2.2  |
| 1   | 2     | 874  | C    | 2.2  |
| 14  | c2    | 43   | ARG  | 2.2  |
| 28  | D6    | 15   | ARG  | 2.2  |
| 32  | e0    | 33   | ARG  | 2.2  |
| 36  | 1     | 1951 | C    | 2.2  |
| 45  | L8    | 48   | ARG  | 2.2  |
| 3   | S1    | 127  | VAL  | 2.2  |
| 20  | c8    | 136  | GLN  | 2.2  |
| 26  | d4    | 113  | ASN  | 2.2  |
| 40  | L3    | 78   | VAL  | 2.2  |
| 2   | S0    | 72   | ASP  | 2.2  |
| 18  | C6    | 120  | ASP  | 2.2  |
| 50  | m4    | 37   | GLU  | 2.2  |
| 14  | c2    | 136  | ILE  | 2.2  |
| 24  | D2    | 75   | ILE  | 2.2  |
| 27  | d5    | 89   | ILE  | 2.2  |
| 58  | N2    | 38   | ILE  | 2.2  |
| 72  | o6    | 9    | ILE  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 5   | S3    | 220  | PRO  | 2.2  |
| 6   | s4    | 9    | LEU  | 2.2  |
| 8   | S6    | 69   | LEU  | 2.2  |
| 9   | s7    | 16   | LEU  | 2.2  |
| 18  | C6    | 18   | ALA  | 2.2  |
| 20  | C8    | 18   | LEU  | 2.2  |
| 22  | D0    | 111  | GLY  | 2.2  |
| 26  | d4    | 4    | ALA  | 2.2  |
| 27  | d5    | 104  | ALA  | 2.2  |
| 30  | d8    | 16   | LEU  | 2.2  |
| 31  | D9    | 17   | GLY  | 2.2  |
| 34  | SR    | 119  | ALA  | 2.2  |
| 42  | l5    | 7    | ALA  | 2.2  |
| 50  | M4    | 9    | ALA  | 2.2  |
| 55  | M9    | 168  | ALA  | 2.2  |
| 60  | N4    | 39   | LEU  | 2.2  |
| 71  | o5    | 87   | ALA  | 2.2  |
| 76  | Q0    | 107  | ALA  | 2.2  |
| 18  | c6    | 46   | PHE  | 2.2  |
| 26  | d4    | 9    | THR  | 2.2  |
| 34  | SR    | 283  | LYS  | 2.2  |
| 45  | l8    | 222  | PHE  | 2.2  |
| 60  | N4    | 70   | LYS  | 2.2  |
| 72  | o6    | 80   | PHE  | 2.2  |
| 78  | Q2    | 36   | PHE  | 2.2  |
| 1   | 2     | 712  | G    | 2.2  |
| 1   | 2     | 1418 | G    | 2.2  |
| 3   | S1    | 119  | THR  | 2.2  |
| 8   | S6    | 189  | HIS  | 2.2  |
| 10  | S8    | 116  | HIS  | 2.2  |
| 36  | 1     | 1577 | G    | 2.2  |
| 60  | n4    | 64   | THR  | 2.2  |
| 64  | N8    | 28   | HIS  | 2.2  |
| 1   | 2     | 1795 | U    | 2.2  |
| 1   | 6     | 1585 | U    | 2.2  |
| 8   | S6    | 137  | ARG  | 2.2  |
| 18  | C6    | 68   | ARG  | 2.2  |
| 18  | c6    | 143  | ARG  | 2.2  |
| 19  | C7    | 67   | ARG  | 2.2  |
| 22  | D0    | 90   | TYR  | 2.2  |
| 36  | 1     | 1094 | U    | 2.2  |
| 36  | 5     | 492  | U    | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 36  | 5     | 3079 | U    | 2.2  |
| 36  | 5     | 3319 | U    | 2.2  |
| 40  | L3    | 146  | ARG  | 2.2  |
| 75  | O9    | 45   | ARG  | 2.2  |
| 1   | 2     | 41   | A    | 2.2  |
| 1   | 2     | 169  | A    | 2.2  |
| 1   | 2     | 733  | A    | 2.2  |
| 1   | 2     | 1202 | A    | 2.2  |
| 1   | 6     | 793  | A    | 2.2  |
| 1   | 6     | 1693 | A    | 2.2  |
| 10  | S8    | 7    | SER  | 2.2  |
| 36  | 5     | 1025 | A    | 2.2  |
| 36  | 5     | 1036 | A    | 2.2  |
| 36  | 5     | 1278 | A    | 2.2  |
| 51  | m5    | 171  | SER  | 2.2  |
| 14  | c2    | 60   | VAL  | 2.2  |
| 30  | D8    | 25   | VAL  | 2.2  |
| 52  | M6    | 3    | VAL  | 2.2  |
| 51  | M5    | 34   | ASN  | 2.2  |
| 21  | C9    | 116  | ILE  | 2.2  |
| 1   | 6     | 731  | C    | 2.2  |
| 2   | S0    | 9    | LEU  | 2.2  |
| 2   | S0    | 35   | PRO  | 2.2  |
| 3   | S1    | 54   | LEU  | 2.2  |
| 3   | S1    | 141  | ALA  | 2.2  |
| 4   | s2    | 61   | LEU  | 2.2  |
| 7   | s5    | 145  | ASP  | 2.2  |
| 11  | s9    | 5    | PRO  | 2.2  |
| 14  | c2    | 28   | LEU  | 2.2  |
| 14  | c2    | 98   | GLY  | 2.2  |
| 18  | C6    | 44   | LEU  | 2.2  |
| 19  | C7    | 115  | LEU  | 2.2  |
| 21  | C9    | 95   | ASP  | 2.2  |
| 36  | 1     | 439  | C    | 2.2  |
| 36  | 1     | 1562 | C    | 2.2  |
| 37  | 3     | 73   | C    | 2.2  |
| 46  | l9    | 190  | ASP  | 2.2  |
| 20  | c8    | 76   | PRO  | 2.2  |
| 21  | C9    | 118  | PRO  | 2.2  |
| 22  | D0    | 110  | PRO  | 2.2  |
| 29  | D7    | 53   | ALA  | 2.2  |
| 33  | E1    | 124  | PRO  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 45  | l8    | 99  | PRO  | 2.2  |
| 57  | N1    | 2   | GLY  | 2.2  |
| 61  | N5    | 113 | LEU  | 2.2  |
| 64  | N8    | 149 | ALA  | 2.2  |
| 65  | N9    | 30  | PRO  | 2.2  |
| 80  | c0    | 23  | ALA  | 2.2  |
| 8   | S6    | 187 | LYS  | 2.2  |
| 11  | S9    | 10  | LYS  | 2.2  |
| 28  | D6    | 70  | LYS  | 2.2  |
| 33  | e1    | 143 | LYS  | 2.2  |
| 34  | SR    | 87  | LYS  | 2.2  |
| 67  | O1    | 27  | LYS  | 2.2  |
| 73  | o7    | 85  | LYS  | 2.2  |
| 78  | q2    | 78  | LYS  | 2.2  |
| 10  | S8    | 27  | PHE  | 2.2  |
| 22  | d0    | 79  | TRP  | 2.2  |
| 48  | M1    | 127 | PHE  | 2.2  |
| 6   | S4    | 252 | ARG  | 2.2  |
| 48  | M1    | 51  | ARG  | 2.2  |
| 69  | o3    | 60  | ARG  | 2.2  |
| 11  | S9    | 7   | THR  | 2.2  |
| 13  | C1    | 31  | THR  | 2.2  |
| 18  | c6    | 21  | HIS  | 2.2  |
| 21  | C9    | 93  | HIS  | 2.2  |
| 22  | D0    | 27  | THR  | 2.2  |
| 26  | d4    | 121 | THR  | 2.2  |
| 7   | S5    | 209 | TYR  | 2.2  |
| 18  | C6    | 142 | TYR  | 2.2  |
| 2   | s0    | 143 | VAL  | 2.2  |
| 8   | S6    | 81  | VAL  | 2.2  |
| 16  | c4    | 67  | VAL  | 2.2  |
| 25  | D3    | 120 | VAL  | 2.2  |
| 35  | SM    | 106 | VAL  | 2.2  |
| 16  | C4    | 22  | SER  | 2.2  |
| 16  | C4    | 123 | SER  | 2.2  |
| 60  | N4    | 95  | SER  | 2.2  |
| 60  | n4    | 95  | SER  | 2.2  |
| 77  | q1    | 24  | SER  | 2.2  |
| 1   | 2     | 626 | U    | 2.2  |
| 1   | 2     | 701 | U    | 2.2  |
| 1   | 2     | 820 | U    | 2.2  |
| 3   | S1    | 92  | GLN  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 4   | S2    | 94   | GLN  | 2.2  |
| 36  | 1     | 1353 | U    | 2.2  |
| 36  | 1     | 2209 | U    | 2.2  |
| 36  | 1     | 2538 | U    | 2.2  |
| 36  | 5     | 2875 | U    | 2.2  |
| 38  | 8     | 82   | U    | 2.2  |
| 2   | s0    | 98   | ILE  | 2.2  |
| 17  | C5    | 84   | ILE  | 2.2  |
| 18  | C6    | 29   | ILE  | 2.2  |
| 19  | C7    | 38   | ILE  | 2.2  |
| 1   | 2     | 236  | A    | 2.2  |
| 1   | 2     | 647  | G    | 2.2  |
| 1   | 2     | 810  | G    | 2.2  |
| 1   | 6     | 669  | G    | 2.2  |
| 1   | 6     | 1265 | G    | 2.2  |
| 1   | 6     | 1601 | G    | 2.2  |
| 26  | D4    | 31   | ASN  | 2.2  |
| 29  | d7    | 57   | GLU  | 2.2  |
| 31  | D9    | 53   | ASN  | 2.2  |
| 35  | sM    | 50   | ASN  | 2.2  |
| 36  | 1     | 243  | G    | 2.2  |
| 36  | 1     | 1024 | G    | 2.2  |
| 36  | 1     | 3291 | G    | 2.2  |
| 36  | 5     | 1152 | G    | 2.2  |
| 5   | s3    | 142  | LEU  | 2.2  |
| 6   | S4    | 9    | LEU  | 2.2  |
| 10  | S8    | 193  | LEU  | 2.2  |
| 14  | c2    | 62   | LEU  | 2.2  |
| 19  | C7    | 119  | LEU  | 2.2  |
| 24  | D2    | 111  | MET  | 2.2  |
| 27  | d5    | 65   | LEU  | 2.2  |
| 22  | d0    | 73   | GLY  | 2.2  |
| 23  | D1    | 45   | ALA  | 2.2  |
| 30  | D8    | 57   | MET  | 2.2  |
| 34  | sR    | 225  | LEU  | 2.2  |
| 36  | 5     | 1352 | A    | 2.2  |
| 79  | Q3    | 22   | LEU  | 2.2  |
| 2   | S0    | 90   | ALA  | 2.2  |
| 4   | S2    | 85   | PRO  | 2.2  |
| 7   | s5    | 191  | ALA  | 2.2  |
| 11  | S9    | 169  | PRO  | 2.2  |
| 16  | c4    | 109  | GLY  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 50  | M4    | 75   | GLY  | 2.2  |
| 55  | m9    | 189  | ALA  | 2.2  |
| 19  | c7    | 27   | ASP  | 2.2  |
| 78  | Q2    | 100  | LYS  | 2.2  |
| 6   | s4    | 200  | ARG  | 2.2  |
| 9   | s7    | 39   | ARG  | 2.2  |
| 10  | S8    | 146  | ARG  | 2.2  |
| 16  | c4    | 135  | ARG  | 2.2  |
| 26  | d4    | 60   | PHE  | 2.2  |
| 34  | sR    | 263  | PHE  | 2.2  |
| 63  | N7    | 65   | ARG  | 2.2  |
| 1   | 2     | 937  | C    | 2.2  |
| 1   | 2     | 1374 | C    | 2.2  |
| 1   | 6     | 1192 | C    | 2.2  |
| 1   | 6     | 1709 | C    | 2.2  |
| 36  | 1     | 1670 | C    | 2.2  |
| 16  | C4    | 91   | THR  | 2.2  |
| 20  | C8    | 78   | HIS  | 2.2  |
| 54  | m8    | 15   | HIS  | 2.2  |
| 71  | O5    | 46   | THR  | 2.2  |
| 2   | S0    | 45   | VAL  | 2.2  |
| 14  | c2    | 121  | VAL  | 2.2  |
| 18  | C6    | 79   | TYR  | 2.2  |
| 62  | N6    | 59   | VAL  | 2.2  |
| 9   | s7    | 125  | ILE  | 2.2  |
| 18  | c6    | 43   | ILE  | 2.2  |
| 27  | D5    | 71   | ILE  | 2.2  |
| 47  | m0    | 113  | GLN  | 2.2  |
| 60  | N4    | 9    | SER  | 2.2  |
| 68  | o2    | 52   | GLN  | 2.2  |
| 4   | S2    | 61   | LEU  | 2.2  |
| 34  | SR    | 225  | LEU  | 2.2  |
| 34  | sR    | 144  | LEU  | 2.2  |
| 39  | l2    | 246  | LEU  | 2.2  |
| 7   | S5    | 99   | MET  | 2.2  |
| 2   | S0    | 49   | ASN  | 2.2  |
| 2   | S0    | 145  | ALA  | 2.2  |
| 6   | S4    | 2    | ALA  | 2.2  |
| 22  | D0    | 83   | GLU  | 2.2  |
| 23  | d1    | 35   | ASN  | 2.2  |
| 27  | d5    | 97   | LYS  | 2.2  |
| 30  | d8    | 43   | ASN  | 2.2  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 34         | sR           | 162        | ALA         | 2.2         |
| 41         | l4           | 63         | GLU         | 2.2         |
| 50         | m4           | 9          | ALA         | 2.2         |
| 52         | M6           | 169        | ALA         | 2.2         |
| 56         | N0           | 2          | ALA         | 2.2         |
| 41         | L4           | 79         | GLY         | 2.2         |
| 41         | L4           | 350        | LYS         | 2.2         |
| 45         | L8           | 45         | ASN         | 2.2         |
| 73         | O7           | 86         | ALA         | 2.2         |
| 1          | 2            | 1240       | U           | 2.2         |
| 1          | 2            | 1582       | U           | 2.2         |
| 1          | 6            | 721        | U           | 2.2         |
| 4          | S2           | 223        | GLY         | 2.2         |
| 30         | D8           | 24         | GLY         | 2.2         |
| 60         | n4           | 62         | GLY         | 2.2         |
| 65         | N9           | 20         | GLY         | 2.2         |
| 24         | D2           | 72         | CYS         | 2.2         |
| 29         | D7           | 37         | CYS         | 2.2         |
| 34         | SR           | 71         | CYS         | 2.2         |
| 55         | M9           | 181        | ARG         | 2.2         |
| 3          | s1           | 89         | ASP         | 2.2         |
| 7          | S5           | 55         | ASP         | 2.2         |
| 7          | s5           | 43         | PHE         | 2.2         |
| 21         | c9           | 95         | ASP         | 2.2         |
| 46         | L9           | 45         | PHE         | 2.2         |
| 1          | 2            | 65         | A           | 2.2         |
| 1          | 2            | 445        | A           | 2.2         |
| 1          | 2            | 1300       | A           | 2.2         |
| 1          | 2            | 1410       | A           | 2.2         |
| 1          | 2            | 1635       | A           | 2.2         |
| 1          | 6            | 218        | A           | 2.2         |
| 1          | 6            | 1069       | A           | 2.2         |
| 36         | 5            | 2626       | A           | 2.2         |
| 1          | 2            | 196        | G           | 2.2         |
| 1          | 2            | 574        | G           | 2.2         |
| 1          | 2            | 938        | G           | 2.2         |
| 36         | 1            | 1243       | G           | 2.2         |
| 36         | 1            | 1281       | G           | 2.2         |
| 36         | 1            | 2169       | G           | 2.2         |
| 36         | 5            | 1236       | G           | 2.2         |
| 36         | 5            | 1811       | G           | 2.2         |
| 70         | o4           | 69         | HIS         | 2.2         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 4   | S2    | 167  | VAL  | 2.1  |
| 27  | d5    | 105  | THR  | 2.1  |
| 33  | E1    | 150  | VAL  | 2.1  |
| 53  | m7    | 24   | VAL  | 2.1  |
| 60  | N4    | 64   | THR  | 2.1  |
| 68  | O2    | 10   | VAL  | 2.1  |
| 70  | o4    | 22   | VAL  | 2.1  |
| 73  | o7    | 80   | THR  | 2.1  |
| 82  | p0    | 50   | VAL  | 2.1  |
| 55  | m9    | 109  | TYR  | 2.1  |
| 1   | 2     | 268  | C    | 2.1  |
| 1   | 2     | 381  | C    | 2.1  |
| 1   | 6     | 700  | C    | 2.1  |
| 1   | 6     | 1581 | C    | 2.1  |
| 10  | S8    | 43   | ILE  | 2.1  |
| 19  | c7    | 38   | ILE  | 2.1  |
| 36  | 1     | 1275 | C    | 2.1  |
| 36  | 1     | 1759 | C    | 2.1  |
| 36  | 1     | 3164 | C    | 2.1  |
| 36  | 5     | 1951 | C    | 2.1  |
| 45  | L8    | 179  | ILE  | 2.1  |
| 82  | p0    | 4    | ILE  | 2.1  |
| 8   | s6    | 216  | LEU  | 2.1  |
| 11  | s9    | 60   | LEU  | 2.1  |
| 17  | c5    | 104  | GLN  | 2.1  |
| 29  | D7    | 51   | GLN  | 2.1  |
| 42  | l5    | 274  | GLN  | 2.1  |
| 51  | M5    | 134  | LEU  | 2.1  |
| 54  | m8    | 166  | LEU  | 2.1  |
| 69  | O3    | 7    | LEU  | 2.1  |
| 75  | O9    | 11   | GLN  | 2.1  |
| 2   | S0    | 78   | SER  | 2.1  |
| 16  | C4    | 36   | LYS  | 2.1  |
| 18  | C6    | 87   | LYS  | 2.1  |
| 20  | c8    | 139  | LYS  | 2.1  |
| 21  | C9    | 75   | LYS  | 2.1  |
| 2   | S0    | 154  | GLU  | 2.1  |
| 10  | S8    | 79   | ALA  | 2.1  |
| 11  | s9    | 162  | SER  | 2.1  |
| 13  | c1    | 2    | SER  | 2.1  |
| 22  | d0    | 77   | LYS  | 2.1  |
| 26  | D4    | 21   | LYS  | 2.1  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 32         | E0           | 53         | LYS         | 2.1         |
| 33         | E1           | 116        | LYS         | 2.1         |
| 34         | SR           | 82         | SER         | 2.1         |
| 34         | sR           | 213        | SER         | 2.1         |
| 39         | l2           | 68         | LYS         | 2.1         |
| 34         | sR           | 257        | ALA         | 2.1         |
| 55         | M9           | 59         | SER         | 2.1         |
| 45         | L8           | 208        | GLU         | 2.1         |
| 45         | L8           | 209        | ALA         | 2.1         |
| 72         | o6           | 32         | ALA         | 2.1         |
| 80         | c0           | 70         | GLU         | 2.1         |
| 82         | p0           | 107        | ALA         | 2.1         |
| 6          | S4           | 255        | ARG         | 2.1         |
| 17         | c5           | 38         | PRO         | 2.1         |
| 21         | C9           | 7          | ARG         | 2.1         |
| 21         | c9           | 90         | PRO         | 2.1         |
| 48         | M1           | 83         | GLY         | 2.1         |
| 64         | N8           | 37         | GLY         | 2.1         |
| 44         | L7           | 166        | ASN         | 2.1         |
| 80         | c0           | 81         | ASN         | 2.1         |
| 15         | C3           | 26         | PHE         | 2.1         |
| 45         | l8           | 34         | PHE         | 2.1         |
| 52         | M6           | 80         | PHE         | 2.1         |
| 58         | N2           | 95         | PHE         | 2.1         |
| 61         | N5           | 32         | PHE         | 2.1         |
| 63         | N7           | 92         | PHE         | 2.1         |
| 1          | 2            | 73         | U           | 2.1         |
| 1          | 2            | 1423       | U           | 2.1         |
| 2          | S0           | 190        | ASP         | 2.1         |
| 14         | C2           | 93         | ASP         | 2.1         |
| 36         | 5            | 2508       | U           | 2.1         |
| 13         | C1           | 140        | VAL         | 2.1         |
| 16         | c4           | 28         | VAL         | 2.1         |
| 22         | d0           | 42         | VAL         | 2.1         |
| 24         | D2           | 120        | HIS         | 2.1         |
| 28         | D6           | 72         | HIS         | 2.1         |
| 29         | d7           | 2          | VAL         | 2.1         |
| 45         | l8           | 116        | VAL         | 2.1         |
| 50         | m4           | 131        | VAL         | 2.1         |
| 57         | N1           | 124        | VAL         | 2.1         |
| 70         | o4           | 5          | VAL         | 2.1         |
| 4          | S2           | 51         | THR         | 2.1         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 74  | O8    | 24   | THR  | 2.1  |
| 1   | 2     | 86   | A    | 2.1  |
| 1   | 2     | 135  | A    | 2.1  |
| 2   | S0    | 175  | TYR  | 2.1  |
| 3   | S1    | 197  | ILE  | 2.1  |
| 11  | S9    | 8    | TYR  | 2.1  |
| 16  | C4    | 20   | TYR  | 2.1  |
| 18  | C6    | 65   | ILE  | 2.1  |
| 34  | SR    | 211  | ILE  | 2.1  |
| 36  | 1     | 440  | A    | 2.1  |
| 72  | O6    | 28   | TYR  | 2.1  |
| 3   | S1    | 86   | LEU  | 2.1  |
| 13  | C1    | 26   | LYS  | 2.1  |
| 21  | C9    | 78   | LYS  | 2.1  |
| 26  | d4    | 128  | LYS  | 2.1  |
| 27  | d5    | 75   | LEU  | 2.1  |
| 30  | D8    | 9    | LEU  | 2.1  |
| 31  | d9    | 30   | LEU  | 2.1  |
| 34  | SR    | 7    | LEU  | 2.1  |
| 41  | l4    | 235  | LEU  | 2.1  |
| 45  | L8    | 92   | LYS  | 2.1  |
| 60  | N4    | 41   | LYS  | 2.1  |
| 60  | n4    | 61   | LYS  | 2.1  |
| 1   | 2     | 127  | G    | 2.1  |
| 1   | 2     | 714  | G    | 2.1  |
| 1   | 2     | 729  | G    | 2.1  |
| 1   | 2     | 834  | G    | 2.1  |
| 1   | 2     | 1521 | G    | 2.1  |
| 1   | 6     | 1241 | G    | 2.1  |
| 4   | s2    | 94   | GLN  | 2.1  |
| 34  | sR    | 177  | MET  | 2.1  |
| 36  | 1     | 2111 | G    | 2.1  |
| 36  | 5     | 2522 | G    | 2.1  |
| 48  | M1    | 9    | MET  | 2.1  |
| 71  | o5    | 108  | GLN  | 2.1  |
| 2   | s0    | 145  | ALA  | 2.1  |
| 9   | S7    | 59   | ALA  | 2.1  |
| 9   | s7    | 3    | ALA  | 2.1  |
| 14  | c2    | 101  | ALA  | 2.1  |
| 15  | C3    | 63   | ALA  | 2.1  |
| 15  | c3    | 15   | ALA  | 2.1  |
| 26  | D4    | 126  | ALA  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 34  | sR    | 24   | ALA  | 2.1  |
| 58  | N2    | 46   | ALA  | 2.1  |
| 8   | s6    | 35   | GLU  | 2.1  |
| 10  | S8    | 71   | GLY  | 2.1  |
| 1   | 2     | 25   | C    | 2.1  |
| 1   | 2     | 54   | C    | 2.1  |
| 1   | 2     | 1045 | C    | 2.1  |
| 1   | 6     | 1159 | C    | 2.1  |
| 2   | S0    | 11   | PRO  | 2.1  |
| 2   | S0    | 97   | PRO  | 2.1  |
| 16  | C4    | 94   | PRO  | 2.1  |
| 29  | d7    | 68   | GLY  | 2.1  |
| 34  | sR    | 247  | PRO  | 2.1  |
| 40  | l3    | 253  | GLY  | 2.1  |
| 42  | l5    | 47   | PRO  | 2.1  |
| 55  | M9    | 48   | GLY  | 2.1  |
| 61  | n5    | 79   | GLY  | 2.1  |
| 66  | O0    | 88   | GLY  | 2.1  |
| 72  | O6    | 14   | GLY  | 2.1  |
| 79  | q3    | 21   | SER  | 2.1  |
| 36  | 1     | 242  | C    | 2.1  |
| 36  | 1     | 648  | C    | 2.1  |
| 36  | 1     | 1254 | C    | 2.1  |
| 36  | 1     | 3285 | C    | 2.1  |
| 36  | 5     | 1092 | C    | 2.1  |
| 36  | 5     | 1633 | C    | 2.1  |
| 36  | 5     | 2539 | C    | 2.1  |
| 7   | S5    | 79   | ASN  | 2.1  |
| 12  | C0    | 28   | ASN  | 2.1  |
| 13  | c1    | 37   | ASN  | 2.1  |
| 17  | C5    | 119  | PHE  | 2.1  |
| 19  | C7    | 71   | PHE  | 2.1  |
| 19  | c7    | 104  | ASN  | 2.1  |
| 26  | d4    | 64   | PHE  | 2.1  |
| 3   | s1    | 114  | VAL  | 2.1  |
| 14  | C2    | 91   | VAL  | 2.1  |
| 17  | c5    | 11   | VAL  | 2.1  |
| 18  | c6    | 67   | VAL  | 2.1  |
| 19  | C7    | 9    | VAL  | 2.1  |
| 21  | c9    | 37   | VAL  | 2.1  |
| 24  | d2    | 85   | ASP  | 2.1  |
| 34  | SR    | 68   | VAL  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 40  | L3    | 229  | VAL  | 2.1  |
| 51  | m5    | 200  | TRP  | 2.1  |
| 69  | o3    | 27   | VAL  | 2.1  |
| 1   | 2     | 216  | U    | 2.1  |
| 1   | 2     | 1473 | U    | 2.1  |
| 2   | S0    | 173  | ILE  | 2.1  |
| 2   | S0    | 177  | LEU  | 2.1  |
| 2   | s0    | 177  | LEU  | 2.1  |
| 5   | s3    | 115  | ILE  | 2.1  |
| 6   | S4    | 173  | ILE  | 2.1  |
| 6   | S4    | 198  | LYS  | 2.1  |
| 8   | s6    | 163  | THR  | 2.1  |
| 11  | S9    | 143  | ILE  | 2.1  |
| 14  | c2    | 53   | THR  | 2.1  |
| 12  | C0    | 41   | TYR  | 2.1  |
| 18  | C6    | 132  | LYS  | 2.1  |
| 18  | c6    | 37   | THR  | 2.1  |
| 25  | d3    | 110  | LYS  | 2.1  |
| 34  | sR    | 81   | LEU  | 2.1  |
| 34  | sR    | 292  | LEU  | 2.1  |
| 37  | 3     | 106  | U    | 2.1  |
| 40  | L3    | 102  | LEU  | 2.1  |
| 45  | l8    | 245  | LYS  | 2.1  |
| 49  | m3    | 7    | LEU  | 2.1  |
| 49  | m3    | 178  | LYS  | 2.1  |
| 61  | n5    | 40   | LEU  | 2.1  |
| 62  | n6    | 113  | LYS  | 2.1  |
| 63  | N7    | 60   | LYS  | 2.1  |
| 64  | N8    | 70   | LYS  | 2.1  |
| 5   | s3    | 150  | MET  | 2.1  |
| 28  | D6    | 22   | ARG  | 2.1  |
| 35  | sM    | 68   | ARG  | 2.1  |
| 62  | N6    | 12   | ARG  | 2.1  |
| 63  | n7    | 15   | ARG  | 2.1  |
| 68  | O2    | 19   | ARG  | 2.1  |
| 77  | Q1    | 6    | ARG  | 2.1  |
| 7   | S5    | 56   | ALA  | 2.1  |
| 10  | s8    | 13   | ALA  | 2.1  |
| 14  | C2    | 101  | ALA  | 2.1  |
| 14  | c2    | 143  | GLN  | 2.1  |
| 18  | c6    | 20   | ALA  | 2.1  |
| 34  | SR    | 24   | ALA  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 56  | n0    | 138  | GLN  | 2.1  |
| 71  | O5    | 65   | ALA  | 2.1  |
| 1   | 2     | 599  | A    | 2.1  |
| 1   | 6     | 579  | A    | 2.1  |
| 2   | S0    | 142  | PRO  | 2.1  |
| 20  | C8    | 82   | PRO  | 2.1  |
| 33  | E1    | 129  | GLY  | 2.1  |
| 34  | SR    | 158  | PRO  | 2.1  |
| 36  | 1     | 1260 | A    | 2.1  |
| 36  | 1     | 1575 | A    | 2.1  |
| 44  | l7    | 217  | PRO  | 2.1  |
| 49  | m3    | 61   | PRO  | 2.1  |
| 49  | m3    | 130  | GLY  | 2.1  |
| 70  | o4    | 26   | PRO  | 2.1  |
| 8   | S6    | 45   | PHE  | 2.1  |
| 10  | S8    | 149  | SER  | 2.1  |
| 21  | C9    | 97   | SER  | 2.1  |
| 30  | D8    | 21   | SER  | 2.1  |
| 33  | e1    | 122  | SER  | 2.1  |
| 34  | SR    | 186  | PHE  | 2.1  |
| 57  | N1    | 47   | SER  | 2.1  |
| 64  | N8    | 16   | SER  | 2.1  |
| 69  | O3    | 62   | SER  | 2.1  |
| 35  | sM    | 71   | ASN  | 2.1  |
| 1   | 2     | 514  | G    | 2.1  |
| 1   | 2     | 628  | G    | 2.1  |
| 1   | 6     | 739  | G    | 2.1  |
| 1   | 6     | 797  | G    | 2.1  |
| 1   | 6     | 1445 | G    | 2.1  |
| 2   | s0    | 139  | VAL  | 2.1  |
| 16  | C4    | 30   | VAL  | 2.1  |
| 18  | C6    | 4    | VAL  | 2.1  |
| 26  | D4    | 100  | VAL  | 2.1  |
| 26  | D4    | 129  | VAL  | 2.1  |
| 32  | E0    | 50   | VAL  | 2.1  |
| 36  | 1     | 1954 | G    | 2.1  |
| 36  | 5     | 443  | G    | 2.1  |
| 1   | 2     | 176  | C    | 2.1  |
| 1   | 2     | 489  | C    | 2.1  |
| 36  | 5     | 439  | C    | 2.1  |
| 5   | S3    | 59   | LEU  | 2.1  |
| 5   | s3    | 174  | HIS  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 8   | S6    | 155  | ASP  | 2.1  |
| 8   | s6    | 79   | LYS  | 2.1  |
| 9   | S7    | 89   | HIS  | 2.1  |
| 14  | c2    | 26   | ASP  | 2.1  |
| 22  | D0    | 21   | LYS  | 2.1  |
| 35  | SM    | 105  | LYS  | 2.1  |
| 55  | m9    | 46   | LYS  | 2.1  |
| 61  | N5    | 22   | LYS  | 2.1  |
| 62  | N6    | 116  | LYS  | 2.1  |
| 65  | N9    | 28   | LYS  | 2.1  |
| 14  | c2    | 32   | LEU  | 2.1  |
| 14  | c2    | 103  | LEU  | 2.1  |
| 20  | c8    | 47   | CYS  | 2.1  |
| 23  | D1    | 69   | LEU  | 2.1  |
| 26  | D4    | 40   | LEU  | 2.1  |
| 27  | d5    | 41   | ILE  | 2.1  |
| 58  | n2    | 105  | LEU  | 2.1  |
| 3   | S1    | 64   | ARG  | 2.1  |
| 3   | s1    | 52   | THR  | 2.1  |
| 4   | s2    | 97   | ARG  | 2.1  |
| 13  | c1    | 129  | ARG  | 2.1  |
| 17  | C5    | 50   | THR  | 2.1  |
| 21  | C9    | 134  | ARG  | 2.1  |
| 29  | D7    | 17   | ARG  | 2.1  |
| 29  | d7    | 52   | THR  | 2.1  |
| 77  | Q1    | 9    | ARG  | 2.1  |
| 82  | p0    | 64   | ARG  | 2.1  |
| 15  | c3    | 72   | MET  | 2.1  |
| 13  | c1    | 145  | ALA  | 2.1  |
| 16  | C4    | 59   | ALA  | 2.1  |
| 16  | c4    | 40   | ALA  | 2.1  |
| 34  | SR    | 244  | ALA  | 2.1  |
| 35  | sM    | 35   | ALA  | 2.1  |
| 1   | 2     | 278  | U    | 2.1  |
| 1   | 2     | 1009 | U    | 2.1  |
| 1   | 6     | 132  | U    | 2.1  |
| 18  | C6    | 8    | GLN  | 2.1  |
| 26  | D4    | 63   | GLN  | 2.1  |
| 36  | 5     | 3287 | U    | 2.1  |
| 21  | C9    | 81   | GLY  | 2.1  |
| 33  | e1    | 127  | GLY  | 2.1  |
| 34  | SR    | 63   | GLY  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 51  | M5    | 88   | GLY  | 2.1  |
| 59  | n3    | 43   | GLY  | 2.1  |
| 2   | S0    | 180  | GLU  | 2.1  |
| 6   | S4    | 172  | PHE  | 2.1  |
| 26  | D4    | 58   | PHE  | 2.1  |
| 45  | L8    | 34   | PHE  | 2.1  |
| 52  | m6    | 174  | PHE  | 2.1  |
| 11  | S9    | 145  | SER  | 2.1  |
| 14  | C2    | 119  | SER  | 2.1  |
| 17  | c5    | 92   | SER  | 2.1  |
| 34  | sR    | 246  | SER  | 2.1  |
| 66  | o0    | 6    | SER  | 2.1  |
| 3   | S1    | 68   | VAL  | 2.1  |
| 8   | S6    | 26   | VAL  | 2.1  |
| 11  | S9    | 127  | VAL  | 2.1  |
| 14  | c2    | 86   | VAL  | 2.1  |
| 16  | C4    | 79   | VAL  | 2.1  |
| 16  | c4    | 121  | VAL  | 2.1  |
| 30  | d8    | 15   | VAL  | 2.1  |
| 70  | O4    | 35   | VAL  | 2.1  |
| 1   | 2     | 168  | A    | 2.1  |
| 1   | 2     | 1341 | A    | 2.1  |
| 1   | 6     | 1503 | A    | 2.1  |
| 2   | S0    | 134  | LYS  | 2.1  |
| 6   | S4    | 10   | LYS  | 2.1  |
| 7   | S5    | 106  | LYS  | 2.1  |
| 13  | C1    | 22   | ASN  | 2.1  |
| 14  | c2    | 70   | ASN  | 2.1  |
| 14  | c2    | 95   | LYS  | 2.1  |
| 18  | C6    | 32   | ASN  | 2.1  |
| 22  | D0    | 69   | LYS  | 2.1  |
| 25  | D3    | 5    | LYS  | 2.1  |
| 27  | d5    | 46   | LYS  | 2.1  |
| 28  | d6    | 8    | ASN  | 2.1  |
| 31  | D9    | 16   | LYS  | 2.1  |
| 33  | E1    | 134  | ASN  | 2.1  |
| 35  | sM    | 29   | ASN  | 2.1  |
| 36  | 1     | 1263 | A    | 2.1  |
| 36  | 1     | 1858 | A    | 2.1  |
| 36  | 1     | 2126 | A    | 2.1  |
| 36  | 1     | 3165 | A    | 2.1  |
| 36  | 5     | 3347 | A    | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 74  | O8    | 29   | LYS  | 2.1  |
| 3   | S1    | 189  | ILE  | 2.1  |
| 8   | S6    | 32   | ILE  | 2.1  |
| 21  | C9    | 113  | ILE  | 2.1  |
| 23  | D1    | 87   | ARG  | 2.1  |
| 29  | D7    | 7    | LEU  | 2.1  |
| 41  | l4    | 198  | ARG  | 2.1  |
| 45  | l8    | 48   | ARG  | 2.1  |
| 71  | o5    | 109  | ILE  | 2.1  |
| 33  | E1    | 135  | HIS  | 2.1  |
| 73  | o7    | 12   | HIS  | 2.1  |
| 7   | S5    | 161  | ASP  | 2.1  |
| 11  | S9    | 147  | MET  | 2.1  |
| 15  | c3    | 110  | ASP  | 2.1  |
| 17  | c5    | 83   | MET  | 2.1  |
| 67  | O1    | 6    | ASP  | 2.1  |
| 12  | C0    | 63   | TYR  | 2.1  |
| 12  | C0    | 66   | TYR  | 2.1  |
| 26  | D4    | 89   | TYR  | 2.1  |
| 28  | d6    | 74   | CYS  | 2.1  |
| 31  | D9    | 24   | CYS  | 2.1  |
| 31  | d9    | 28   | THR  | 2.1  |
| 33  | e1    | 86   | THR  | 2.1  |
| 45  | L8    | 134  | TYR  | 2.1  |
| 56  | n0    | 145  | THR  | 2.1  |
| 80  | c0    | 67   | THR  | 2.1  |
| 82  | p0    | 18   | TYR  | 2.1  |
| 1   | 2     | 239  | C    | 2.1  |
| 1   | 2     | 321  | C    | 2.1  |
| 1   | 2     | 479  | C    | 2.1  |
| 1   | 2     | 1068 | C    | 2.1  |
| 1   | 6     | 490  | C    | 2.1  |
| 1   | 2     | 284  | G    | 2.1  |
| 1   | 2     | 291  | G    | 2.1  |
| 1   | 2     | 901  | G    | 2.1  |
| 1   | 2     | 1233 | G    | 2.1  |
| 1   | 6     | 1165 | G    | 2.1  |
| 2   | s0    | 60   | ALA  | 2.1  |
| 10  | S8    | 150  | ALA  | 2.1  |
| 13  | c1    | 48   | ALA  | 2.1  |
| 36  | 1     | 765  | C    | 2.1  |
| 36  | 1     | 1232 | C    | 2.1  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 36         | 5            | 1237       | G           | 2.1         |
| 48         | M1           | 169        | ALA         | 2.1         |
| 49         | M3           | 38         | ALA         | 2.1         |
| 2          | S0           | 193        | GLN         | 2.1         |
| 6          | s4           | 132        | GLY         | 2.1         |
| 7          | S5           | 86         | GLN         | 2.1         |
| 32         | e0           | 32         | GLY         | 2.1         |
| 40         | l3           | 330        | GLY         | 2.1         |
| 6          | S4           | 152        | PRO         | 2.1         |
| 14         | C2           | 99         | GLU         | 2.1         |
| 21         | c9           | 47         | PRO         | 2.1         |
| 34         | sR           | 245        | PHE         | 2.1         |
| 42         | l5           | 217        | GLU         | 2.1         |
| 45         | l8           | 25         | PRO         | 2.1         |
| 60         | N4           | 65         | GLU         | 2.1         |
| 1          | 2            | 240        | U           | 2.0         |
| 1          | 2            | 928        | U           | 2.0         |
| 1          | 2            | 1413       | U           | 2.0         |
| 1          | 6            | 227        | U           | 2.0         |
| 1          | 6            | 499        | U           | 2.0         |
| 1          | 6            | 836        | U           | 2.0         |
| 2          | S0           | 29         | VAL         | 2.0         |
| 5          | S3           | 48         | VAL         | 2.0         |
| 17         | C5           | 11         | VAL         | 2.0         |
| 19         | C7           | 10         | LYS         | 2.0         |
| 33         | E1           | 130        | VAL         | 2.0         |
| 36         | 1            | 2875       | U           | 2.0         |
| 36         | 1            | 3156       | U           | 2.0         |
| 36         | 5            | 2504       | U           | 2.0         |
| 51         | m5           | 192        | LYS         | 2.0         |
| 60         | N4           | 61         | LYS         | 2.0         |
| 63         | n7           | 73         | LYS         | 2.0         |
| 67         | O1           | 67         | VAL         | 2.0         |
| 70         | O4           | 19         | LYS         | 2.0         |
| 79         | q3           | 3          | LYS         | 2.0         |
| 21         | C9           | 40         | SER         | 2.0         |
| 26         | D4           | 104        | SER         | 2.0         |
| 27         | d5           | 61         | SER         | 2.0         |
| 48         | m1           | 22         | SER         | 2.0         |
| 50         | m4           | 10         | SER         | 2.0         |
| 2          | S0           | 111        | ILE         | 2.0         |
| 6          | s4           | 59         | ARG         | 2.0         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 12         | C0           | 43         | ILE         | 2.0         |
| 14         | c2           | 36         | LEU         | 2.0         |
| 23         | d1           | 11         | LEU         | 2.0         |
| 26         | D4           | 28         | LEU         | 2.0         |
| 28         | D6           | 44         | ILE         | 2.0         |
| 31         | d9           | 56         | ARG         | 2.0         |
| 34         | SR           | 59         | ARG         | 2.0         |
| 34         | SR           | 274        | LEU         | 2.0         |
| 45         | l8           | 45         | ASN         | 2.0         |
| 46         | L9           | 144        | ILE         | 2.0         |
| 55         | m9           | 185        | LEU         | 2.0         |
| 60         | n4           | 71         | ARG         | 2.0         |
| 70         | o4           | 54         | ILE         | 2.0         |
| 75         | o9           | 30         | ARG         | 2.0         |
| 76         | Q0           | 113        | ARG         | 2.0         |
| 6          | S4           | 16         | HIS         | 2.0         |
| 29         | d7           | 49         | HIS         | 2.0         |
| 35         | SM           | 110        | TRP         | 2.0         |
| 51         | m5           | 191        | TRP         | 2.0         |
| 21         | C9           | 67         | MET         | 2.0         |
| 60         | N4           | 59         | HIS         | 2.0         |
| 3          | S1           | 200        | ALA         | 2.0         |
| 5          | S3           | 205        | ALA         | 2.0         |
| 13         | C1           | 145        | ALA         | 2.0         |
| 34         | sR           | 100        | TYR         | 2.0         |
| 36         | 5            | 1813       | A           | 2.0         |
| 36         | 5            | 2443       | A           | 2.0         |
| 40         | l3           | 386        | ASP         | 2.0         |
| 41         | l4           | 194        | TYR         | 2.0         |
| 51         | m5           | 129        | TYR         | 2.0         |
| 60         | n4           | 125        | ALA         | 2.0         |
| 75         | O9           | 2          | ALA         | 2.0         |
| 77         | q1           | 10         | THR         | 2.0         |
| 10         | S8           | 30         | GLY         | 2.0         |
| 10         | s8           | 103        | GLN         | 2.0         |
| 11         | S9           | 139        | GLN         | 2.0         |
| 26         | D4           | 66         | GLY         | 2.0         |
| 26         | d4           | 23         | PHE         | 2.0         |
| 45         | l8           | 123        | GLN         | 2.0         |
| 73         | o7           | 79         | GLN         | 2.0         |
| 31         | d9           | 11         | PRO         | 2.0         |
| 35         | sM           | 52         | PRO         | 2.0         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | S1    | 122  | GLU  | 2.0  |
| 11  | s9    | 41   | GLU  | 2.0  |
| 1   | 2     | 443  | C    | 2.0  |
| 1   | 2     | 708  | C    | 2.0  |
| 1   | 2     | 724  | C    | 2.0  |
| 1   | 6     | 717  | C    | 2.0  |
| 4   | s2    | 161  | LYS  | 2.0  |
| 17  | C5    | 52   | LYS  | 2.0  |
| 34  | sR    | 216  | LYS  | 2.0  |
| 2   | S0    | 31   | VAL  | 2.0  |
| 3   | S1    | 150  | VAL  | 2.0  |
| 4   | S2    | 63   | VAL  | 2.0  |
| 6   | s4    | 129  | VAL  | 2.0  |
| 9   | s7    | 152  | VAL  | 2.0  |
| 17  | C5    | 76   | VAL  | 2.0  |
| 22  | d0    | 97   | VAL  | 2.0  |
| 34  | sR    | 104  | VAL  | 2.0  |
| 36  | 1     | 1693 | C    | 2.0  |
| 54  | m8    | 186  | VAL  | 2.0  |
| 67  | o1    | 7    | VAL  | 2.0  |
| 71  | o5    | 54   | VAL  | 2.0  |
| 1   | 2     | 1663 | G    | 2.0  |
| 1   | 6     | 487  | G    | 2.0  |
| 1   | 6     | 1698 | G    | 2.0  |
| 4   | s2    | 95   | ARG  | 2.0  |
| 8   | S6    | 159  | ARG  | 2.0  |
| 11  | S9    | 97   | LEU  | 2.0  |
| 29  | D7    | 73   | LEU  | 2.0  |
| 36  | 1     | 1250 | G    | 2.0  |
| 36  | 1     | 2110 | G    | 2.0  |
| 36  | 5     | 3036 | G    | 2.0  |
| 42  | L5    | 54   | ARG  | 2.0  |
| 57  | n1    | 128  | LEU  | 2.0  |
| 5   | s3    | 160  | SER  | 2.0  |
| 9   | S7    | 66   | SER  | 2.0  |
| 20  | C8    | 2    | SER  | 2.0  |
| 22  | D0    | 76   | SER  | 2.0  |
| 22  | d0    | 19   | ILE  | 2.0  |
| 31  | d9    | 9    | SER  | 2.0  |
| 34  | sR    | 211  | ILE  | 2.0  |
| 48  | M1    | 79   | ILE  | 2.0  |
| 60  | n4    | 130  | SER  | 2.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | 2     | 1468 | U    | 2.0  |
| 1   | 6     | 185  | U    | 2.0  |
| 1   | 6     | 710  | U    | 2.0  |
| 1   | 6     | 1687 | U    | 2.0  |
| 4   | S2    | 82   | ASN  | 2.0  |
| 33  | e1    | 134  | ASN  | 2.0  |
| 34  | SR    | 308  | ASN  | 2.0  |
| 36  | 1     | 1765 | U    | 2.0  |
| 6   | S4    | 17   | HIS  | 2.0  |
| 10  | S8    | 9    | HIS  | 2.0  |
| 12  | C0    | 12   | HIS  | 2.0  |
| 19  | c7    | 58   | MET  | 2.0  |
| 55  | M9    | 3    | ASN  | 2.0  |
| 75  | O9    | 32   | ASN  | 2.0  |
| 3   | S1    | 126  | THR  | 2.0  |
| 20  | c8    | 58   | ALA  | 2.0  |
| 34  | sR    | 2    | ALA  | 2.0  |
| 34  | sR    | 48   | THR  | 2.0  |
| 55  | m9    | 65   | ALA  | 2.0  |
| 67  | O1    | 99   | ALA  | 2.0  |
| 71  | O5    | 120  | ALA  | 2.0  |
| 77  | q1    | 22   | ALA  | 2.0  |
| 6   | s4    | 54   | TYR  | 2.0  |
| 82  | p0    | 31   | ASP  | 2.0  |
| 3   | s1    | 205  | PHE  | 2.0  |
| 11  | S9    | 35   | GLY  | 2.0  |
| 13  | C1    | 42   | PHE  | 2.0  |
| 26  | D4    | 119  | PHE  | 2.0  |
| 29  | d7    | 76   | GLY  | 2.0  |
| 7   | s5    | 188  | LYS  | 2.0  |
| 8   | s6    | 182  | GLN  | 2.0  |
| 10  | s8    | 159  | GLN  | 2.0  |
| 13  | C1    | 46   | LYS  | 2.0  |
| 13  | c1    | 36   | LYS  | 2.0  |
| 17  | c5    | 52   | LYS  | 2.0  |
| 29  | D7    | 22   | LYS  | 2.0  |
| 46  | l9    | 165  | CYS  | 2.0  |
| 51  | M5    | 137  | PRO  | 2.0  |
| 70  | O4    | 70   | LYS  | 2.0  |
| 72  | O6    | 52   | PRO  | 2.0  |
| 77  | Q1    | 25   | LYS  | 2.0  |
| 1   | 2     | 219  | A    | 2.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | 2     | 713  | A    | 2.0  |
| 1   | 2     | 793  | A    | 2.0  |
| 1   | 2     | 1329 | A    | 2.0  |
| 1   | 2     | 1689 | A    | 2.0  |
| 1   | 6     | 104  | A    | 2.0  |
| 8   | S6    | 196  | ARG  | 2.0  |
| 14  | c2    | 66   | VAL  | 2.0  |
| 16  | C4    | 28   | VAL  | 2.0  |
| 17  | C5    | 126  | VAL  | 2.0  |
| 18  | c6    | 42   | GLU  | 2.0  |
| 23  | D1    | 36   | VAL  | 2.0  |
| 24  | D2    | 18   | GLU  | 2.0  |
| 36  | 1     | 1245 | A    | 2.0  |
| 36  | 1     | 2312 | A    | 2.0  |
| 36  | 5     | 219  | A    | 2.0  |
| 36  | 5     | 621  | A    | 2.0  |
| 36  | 5     | 1816 | A    | 2.0  |
| 58  | N2    | 43   | VAL  | 2.0  |
| 63  | n7    | 43   | VAL  | 2.0  |
| 6   | S4    | 180  | LEU  | 2.0  |
| 10  | S8    | 29   | LEU  | 2.0  |
| 11  | S9    | 116  | LEU  | 2.0  |
| 13  | c1    | 5    | LEU  | 2.0  |
| 14  | c2    | 78   | LEU  | 2.0  |
| 16  | c4    | 137  | LEU  | 2.0  |
| 19  | C7    | 34   | LEU  | 2.0  |
| 19  | c7    | 46   | LEU  | 2.0  |
| 30  | d8    | 54   | LEU  | 2.0  |
| 34  | SR    | 252  | LEU  | 2.0  |
| 46  | L9    | 161  | LEU  | 2.0  |
| 51  | m5    | 197  | LEU  | 2.0  |
| 8   | S6    | 52   | ILE  | 2.0  |
| 8   | s6    | 52   | ILE  | 2.0  |
| 22  | D0    | 22   | ILE  | 2.0  |
| 45  | L8    | 75   | ILE  | 2.0  |
| 1   | 2     | 1159 | C    | 2.0  |
| 1   | 6     | 668  | C    | 2.0  |
| 1   | 6     | 1070 | C    | 2.0  |
| 36  | 1     | 1228 | C    | 2.0  |
| 36  | 1     | 2374 | C    | 2.0  |
| 36  | 5     | 757  | C    | 2.0  |
| 36  | 5     | 1706 | C    | 2.0  |

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

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

## 5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.4 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( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|-----------------------------|-------|
| 86  | MG   | MG    | 2215 | 1/1   | -0.40 | 0.28 | 126,126,126,126             | 0     |
| 86  | MG   | 1     | 4090 | 1/1   | -0.15 | 0.20 | 129,129,129,129             | 0     |
| 86  | MG   | 2     | 2120 | 1/1   | -0.11 | 0.39 | 128,128,128,128             | 0     |
| 86  | MG   | 2     | 2101 | 1/1   | -0.04 | 0.50 | 126,126,126,126             | 0     |
| 86  | MG   | N4    | 201  | 1/1   | -0.01 | 0.30 | 142,142,142,142             | 0     |
| 86  | MG   | 2     | 2098 | 1/1   | -0.01 | 0.38 | 135,135,135,135             | 0     |
| 86  | MG   | 1     | 4094 | 1/1   | 0.08  | 0.39 | 68,68,68,68                 | 0     |
| 86  | MG   | C2    | 202  | 1/1   | 0.11  | 0.40 | 88,88,88,88                 | 0     |
| 86  | MG   | 1     | 4087 | 1/1   | 0.11  | 0.89 | 84,84,84,84                 | 0     |
| 86  | MG   | C2    | 207  | 1/1   | 0.13  | 0.18 | 105,105,105,105             | 0     |
| 86  | MG   | 1     | 4027 | 1/1   | 0.14  | 0.39 | 120,120,120,120             | 0     |
| 86  | MG   | M3    | 201  | 1/1   | 0.15  | 0.31 | 94,94,94,94                 | 0     |
| 86  | MG   | L5    | 301  | 1/1   | 0.20  | 0.16 | 110,110,110,110             | 0     |
| 86  | MG   | 1     | 4095 | 1/1   | 0.21  | 0.19 | 70,70,70,70                 | 0     |
| 86  | MG   | 5     | 4065 | 1/1   | 0.21  | 0.26 | 75,75,75,75                 | 0     |
| 86  | MG   | 1     | 4111 | 1/1   | 0.21  | 0.25 | 145,145,145,145             | 0     |
| 86  | MG   | MG    | 2224 | 1/1   | 0.25  | 0.52 | 243,243,243,243             | 0     |
| 86  | MG   | 14    | 403  | 1/1   | 0.26  | 0.23 | 52,52,52,52                 | 0     |
| 86  | MG   | 2     | 2079 | 1/1   | 0.27  | 0.30 | 154,154,154,154             | 0     |
| 86  | MG   | 2     | 2124 | 1/1   | 0.29  | 0.40 | 113,113,113,113             | 0     |
| 86  | MG   | 6     | 2151 | 1/1   | 0.30  | 0.28 | 140,140,140,140             | 0     |
| 86  | MG   | MG    | 2217 | 1/1   | 0.31  | 0.18 | 77,77,77,77                 | 0     |
| 86  | MG   | 6     | 2178 | 1/1   | 0.32  | 0.42 | 56,56,56,56                 | 0     |
| 86  | MG   | 6     | 2065 | 1/1   | 0.33  | 0.45 | 60,60,60,60                 | 0     |
| 86  | MG   | 6     | 2175 | 1/1   | 0.35  | 0.16 | 84,84,84,84                 | 0     |
| 86  | MG   | C9    | 201  | 1/1   | 0.36  | 0.35 | 95,95,95,95                 | 0     |
| 86  | MG   | 6     | 2150 | 1/1   | 0.36  | 0.30 | 113,113,113,113             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 2     | 2093 | 1/1   | 0.37 | 0.47 | 125,125,125,125             | 0     |
| 86  | MG   | 1     | 4089 | 1/1   | 0.37 | 0.75 | 56,56,56,56                 | 0     |
| 86  | MG   | 6     | 2122 | 1/1   | 0.37 | 0.33 | 105,105,105,105             | 0     |
| 86  | MG   | 1     | 4101 | 1/1   | 0.38 | 0.14 | 95,95,95,95                 | 0     |
| 86  | MG   | 6     | 2161 | 1/1   | 0.39 | 0.27 | 149,149,149,149             | 0     |
| 86  | MG   | 2     | 2096 | 1/1   | 0.40 | 0.33 | 66,66,66,66                 | 0     |
| 86  | MG   | 1     | 3742 | 1/1   | 0.41 | 0.33 | 138,138,138,138             | 0     |
| 86  | MG   | 5     | 3807 | 1/1   | 0.41 | 0.37 | 102,102,102,102             | 0     |
| 86  | MG   | 5     | 4048 | 1/1   | 0.41 | 0.24 | 106,106,106,106             | 0     |
| 86  | MG   | 2     | 2063 | 1/1   | 0.41 | 0.46 | 70,70,70,70                 | 0     |
| 86  | MG   | C2    | 201  | 1/1   | 0.42 | 0.64 | 78,78,78,78                 | 0     |
| 86  | MG   | 2     | 2092 | 1/1   | 0.42 | 0.36 | 98,98,98,98                 | 0     |
| 86  | MG   | 1     | 4054 | 1/1   | 0.42 | 0.22 | 86,86,86,86                 | 0     |
| 86  | MG   | 1     | 4105 | 1/1   | 0.43 | 0.41 | 62,62,62,62                 | 0     |
| 86  | MG   | 8     | 222  | 1/1   | 0.44 | 0.28 | 53,53,53,53                 | 0     |
| 86  | MG   | 1     | 3932 | 1/1   | 0.44 | 0.30 | 78,78,78,78                 | 0     |
| 86  | MG   | 2     | 2114 | 1/1   | 0.44 | 0.47 | 67,67,67,67                 | 0     |
| 86  | MG   | 2     | 2105 | 1/1   | 0.44 | 0.40 | 90,90,90,90                 | 0     |
| 86  | MG   | 7     | 213  | 1/1   | 0.44 | 0.36 | 49,49,49,49                 | 0     |
| 86  | MG   | 5     | 3994 | 1/1   | 0.46 | 0.47 | 44,44,44,44                 | 0     |
| 86  | MG   | 2     | 2048 | 1/1   | 0.46 | 0.36 | 73,73,73,73                 | 0     |
| 86  | MG   | n0    | 204  | 1/1   | 0.46 | 0.49 | 42,42,42,42                 | 0     |
| 86  | MG   | 5     | 4134 | 1/1   | 0.47 | 0.45 | 69,69,69,69                 | 0     |
| 86  | MG   | 2     | 2089 | 1/1   | 0.47 | 0.29 | 102,102,102,102             | 0     |
| 86  | MG   | 1     | 4050 | 1/1   | 0.47 | 0.35 | 92,92,92,92                 | 0     |
| 86  | MG   | 6     | 2130 | 1/1   | 0.47 | 0.59 | 82,82,82,82                 | 0     |
| 86  | MG   | 5     | 4144 | 1/1   | 0.48 | 0.33 | 85,85,85,85                 | 0     |
| 86  | MG   | M9    | 202  | 1/1   | 0.48 | 0.27 | 74,74,74,74                 | 0     |
| 86  | MG   | 2     | 2109 | 1/1   | 0.48 | 0.54 | 73,73,73,73                 | 0     |
| 86  | MG   | 5     | 4039 | 1/1   | 0.48 | 0.21 | 52,52,52,52                 | 0     |
| 86  | MG   | 2     | 2117 | 1/1   | 0.49 | 0.16 | 68,68,68,68                 | 0     |
| 86  | MG   | Q1    | 101  | 1/1   | 0.49 | 0.46 | 66,66,66,66                 | 0     |
| 86  | MG   | 2     | 2125 | 1/1   | 0.49 | 0.23 | 123,123,123,123             | 0     |
| 86  | MG   | 1     | 4097 | 1/1   | 0.49 | 0.68 | 70,70,70,70                 | 0     |
| 86  | MG   | 2     | 2102 | 1/1   | 0.50 | 0.39 | 79,79,79,79                 | 0     |
| 86  | MG   | 5     | 4054 | 1/1   | 0.50 | 0.39 | 56,56,56,56                 | 0     |
| 86  | MG   | 1     | 3802 | 1/1   | 0.50 | 0.20 | 93,93,93,93                 | 0     |
| 86  | MG   | C2    | 206  | 1/1   | 0.50 | 0.12 | 170,170,170,170             | 0     |
| 86  | MG   | 5     | 4017 | 1/1   | 0.50 | 0.26 | 131,131,131,131             | 0     |
| 86  | MG   | 1     | 4008 | 1/1   | 0.50 | 0.28 | 49,49,49,49                 | 0     |
| 87  | ZN   | d7    | 101  | 1/1   | 0.50 | 0.21 | 133,133,133,133             | 0     |
| 86  | MG   | L2    | 302  | 1/1   | 0.52 | 1.12 | 73,73,73,73                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | MG    | 2222 | 1/1   | 0.53 | 0.21 | 136,136,136,136             | 0     |
| 86  | MG   | 2     | 2099 | 1/1   | 0.53 | 0.39 | 62,62,62,62                 | 0     |
| 86  | MG   | 5     | 4112 | 1/1   | 0.53 | 0.26 | 103,103,103,103             | 0     |
| 86  | MG   | 2     | 2097 | 1/1   | 0.54 | 0.48 | 82,82,82,82                 | 0     |
| 86  | MG   | 1     | 4070 | 1/1   | 0.54 | 0.17 | 203,203,203,203             | 0     |
| 86  | MG   | 5     | 3817 | 1/1   | 0.54 | 0.32 | 66,66,66,66                 | 0     |
| 86  | MG   | c8    | 202  | 1/1   | 0.55 | 0.12 | 94,94,94,94                 | 0     |
| 86  | MG   | 6     | 2173 | 1/1   | 0.55 | 0.17 | 58,58,58,58                 | 0     |
| 86  | MG   | 6     | 2074 | 1/1   | 0.55 | 0.34 | 76,76,76,76                 | 0     |
| 86  | MG   | 1     | 4127 | 1/1   | 0.55 | 0.54 | 113,113,113,113             | 0     |
| 86  | MG   | MG    | 2196 | 1/1   | 0.55 | 0.22 | 77,77,77,77                 | 0     |
| 86  | MG   | 5     | 3967 | 1/1   | 0.56 | 0.18 | 54,54,54,54                 | 0     |
| 86  | MG   | 6     | 2061 | 1/1   | 0.56 | 0.28 | 88,88,88,88                 | 0     |
| 86  | MG   | 1     | 4118 | 1/1   | 0.56 | 0.25 | 54,54,54,54                 | 0     |
| 86  | MG   | 5     | 3779 | 1/1   | 0.56 | 0.25 | 103,103,103,103             | 0     |
| 86  | MG   | 5     | 4162 | 1/1   | 0.56 | 0.27 | 76,76,76,76                 | 0     |
| 86  | MG   | 6     | 2143 | 1/1   | 0.56 | 0.44 | 82,82,82,82                 | 0     |
| 86  | MG   | 7     | 223  | 1/1   | 0.56 | 0.21 | 71,71,71,71                 | 0     |
| 86  | MG   | 1     | 4005 | 1/1   | 0.56 | 0.27 | 69,69,69,69                 | 0     |
| 86  | MG   | 1     | 4021 | 1/1   | 0.57 | 0.33 | 77,77,77,77                 | 0     |
| 86  | MG   | 6     | 2128 | 1/1   | 0.57 | 0.29 | 81,81,81,81                 | 0     |
| 86  | MG   | 6     | 2058 | 1/1   | 0.57 | 0.36 | 109,109,109,109             | 0     |
| 86  | MG   | D9    | 103  | 1/1   | 0.57 | 0.31 | 88,88,88,88                 | 0     |
| 86  | MG   | N3    | 202  | 1/1   | 0.57 | 0.18 | 59,59,59,59                 | 0     |
| 86  | MG   | 1     | 3939 | 1/1   | 0.57 | 0.19 | 65,65,65,65                 | 0     |
| 86  | MG   | 5     | 3776 | 1/1   | 0.58 | 0.20 | 33,33,33,33                 | 0     |
| 86  | MG   | 5     | 4139 | 1/1   | 0.58 | 0.37 | 52,52,52,52                 | 0     |
| 86  | MG   | 1     | 3987 | 1/1   | 0.58 | 0.14 | 70,70,70,70                 | 0     |
| 86  | MG   | 6     | 2180 | 1/1   | 0.58 | 0.22 | 88,88,88,88                 | 0     |
| 86  | MG   | O5    | 201  | 1/1   | 0.58 | 0.16 | 144,144,144,144             | 0     |
| 86  | MG   | 2     | 2075 | 1/1   | 0.59 | 0.38 | 72,72,72,72                 | 0     |
| 86  | MG   | 2     | 2133 | 1/1   | 0.59 | 0.21 | 66,66,66,66                 | 0     |
| 86  | MG   | 1     | 3805 | 1/1   | 0.59 | 0.35 | 97,97,97,97                 | 0     |
| 86  | MG   | 1     | 3929 | 1/1   | 0.59 | 0.22 | 42,42,42,42                 | 0     |
| 86  | MG   | 2     | 2113 | 1/1   | 0.59 | 0.33 | 105,105,105,105             | 0     |
| 86  | MG   | 2     | 2057 | 1/1   | 0.59 | 0.39 | 57,57,57,57                 | 0     |
| 86  | MG   | 1     | 3984 | 1/1   | 0.59 | 0.25 | 75,75,75,75                 | 0     |
| 86  | MG   | 1     | 4031 | 1/1   | 0.60 | 0.23 | 121,121,121,121             | 0     |
| 86  | MG   | 6     | 2127 | 1/1   | 0.60 | 0.23 | 57,57,57,57                 | 0     |
| 86  | MG   | 6     | 2183 | 1/1   | 0.60 | 0.23 | 64,64,64,64                 | 0     |
| 86  | MG   | 5     | 4073 | 1/1   | 0.60 | 0.23 | 72,72,72,72                 | 0     |
| 86  | MG   | 1     | 4065 | 1/1   | 0.61 | 0.22 | 47,47,47,47                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 5     | 4113 | 1/1   | 0.61 | 0.25 | 44,44,44,44                 | 0     |
| 86  | MG   | 6     | 2113 | 1/1   | 0.61 | 0.41 | 50,50,50,50                 | 0     |
| 86  | MG   | 2     | 2055 | 1/1   | 0.61 | 0.46 | 77,77,77,77                 | 0     |
| 86  | MG   | 5     | 4143 | 1/1   | 0.61 | 0.34 | 55,55,55,55                 | 0     |
| 86  | MG   | 1     | 3889 | 1/1   | 0.61 | 0.29 | 36,36,36,36                 | 0     |
| 86  | MG   | 6     | 2154 | 1/1   | 0.61 | 0.25 | 92,92,92,92                 | 0     |
| 86  | MG   | 5     | 4069 | 1/1   | 0.61 | 0.20 | 49,49,49,49                 | 0     |
| 86  | MG   | 1     | 4123 | 1/1   | 0.61 | 0.26 | 47,47,47,47                 | 0     |
| 86  | MG   | 5     | 4044 | 1/1   | 0.62 | 0.14 | 46,46,46,46                 | 0     |
| 86  | MG   | C2    | 203  | 1/1   | 0.62 | 0.36 | 132,132,132,132             | 0     |
| 86  | MG   | 1     | 4085 | 1/1   | 0.62 | 0.17 | 47,47,47,47                 | 0     |
| 86  | MG   | 5     | 3806 | 1/1   | 0.62 | 0.26 | 57,57,57,57                 | 0     |
| 86  | MG   | 2     | 2106 | 1/1   | 0.62 | 0.30 | 103,103,103,103             | 0     |
| 86  | MG   | 5     | 3812 | 1/1   | 0.62 | 0.23 | 57,57,57,57                 | 0     |
| 86  | MG   | 1     | 3973 | 1/1   | 0.63 | 0.28 | 55,55,55,55                 | 0     |
| 86  | MG   | 1     | 4093 | 1/1   | 0.63 | 0.17 | 78,78,78,78                 | 0     |
| 86  | MG   | 6     | 2132 | 1/1   | 0.63 | 0.18 | 65,65,65,65                 | 0     |
| 86  | MG   | 1     | 3997 | 1/1   | 0.64 | 0.34 | 58,58,58,58                 | 0     |
| 86  | MG   | 2     | 2077 | 1/1   | 0.64 | 0.30 | 71,71,71,71                 | 0     |
| 86  | MG   | 2     | 2082 | 1/1   | 0.64 | 0.35 | 104,104,104,104             | 0     |
| 86  | MG   | 6     | 2144 | 1/1   | 0.64 | 0.26 | 75,75,75,75                 | 0     |
| 86  | MG   | 6     | 2145 | 1/1   | 0.64 | 0.27 | 92,92,92,92                 | 0     |
| 86  | MG   | 4     | 216  | 1/1   | 0.64 | 0.31 | 55,55,55,55                 | 0     |
| 86  | MG   | 1     | 4116 | 1/1   | 0.64 | 0.30 | 67,67,67,67                 | 0     |
| 86  | MG   | 1     | 4108 | 1/1   | 0.65 | 0.23 | 66,66,66,66                 | 0     |
| 86  | MG   | 1     | 3944 | 1/1   | 0.65 | 0.28 | 59,59,59,59                 | 0     |
| 86  | MG   | 6     | 2177 | 1/1   | 0.65 | 0.22 | 99,99,99,99                 | 0     |
| 86  | MG   | 5     | 3851 | 1/1   | 0.65 | 0.36 | 48,48,48,48                 | 0     |
| 86  | MG   | 5     | 4115 | 1/1   | 0.65 | 0.34 | 47,47,47,47                 | 0     |
| 86  | MG   | C2    | 205  | 1/1   | 0.65 | 0.28 | 170,170,170,170             | 0     |
| 86  | MG   | 2     | 2083 | 1/1   | 0.65 | 0.28 | 73,73,73,73                 | 0     |
| 86  | MG   | 4     | 218  | 1/1   | 0.66 | 0.35 | 49,49,49,49                 | 0     |
| 86  | MG   | 8     | 227  | 1/1   | 0.66 | 0.18 | 54,54,54,54                 | 0     |
| 86  | MG   | 1     | 3985 | 1/1   | 0.66 | 0.31 | 61,61,61,61                 | 0     |
| 86  | MG   | 19    | 202  | 1/1   | 0.66 | 0.18 | 46,46,46,46                 | 0     |
| 86  | MG   | 1     | 4120 | 1/1   | 0.66 | 0.28 | 76,76,76,76                 | 0     |
| 86  | MG   | 5     | 4147 | 1/1   | 0.66 | 0.21 | 88,88,88,88                 | 0     |
| 86  | MG   | 1     | 4017 | 1/1   | 0.66 | 0.20 | 50,50,50,50                 | 0     |
| 86  | MG   | 5     | 4166 | 1/1   | 0.66 | 0.25 | 51,51,51,51                 | 0     |
| 86  | MG   | 5     | 4171 | 1/1   | 0.66 | 0.28 | 35,35,35,35                 | 0     |
| 86  | MG   | 1     | 4042 | 1/1   | 0.66 | 0.19 | 79,79,79,79                 | 0     |
| 86  | MG   | 2     | 2123 | 1/1   | 0.66 | 0.16 | 97,97,97,97                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 2     | 2088 | 1/1   | 0.67 | 0.31 | 101,101,101,101             | 0     |
| 86  | MG   | 5     | 3789 | 1/1   | 0.67 | 0.20 | 36,36,36,36                 | 0     |
| 86  | MG   | 1     | 3955 | 1/1   | 0.67 | 0.26 | 42,42,42,42                 | 0     |
| 86  | MG   | 6     | 2103 | 1/1   | 0.67 | 0.38 | 62,62,62,62                 | 0     |
| 86  | MG   | 1     | 3928 | 1/1   | 0.67 | 0.18 | 44,44,44,44                 | 0     |
| 86  | MG   | 1     | 3752 | 1/1   | 0.67 | 0.23 | 41,41,41,41                 | 0     |
| 86  | MG   | 5     | 4150 | 1/1   | 0.67 | 0.33 | 79,79,79,79                 | 0     |
| 86  | MG   | 2     | 2111 | 1/1   | 0.67 | 0.18 | 77,77,77,77                 | 0     |
| 86  | MG   | 5     | 3957 | 1/1   | 0.67 | 0.40 | 83,83,83,83                 | 0     |
| 86  | MG   | 1     | 4026 | 1/1   | 0.67 | 0.26 | 69,69,69,69                 | 0     |
| 86  | MG   | 2     | 2046 | 1/1   | 0.67 | 0.36 | 84,84,84,84                 | 0     |
| 87  | ZN   | D7    | 101  | 1/1   | 0.67 | 0.15 | 147,147,147,147             | 0     |
| 86  | MG   | 7     | 221  | 1/1   | 0.67 | 0.18 | 51,51,51,51                 | 0     |
| 86  | MG   | 5     | 4045 | 1/1   | 0.68 | 0.20 | 42,42,42,42                 | 0     |
| 86  | MG   | 6     | 2102 | 1/1   | 0.68 | 0.48 | 68,68,68,68                 | 0     |
| 86  | MG   | 5     | 4172 | 1/1   | 0.68 | 0.34 | 70,70,70,70                 | 0     |
| 86  | MG   | 1     | 3920 | 1/1   | 0.68 | 0.43 | 70,70,70,70                 | 0     |
| 86  | MG   | 1     | 3956 | 1/1   | 0.68 | 0.42 | 81,81,81,81                 | 0     |
| 86  | MG   | 1     | 3744 | 1/1   | 0.68 | 0.30 | 36,36,36,36                 | 0     |
| 86  | MG   | 5     | 4072 | 1/1   | 0.68 | 0.29 | 60,60,60,60                 | 0     |
| 86  | MG   | 6     | 2164 | 1/1   | 0.68 | 0.21 | 90,90,90,90                 | 0     |
| 86  | MG   | 1     | 3974 | 1/1   | 0.68 | 0.14 | 52,52,52,52                 | 0     |
| 86  | MG   | 1     | 4079 | 1/1   | 0.68 | 0.16 | 82,82,82,82                 | 0     |
| 86  | MG   | 5     | 3944 | 1/1   | 0.68 | 0.20 | 39,39,39,39                 | 0     |
| 86  | MG   | p0    | 401  | 1/1   | 0.68 | 0.29 | 89,89,89,89                 | 0     |
| 86  | MG   | C2    | 208  | 1/1   | 0.68 | 0.45 | 88,88,88,88                 | 0     |
| 86  | MG   | 2     | 2119 | 1/1   | 0.68 | 0.24 | 81,81,81,81                 | 0     |
| 86  | MG   | 6     | 2134 | 1/1   | 0.68 | 0.41 | 56,56,56,56                 | 0     |
| 86  | MG   | 2     | 2126 | 1/1   | 0.68 | 0.18 | 82,82,82,82                 | 0     |
| 86  | MG   | 5     | 4025 | 1/1   | 0.68 | 0.22 | 56,56,56,56                 | 0     |
| 86  | MG   | 2     | 2095 | 1/1   | 0.68 | 0.36 | 72,72,72,72                 | 0     |
| 86  | MG   | 6     | 2077 | 1/1   | 0.68 | 0.29 | 62,62,62,62                 | 0     |
| 86  | MG   | 1     | 3902 | 1/1   | 0.69 | 0.52 | 51,51,51,51                 | 0     |
| 86  | MG   | 5     | 3962 | 1/1   | 0.69 | 0.33 | 42,42,42,42                 | 0     |
| 86  | MG   | 5     | 3964 | 1/1   | 0.69 | 0.11 | 57,57,57,57                 | 0     |
| 86  | MG   | 5     | 4103 | 1/1   | 0.69 | 0.13 | 92,92,92,92                 | 0     |
| 86  | MG   | 6     | 2131 | 1/1   | 0.69 | 0.20 | 102,102,102,102             | 0     |
| 86  | MG   | 2     | 2116 | 1/1   | 0.69 | 0.26 | 82,82,82,82                 | 0     |
| 86  | MG   | 5     | 3998 | 1/1   | 0.69 | 0.32 | 76,76,76,76                 | 0     |
| 86  | MG   | 2     | 2108 | 1/1   | 0.69 | 0.31 | 73,73,73,73                 | 0     |
| 86  | MG   | m0    | 304  | 1/1   | 0.69 | 0.37 | 88,88,88,88                 | 0     |
| 86  | MG   | 4     | 217  | 1/1   | 0.70 | 0.40 | 69,69,69,69                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 5     | 3934 | 1/1   | 0.70 | 0.25 | 44,44,44,44                 | 0     |
| 86  | MG   | 2     | 2069 | 1/1   | 0.70 | 0.39 | 67,67,67,67                 | 0     |
| 86  | MG   | 5     | 4070 | 1/1   | 0.70 | 0.27 | 68,68,68,68                 | 0     |
| 86  | MG   | 6     | 2064 | 1/1   | 0.70 | 0.47 | 75,75,75,75                 | 0     |
| 86  | MG   | 1     | 3769 | 1/1   | 0.70 | 0.28 | 56,56,56,56                 | 0     |
| 86  | MG   | 5     | 4092 | 1/1   | 0.70 | 0.12 | 58,58,58,58                 | 0     |
| 86  | MG   | 1     | 4073 | 1/1   | 0.70 | 0.14 | 47,47,47,47                 | 0     |
| 86  | MG   | M1    | 201  | 1/1   | 0.70 | 0.52 | 74,74,74,74                 | 0     |
| 86  | MG   | 2     | 2052 | 1/1   | 0.70 | 0.33 | 64,64,64,64                 | 0     |
| 86  | MG   | 2     | 2064 | 1/1   | 0.70 | 0.46 | 83,83,83,83                 | 0     |
| 86  | MG   | 5     | 4014 | 1/1   | 0.70 | 0.23 | 66,66,66,66                 | 0     |
| 86  | MG   | 6     | 2106 | 1/1   | 0.70 | 0.30 | 87,87,87,87                 | 0     |
| 86  | MG   | 5     | 4019 | 1/1   | 0.70 | 0.39 | 68,68,68,68                 | 0     |
| 86  | MG   | 1     | 4098 | 1/1   | 0.70 | 0.41 | 106,106,106,106             | 0     |
| 86  | MG   | 2     | 2068 | 1/1   | 0.70 | 0.25 | 74,74,74,74                 | 0     |
| 86  | MG   | 3     | 212  | 1/1   | 0.70 | 0.26 | 78,78,78,78                 | 0     |
| 86  | MG   | 1     | 4055 | 1/1   | 0.70 | 0.18 | 78,78,78,78                 | 0     |
| 86  | MG   | 5     | 3839 | 1/1   | 0.70 | 0.29 | 47,47,47,47                 | 0     |
| 86  | MG   | 1     | 4132 | 1/1   | 0.71 | 0.38 | 53,53,53,53                 | 0     |
| 86  | MG   | 2     | 2107 | 1/1   | 0.71 | 0.37 | 65,65,65,65                 | 0     |
| 86  | MG   | L9    | 201  | 1/1   | 0.71 | 0.23 | 57,57,57,57                 | 0     |
| 86  | MG   | 5     | 3881 | 1/1   | 0.71 | 0.24 | 49,49,49,49                 | 0     |
| 86  | MG   | 1     | 3806 | 1/1   | 0.71 | 0.16 | 56,56,56,56                 | 0     |
| 86  | MG   | 5     | 4128 | 1/1   | 0.71 | 0.29 | 87,87,87,87                 | 0     |
| 86  | MG   | 5     | 3766 | 1/1   | 0.71 | 0.25 | 88,88,88,88                 | 0     |
| 86  | MG   | 5     | 3953 | 1/1   | 0.71 | 0.18 | 43,43,43,43                 | 0     |
| 86  | MG   | 6     | 2055 | 1/1   | 0.71 | 0.27 | 51,51,51,51                 | 0     |
| 86  | MG   | 1     | 3807 | 1/1   | 0.71 | 0.24 | 59,59,59,59                 | 0     |
| 86  | MG   | 6     | 2167 | 1/1   | 0.71 | 0.23 | 60,60,60,60                 | 0     |
| 86  | MG   | 6     | 2059 | 1/1   | 0.71 | 0.18 | 80,80,80,80                 | 0     |
| 86  | MG   | 5     | 4151 | 1/1   | 0.71 | 0.25 | 99,99,99,99                 | 0     |
| 86  | MG   | 5     | 3969 | 1/1   | 0.71 | 0.10 | 64,64,64,64                 | 0     |
| 86  | MG   | 2     | 2134 | 1/1   | 0.71 | 0.37 | 116,116,116,116             | 0     |
| 86  | MG   | 6     | 2114 | 1/1   | 0.71 | 0.35 | 78,78,78,78                 | 0     |
| 86  | MG   | 5     | 4082 | 1/1   | 0.71 | 0.24 | 66,66,66,66                 | 0     |
| 86  | MG   | 6     | 2139 | 1/1   | 0.72 | 0.31 | 112,112,112,112             | 0     |
| 86  | MG   | 1     | 3815 | 1/1   | 0.72 | 0.27 | 54,54,54,54                 | 0     |
| 86  | MG   | 1     | 3830 | 1/1   | 0.72 | 0.36 | 29,29,29,29                 | 0     |
| 86  | MG   | 5     | 4152 | 1/1   | 0.72 | 0.30 | 48,48,48,48                 | 0     |
| 86  | MG   | 1     | 4045 | 1/1   | 0.72 | 0.15 | 106,106,106,106             | 0     |
| 86  | MG   | 6     | 2081 | 1/1   | 0.72 | 0.26 | 85,85,85,85                 | 0     |
| 86  | MG   | 5     | 4170 | 1/1   | 0.72 | 0.24 | 55,55,55,55                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 5     | 3831 | 1/1   | 0.72 | 0.39 | 32,32,32,32                 | 0     |
| 86  | MG   | 6     | 2089 | 1/1   | 0.72 | 0.41 | 84,84,84,84                 | 0     |
| 86  | MG   | 1     | 3834 | 1/1   | 0.72 | 0.44 | 43,43,43,43                 | 0     |
| 86  | MG   | 2     | 2060 | 1/1   | 0.72 | 0.28 | 75,75,75,75                 | 0     |
| 85  | OHX  | 4     | 212  | 7/7   | 0.72 | 0.26 | 135,135,135,135             | 0     |
| 86  | MG   | 6     | 2111 | 1/1   | 0.72 | 0.26 | 86,86,86,86                 | 0     |
| 86  | MG   | 5     | 3952 | 1/1   | 0.73 | 0.12 | 38,38,38,38                 | 0     |
| 86  | MG   | 6     | 2179 | 1/1   | 0.73 | 0.42 | 55,55,55,55                 | 0     |
| 86  | MG   | 1     | 4076 | 1/1   | 0.73 | 0.15 | 45,45,45,45                 | 0     |
| 86  | MG   | 5     | 4095 | 1/1   | 0.73 | 0.11 | 59,59,59,59                 | 0     |
| 85  | OHX  | 1     | 3725 | 7/7   | 0.73 | 0.17 | 178,178,178,178             | 0     |
| 86  | MG   | n6    | 202  | 1/1   | 0.73 | 0.29 | 44,44,44,44                 | 0     |
| 86  | MG   | 1     | 3893 | 1/1   | 0.73 | 0.35 | 52,52,52,52                 | 0     |
| 86  | MG   | 1     | 3896 | 1/1   | 0.73 | 0.37 | 47,47,47,47                 | 0     |
| 86  | MG   | 5     | 4053 | 1/1   | 0.73 | 0.33 | 77,77,77,77                 | 0     |
| 86  | MG   | 2     | 2122 | 1/1   | 0.73 | 0.25 | 74,74,74,74                 | 0     |
| 86  | MG   | 5     | 3858 | 1/1   | 0.73 | 0.32 | 39,39,39,39                 | 0     |
| 86  | MG   | 2     | 2085 | 1/1   | 0.73 | 0.34 | 97,97,97,97                 | 0     |
| 86  | MG   | 2     | 2066 | 1/1   | 0.73 | 0.41 | 98,98,98,98                 | 0     |
| 86  | MG   | 1     | 3971 | 1/1   | 0.73 | 0.21 | 46,46,46,46                 | 0     |
| 86  | MG   | 5     | 4148 | 1/1   | 0.74 | 0.27 | 52,52,52,52                 | 0     |
| 86  | MG   | 1     | 3919 | 1/1   | 0.74 | 0.29 | 67,67,67,67                 | 0     |
| 86  | MG   | 6     | 2108 | 1/1   | 0.74 | 0.42 | 77,77,77,77                 | 0     |
| 86  | MG   | 6     | 2110 | 1/1   | 0.74 | 0.29 | 85,85,85,85                 | 0     |
| 86  | MG   | O2    | 201  | 1/1   | 0.74 | 0.20 | 48,48,48,48                 | 0     |
| 86  | MG   | 2     | 2049 | 1/1   | 0.74 | 0.33 | 58,58,58,58                 | 0     |
| 86  | MG   | 5     | 3884 | 1/1   | 0.74 | 0.46 | 47,47,47,47                 | 0     |
| 86  | MG   | 5     | 4055 | 1/1   | 0.74 | 0.14 | 47,47,47,47                 | 0     |
| 86  | MG   | 2     | 2078 | 1/1   | 0.74 | 0.23 | 77,77,77,77                 | 0     |
| 86  | MG   | 1     | 4011 | 1/1   | 0.74 | 0.20 | 41,41,41,41                 | 0     |
| 86  | MG   | 5     | 3948 | 1/1   | 0.74 | 0.22 | 50,50,50,50                 | 0     |
| 86  | MG   | 6     | 2126 | 1/1   | 0.74 | 0.19 | 82,82,82,82                 | 0     |
| 86  | MG   | 1     | 4016 | 1/1   | 0.74 | 0.24 | 61,61,61,61                 | 0     |
| 86  | MG   | 1     | 3972 | 1/1   | 0.74 | 0.21 | 49,49,49,49                 | 0     |
| 86  | MG   | S4    | 301  | 1/1   | 0.74 | 0.33 | 82,82,82,82                 | 0     |
| 86  | MG   | 1     | 4106 | 1/1   | 0.74 | 0.29 | 55,55,55,55                 | 0     |
| 86  | MG   | 1     | 4107 | 1/1   | 0.74 | 0.13 | 44,44,44,44                 | 0     |
| 86  | MG   | 6     | 2071 | 1/1   | 0.74 | 0.27 | 73,73,73,73                 | 0     |
| 86  | MG   | 5     | 3981 | 1/1   | 0.74 | 0.48 | 58,58,58,58                 | 0     |
| 86  | MG   | 5     | 3983 | 1/1   | 0.74 | 0.22 | 36,36,36,36                 | 0     |
| 86  | MG   | 2     | 2128 | 1/1   | 0.74 | 0.17 | 56,56,56,56                 | 0     |
| 86  | MG   | 5     | 4129 | 1/1   | 0.74 | 0.36 | 66,66,66,66                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 1     | 3977 | 1/1   | 0.74 | 0.38 | 48,48,48,48                 | 0     |
| 86  | MG   | 1     | 3786 | 1/1   | 0.74 | 0.42 | 37,37,37,37                 | 0     |
| 86  | MG   | M7    | 203  | 1/1   | 0.74 | 0.53 | 65,65,65,65                 | 0     |
| 86  | MG   | 1     | 3818 | 1/1   | 0.74 | 0.34 | 38,38,38,38                 | 0     |
| 86  | MG   | 1     | 3954 | 1/1   | 0.74 | 0.25 | 58,58,58,58                 | 0     |
| 86  | MG   | 6     | 2115 | 1/1   | 0.75 | 0.17 | 56,56,56,56                 | 0     |
| 86  | MG   | 6     | 2181 | 1/1   | 0.75 | 0.27 | 62,62,62,62                 | 0     |
| 86  | MG   | 8     | 226  | 1/1   | 0.75 | 0.20 | 55,55,55,55                 | 0     |
| 86  | MG   | 1     | 4102 | 1/1   | 0.75 | 0.66 | 77,77,77,77                 | 0     |
| 86  | MG   | 5     | 3988 | 1/1   | 0.75 | 0.18 | 68,68,68,68                 | 0     |
| 86  | MG   | 6     | 2185 | 1/1   | 0.75 | 0.25 | 71,71,71,71                 | 0     |
| 86  | MG   | 5     | 3997 | 1/1   | 0.75 | 0.24 | 76,76,76,76                 | 0     |
| 86  | MG   | 1     | 4121 | 1/1   | 0.75 | 0.26 | 56,56,56,56                 | 0     |
| 86  | MG   | 1     | 3949 | 1/1   | 0.75 | 0.32 | 43,43,43,43                 | 0     |
| 86  | MG   | 6     | 2056 | 1/1   | 0.75 | 0.29 | 82,82,82,82                 | 0     |
| 86  | MG   | 1     | 3841 | 1/1   | 0.75 | 0.41 | 42,42,42,42                 | 0     |
| 86  | MG   | 1     | 4048 | 1/1   | 0.75 | 0.40 | 67,67,67,67                 | 0     |
| 86  | MG   | 2     | 2056 | 1/1   | 0.75 | 0.28 | 57,57,57,57                 | 0     |
| 86  | MG   | 3     | 216  | 1/1   | 0.75 | 0.27 | 71,71,71,71                 | 0     |
| 86  | MG   | 1     | 3836 | 1/1   | 0.75 | 0.41 | 30,30,30,30                 | 0     |
| 86  | MG   | 1     | 3992 | 1/1   | 0.75 | 0.15 | 51,51,51,51                 | 0     |
| 86  | MG   | 1     | 4036 | 1/1   | 0.75 | 0.19 | 58,58,58,58                 | 0     |
| 86  | MG   | 1     | 3760 | 1/1   | 0.76 | 0.38 | 47,47,47,47                 | 0     |
| 86  | MG   | 5     | 3990 | 1/1   | 0.76 | 0.22 | 36,36,36,36                 | 0     |
| 86  | MG   | 6     | 2148 | 1/1   | 0.76 | 0.15 | 65,65,65,65                 | 0     |
| 85  | OHX  | 6     | 2039 | 7/7   | 0.76 | 0.16 | 166,166,166,166             | 0     |
| 86  | MG   | 1     | 3738 | 1/1   | 0.76 | 0.26 | 50,50,50,50                 | 0     |
| 86  | MG   | 5     | 4001 | 1/1   | 0.76 | 0.14 | 38,38,38,38                 | 0     |
| 86  | MG   | 1     | 3795 | 1/1   | 0.76 | 0.24 | 39,39,39,39                 | 0     |
| 86  | MG   | 2     | 2071 | 1/1   | 0.76 | 0.35 | 74,74,74,74                 | 0     |
| 86  | MG   | 6     | 2162 | 1/1   | 0.76 | 0.37 | 71,71,71,71                 | 0     |
| 86  | MG   | 5     | 4022 | 1/1   | 0.76 | 0.29 | 41,41,41,41                 | 0     |
| 86  | MG   | 6     | 2163 | 1/1   | 0.76 | 0.47 | 79,79,79,79                 | 0     |
| 86  | MG   | 5     | 3846 | 1/1   | 0.76 | 0.47 | 38,38,38,38                 | 0     |
| 85  | OHX  | 5     | 3746 | 7/7   | 0.76 | 0.17 | 172,172,172,172             | 0     |
| 86  | MG   | 1     | 3845 | 1/1   | 0.76 | 0.39 | 59,59,59,59                 | 0     |
| 86  | MG   | 1     | 3866 | 1/1   | 0.76 | 0.38 | 47,47,47,47                 | 0     |
| 86  | MG   | 1     | 4126 | 1/1   | 0.76 | 0.39 | 87,87,87,87                 | 0     |
| 86  | MG   | 5     | 3903 | 1/1   | 0.76 | 0.30 | 37,37,37,37                 | 0     |
| 86  | MG   | 5     | 3904 | 1/1   | 0.76 | 0.37 | 35,35,35,35                 | 0     |
| 86  | MG   | 5     | 4059 | 1/1   | 0.76 | 0.24 | 74,74,74,74                 | 0     |
| 86  | MG   | 1     | 3750 | 1/1   | 0.76 | 0.38 | 39,39,39,39                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 2     | 2087 | 1/1   | 0.76 | 0.49 | 95,95,95,95                 | 0     |
| 86  | MG   | 1     | 4080 | 1/1   | 0.76 | 0.21 | 46,46,46,46                 | 0     |
| 86  | MG   | 6     | 2085 | 1/1   | 0.76 | 0.40 | 74,74,74,74                 | 0     |
| 86  | MG   | N8    | 201  | 1/1   | 0.76 | 0.21 | 48,48,48,48                 | 0     |
| 86  | MG   | 6     | 2093 | 1/1   | 0.76 | 0.27 | 42,42,42,42                 | 0     |
| 86  | MG   | 6     | 2099 | 1/1   | 0.76 | 0.25 | 57,57,57,57                 | 0     |
| 86  | MG   | n8    | 201  | 1/1   | 0.76 | 0.28 | 49,49,49,49                 | 0     |
| 86  | MG   | 5     | 4093 | 1/1   | 0.76 | 0.17 | 49,49,49,49                 | 0     |
| 86  | MG   | 6     | 2141 | 1/1   | 0.76 | 0.37 | 59,59,59,59                 | 0     |
| 86  | MG   | 5     | 4101 | 1/1   | 0.76 | 0.24 | 34,34,34,34                 | 0     |
| 86  | MG   | 5     | 3965 | 1/1   | 0.76 | 0.22 | 56,56,56,56                 | 0     |
| 86  | MG   | 5     | 3763 | 1/1   | 0.76 | 0.32 | 28,28,28,28                 | 0     |
| 86  | MG   | 5     | 3765 | 1/1   | 0.76 | 0.19 | 68,68,68,68                 | 0     |
| 86  | MG   | 3     | 214  | 1/1   | 0.76 | 0.37 | 68,68,68,68                 | 0     |
| 86  | MG   | 1     | 3809 | 1/1   | 0.76 | 0.45 | 41,41,41,41                 | 0     |
| 85  | OHX  | 2     | 2022 | 7/7   | 0.77 | 0.48 | 127,127,127,127             | 0     |
| 86  | MG   | 5     | 3840 | 1/1   | 0.77 | 0.33 | 34,34,34,34                 | 0     |
| 86  | MG   | 1     | 4071 | 1/1   | 0.77 | 0.14 | 38,38,38,38                 | 0     |
| 86  | MG   | 5     | 3982 | 1/1   | 0.77 | 0.16 | 36,36,36,36                 | 0     |
| 85  | OHX  | 5     | 3730 | 7/7   | 0.77 | 0.17 | 158,158,158,158             | 0     |
| 85  | OHX  | 2     | 2024 | 7/7   | 0.77 | 0.18 | 154,154,154,154             | 0     |
| 86  | MG   | 5     | 3989 | 1/1   | 0.77 | 0.19 | 50,50,50,50                 | 0     |
| 86  | MG   | 5     | 3873 | 1/1   | 0.77 | 0.25 | 36,36,36,36                 | 0     |
| 86  | MG   | 1     | 4000 | 1/1   | 0.77 | 0.29 | 58,58,58,58                 | 0     |
| 86  | MG   | 7     | 220  | 1/1   | 0.77 | 0.26 | 44,44,44,44                 | 0     |
| 86  | MG   | 6     | 2086 | 1/1   | 0.77 | 0.28 | 61,61,61,61                 | 0     |
| 86  | MG   | 5     | 3893 | 1/1   | 0.77 | 0.28 | 48,48,48,48                 | 0     |
| 86  | MG   | 5     | 4000 | 1/1   | 0.77 | 0.21 | 42,42,42,42                 | 0     |
| 86  | MG   | 5     | 4097 | 1/1   | 0.77 | 0.09 | 75,75,75,75                 | 0     |
| 86  | MG   | 2     | 2072 | 1/1   | 0.77 | 0.26 | 62,62,62,62                 | 0     |
| 86  | MG   | 5     | 3780 | 1/1   | 0.77 | 0.20 | 41,41,41,41                 | 0     |
| 86  | MG   | 1     | 3740 | 1/1   | 0.77 | 0.23 | 41,41,41,41                 | 0     |
| 86  | MG   | 5     | 4018 | 1/1   | 0.77 | 0.38 | 54,54,54,54                 | 0     |
| 86  | MG   | 5     | 3792 | 1/1   | 0.77 | 0.18 | 52,52,52,52                 | 0     |
| 86  | MG   | 6     | 2118 | 1/1   | 0.77 | 0.29 | 59,59,59,59                 | 0     |
| 86  | MG   | 6     | 2095 | 1/1   | 0.77 | 0.31 | 47,47,47,47                 | 0     |
| 86  | MG   | q1    | 101  | 1/1   | 0.77 | 0.86 | 52,52,52,52                 | 0     |
| 86  | MG   | 5     | 4133 | 1/1   | 0.77 | 0.22 | 55,55,55,55                 | 0     |
| 86  | MG   | 6     | 2097 | 1/1   | 0.77 | 0.19 | 76,76,76,76                 | 0     |
| 86  | MG   | 5     | 4040 | 1/1   | 0.77 | 0.31 | 46,46,46,46                 | 0     |
| 86  | MG   | 2     | 2050 | 1/1   | 0.77 | 0.22 | 87,87,87,87                 | 0     |
| 86  | MG   | 5     | 3821 | 1/1   | 0.77 | 0.13 | 72,72,72,72                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 5     | 3822 | 1/1   | 0.77 | 0.23 | 50,50,50,50                 | 0     |
| 86  | MG   | 6     | 2069 | 1/1   | 0.77 | 0.34 | 71,71,71,71                 | 0     |
| 86  | MG   | 5     | 4149 | 1/1   | 0.77 | 0.25 | 51,51,51,51                 | 0     |
| 85  | OHX  | 2     | 2041 | 7/7   | 0.78 | 0.17 | 159,159,159,159             | 0     |
| 86  | MG   | 1     | 4043 | 1/1   | 0.78 | 0.24 | 52,52,52,52                 | 0     |
| 86  | MG   | 6     | 2109 | 1/1   | 0.78 | 0.23 | 65,65,65,65                 | 0     |
| 86  | MG   | 5     | 4098 | 1/1   | 0.78 | 0.28 | 54,54,54,54                 | 0     |
| 86  | MG   | 1     | 4082 | 1/1   | 0.78 | 0.13 | 53,53,53,53                 | 0     |
| 85  | OHX  | 1     | 3726 | 7/7   | 0.78 | 0.20 | 140,140,140,140             | 0     |
| 86  | MG   | 1     | 3796 | 1/1   | 0.78 | 0.26 | 31,31,31,31                 | 0     |
| 86  | MG   | 5     | 4029 | 1/1   | 0.78 | 0.19 | 62,62,62,62                 | 0     |
| 85  | OHX  | 1     | 3734 | 7/7   | 0.78 | 0.20 | 136,136,136,136             | 0     |
| 86  | MG   | C2    | 204  | 1/1   | 0.78 | 0.41 | 69,69,69,69                 | 0     |
| 86  | MG   | s6    | 301  | 1/1   | 0.78 | 0.20 | 105,105,105,105             | 0     |
| 86  | MG   | 5     | 3970 | 1/1   | 0.78 | 0.32 | 49,49,49,49                 | 0     |
| 86  | MG   | 4     | 223  | 1/1   | 0.78 | 0.22 | 65,65,65,65                 | 0     |
| 86  | MG   | 5     | 3756 | 1/1   | 0.78 | 0.39 | 46,46,46,46                 | 0     |
| 86  | MG   | 1     | 4024 | 1/1   | 0.78 | 0.19 | 57,57,57,57                 | 0     |
| 86  | MG   | 5     | 3984 | 1/1   | 0.78 | 0.19 | 30,30,30,30                 | 0     |
| 86  | MG   | 6     | 2159 | 1/1   | 0.78 | 0.18 | 81,81,81,81                 | 0     |
| 86  | MG   | 2     | 2080 | 1/1   | 0.78 | 0.15 | 78,78,78,78                 | 0     |
| 86  | MG   | 1     | 3762 | 1/1   | 0.78 | 0.26 | 44,44,44,44                 | 0     |
| 86  | MG   | 1     | 3861 | 1/1   | 0.78 | 0.24 | 65,65,65,65                 | 0     |
| 86  | MG   | 6     | 2100 | 1/1   | 0.78 | 0.46 | 42,42,42,42                 | 0     |
| 86  | MG   | 1     | 4034 | 1/1   | 0.78 | 0.15 | 51,51,51,51                 | 0     |
| 86  | MG   | 5     | 4156 | 1/1   | 0.78 | 0.27 | 55,55,55,55                 | 0     |
| 85  | OHX  | 1     | 3715 | 7/7   | 0.78 | 0.17 | 147,147,147,147             | 0     |
| 86  | MG   | 5     | 3794 | 1/1   | 0.78 | 0.31 | 56,56,56,56                 | 0     |
| 86  | MG   | 5     | 4042 | 1/1   | 0.79 | 0.26 | 35,35,35,35                 | 0     |
| 85  | OHX  | 6     | 2029 | 7/7   | 0.79 | 0.17 | 159,159,159,159             | 0     |
| 86  | MG   | 2     | 2070 | 1/1   | 0.79 | 0.32 | 62,62,62,62                 | 0     |
| 85  | OHX  | 5     | 3731 | 7/7   | 0.79 | 0.19 | 146,146,146,146             | 0     |
| 86  | MG   | 1     | 3778 | 1/1   | 0.79 | 0.30 | 40,40,40,40                 | 0     |
| 86  | MG   | 5     | 3808 | 1/1   | 0.79 | 0.20 | 114,114,114,114             | 0     |
| 86  | MG   | 1     | 3858 | 1/1   | 0.79 | 0.30 | 45,45,45,45                 | 0     |
| 86  | MG   | 1     | 4086 | 1/1   | 0.79 | 0.41 | 55,55,55,55                 | 0     |
| 86  | MG   | 1     | 3938 | 1/1   | 0.79 | 0.28 | 60,60,60,60                 | 0     |
| 86  | MG   | 1     | 3780 | 1/1   | 0.79 | 0.30 | 42,42,42,42                 | 0     |
| 86  | MG   | 6     | 2094 | 1/1   | 0.79 | 0.34 | 52,52,52,52                 | 0     |
| 86  | MG   | 5     | 3833 | 1/1   | 0.79 | 0.41 | 70,70,70,70                 | 0     |
| 86  | MG   | 7     | 219  | 1/1   | 0.79 | 0.17 | 50,50,50,50                 | 0     |
| 85  | OHX  | 6     | 2049 | 7/7   | 0.79 | 0.17 | 157,157,157,157             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 1     | 3876 | 1/1   | 0.79 | 0.17 | 48,48,48,48                 | 0     |
| 86  | MG   | 1     | 3816 | 1/1   | 0.79 | 0.25 | 40,40,40,40                 | 0     |
| 86  | MG   | 5     | 3850 | 1/1   | 0.79 | 0.34 | 27,27,27,27                 | 0     |
| 86  | MG   | O7    | 104  | 1/1   | 0.79 | 0.28 | 58,58,58,58                 | 0     |
| 86  | MG   | 3     | 201  | 1/1   | 0.79 | 0.38 | 33,33,33,33                 | 0     |
| 86  | MG   | 5     | 3861 | 1/1   | 0.79 | 0.30 | 33,33,33,33                 | 0     |
| 86  | MG   | 5     | 3870 | 1/1   | 0.79 | 0.25 | 43,43,43,43                 | 0     |
| 86  | MG   | 5     | 3749 | 1/1   | 0.79 | 0.20 | 52,52,52,52                 | 0     |
| 86  | MG   | m1    | 202  | 1/1   | 0.79 | 0.17 | 59,59,59,59                 | 0     |
| 86  | MG   | 1     | 3817 | 1/1   | 0.79 | 0.25 | 53,53,53,53                 | 0     |
| 86  | MG   | 5     | 3882 | 1/1   | 0.79 | 0.25 | 44,44,44,44                 | 0     |
| 85  | OHX  | 5     | 3669 | 7/7   | 0.79 | 0.18 | 192,192,192,192             | 0     |
| 86  | MG   | o2    | 202  | 1/1   | 0.79 | 0.21 | 38,38,38,38                 | 0     |
| 86  | MG   | 5     | 4121 | 1/1   | 0.79 | 0.32 | 44,44,44,44                 | 0     |
| 86  | MG   | 1     | 3959 | 1/1   | 0.79 | 0.13 | 74,74,74,74                 | 0     |
| 86  | MG   | 1     | 3963 | 1/1   | 0.79 | 0.29 | 70,70,70,70                 | 0     |
| 86  | MG   | 1     | 3969 | 1/1   | 0.79 | 0.12 | 35,35,35,35                 | 0     |
| 86  | MG   | 5     | 3915 | 1/1   | 0.79 | 0.35 | 38,38,38,38                 | 0     |
| 86  | MG   | 1     | 4103 | 1/1   | 0.79 | 0.26 | 51,51,51,51                 | 0     |
| 86  | MG   | 5     | 4032 | 1/1   | 0.79 | 0.39 | 70,70,70,70                 | 0     |
| 86  | MG   | SM    | 301  | 1/1   | 0.79 | 0.19 | 57,57,57,57                 | 0     |
| 86  | MG   | 1     | 4022 | 1/1   | 0.79 | 0.36 | 56,56,56,56                 | 0     |
| 86  | MG   | 6     | 2120 | 1/1   | 0.80 | 0.32 | 62,62,62,62                 | 0     |
| 86  | MG   | 2     | 2118 | 1/1   | 0.80 | 0.31 | 51,51,51,51                 | 0     |
| 86  | MG   | 5     | 4012 | 1/1   | 0.80 | 0.17 | 69,69,69,69                 | 0     |
| 86  | MG   | 5     | 4013 | 1/1   | 0.80 | 0.16 | 48,48,48,48                 | 0     |
| 85  | OHX  | 1     | 3704 | 7/7   | 0.80 | 0.14 | 190,190,190,190             | 0     |
| 85  | OHX  | 5     | 3726 | 7/7   | 0.80 | 0.17 | 151,151,151,151             | 0     |
| 86  | MG   | 5     | 3876 | 1/1   | 0.80 | 0.39 | 34,34,34,34                 | 0     |
| 86  | MG   | 1     | 4039 | 1/1   | 0.80 | 0.24 | 44,44,44,44                 | 0     |
| 86  | MG   | 4     | 222  | 1/1   | 0.80 | 0.17 | 43,43,43,43                 | 0     |
| 86  | MG   | 6     | 2080 | 1/1   | 0.80 | 0.55 | 69,69,69,69                 | 0     |
| 86  | MG   | 1     | 3912 | 1/1   | 0.80 | 0.23 | 34,34,34,34                 | 0     |
| 86  | MG   | 1     | 3913 | 1/1   | 0.80 | 0.30 | 39,39,39,39                 | 0     |
| 86  | MG   | 5     | 4155 | 1/1   | 0.80 | 0.28 | 62,62,62,62                 | 0     |
| 86  | MG   | 1     | 3983 | 1/1   | 0.80 | 0.27 | 80,80,80,80                 | 0     |
| 86  | MG   | 2     | 2103 | 1/1   | 0.80 | 0.26 | 93,93,93,93                 | 0     |
| 86  | MG   | 5     | 3921 | 1/1   | 0.80 | 0.30 | 28,28,28,28                 | 0     |
| 86  | MG   | 5     | 3932 | 1/1   | 0.80 | 0.26 | 42,42,42,42                 | 0     |
| 86  | MG   | 1     | 3822 | 1/1   | 0.80 | 0.27 | 56,56,56,56                 | 0     |
| 85  | OHX  | M9    | 201  | 7/7   | 0.80 | 0.15 | 163,163,163,163             | 0     |
| 86  | MG   | 1     | 3833 | 1/1   | 0.80 | 0.41 | 39,39,39,39                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 6     | 2146 | 1/1   | 0.80 | 0.28 | 55,55,55,55                 | 0     |
| 86  | MG   | 6     | 2147 | 1/1   | 0.80 | 0.35 | 62,62,62,62                 | 0     |
| 86  | MG   | 1     | 3996 | 1/1   | 0.80 | 0.09 | 47,47,47,47                 | 0     |
| 86  | MG   | 7     | 222  | 1/1   | 0.80 | 0.16 | 48,48,48,48                 | 0     |
| 86  | MG   | 5     | 3799 | 1/1   | 0.80 | 0.25 | 43,43,43,43                 | 0     |
| 86  | MG   | 1     | 4109 | 1/1   | 0.80 | 0.31 | 36,36,36,36                 | 0     |
| 85  | OHX  | 1     | 3718 | 7/7   | 0.80 | 0.12 | 204,204,204,204             | 0     |
| 86  | MG   | 5     | 3966 | 1/1   | 0.80 | 0.28 | 38,38,38,38                 | 0     |
| 86  | MG   | l3    | 406  | 1/1   | 0.80 | 0.24 | 44,44,44,44                 | 0     |
| 85  | OHX  | 6     | 2035 | 7/7   | 0.80 | 0.22 | 144,144,144,144             | 0     |
| 86  | MG   | 1     | 3839 | 1/1   | 0.80 | 0.37 | 39,39,39,39                 | 0     |
| 86  | MG   | 5     | 4086 | 1/1   | 0.80 | 0.23 | 92,92,92,92                 | 0     |
| 85  | OHX  | 7     | 210  | 7/7   | 0.80 | 0.19 | 140,140,140,140             | 0     |
| 86  | MG   | m4    | 202  | 1/1   | 0.80 | 0.13 | 42,42,42,42                 | 0     |
| 86  | MG   | 5     | 3980 | 1/1   | 0.80 | 0.23 | 46,46,46,46                 | 0     |
| 85  | OHX  | l4    | 402  | 7/7   | 0.80 | 0.37 | 134,134,134,134             | 0     |
| 85  | OHX  | m4    | 201  | 7/7   | 0.80 | 0.14 | 181,181,181,181             | 0     |
| 86  | MG   | n9    | 103  | 1/1   | 0.80 | 0.27 | 40,40,40,40                 | 0     |
| 85  | OHX  | 1     | 3731 | 7/7   | 0.80 | 0.16 | 144,144,144,144             | 0     |
| 86  | MG   | o4    | 202  | 1/1   | 0.80 | 0.49 | 61,61,61,61                 | 0     |
| 86  | MG   | 2     | 2065 | 1/1   | 0.80 | 0.29 | 50,50,50,50                 | 0     |
| 86  | MG   | 2     | 2081 | 1/1   | 0.80 | 0.40 | 77,77,77,77                 | 0     |
| 86  | MG   | 5     | 4109 | 1/1   | 0.80 | 0.24 | 31,31,31,31                 | 0     |
| 85  | OHX  | 1     | 3721 | 7/7   | 0.80 | 0.20 | 137,137,137,137             | 0     |
| 86  | MG   | 5     | 3841 | 1/1   | 0.80 | 0.31 | 53,53,53,53                 | 0     |
| 86  | MG   | 1     | 3966 | 1/1   | 0.80 | 0.20 | 64,64,64,64                 | 0     |
| 86  | MG   | 5     | 4116 | 1/1   | 0.80 | 0.20 | 67,67,67,67                 | 0     |
| 86  | MG   | 1     | 3891 | 1/1   | 0.80 | 0.30 | 36,36,36,36                 | 0     |
| 86  | MG   | 6     | 2119 | 1/1   | 0.80 | 0.19 | 76,76,76,76                 | 0     |
| 86  | MG   | 6     | 2155 | 1/1   | 0.81 | 0.21 | 108,108,108,108             | 0     |
| 86  | MG   | 5     | 3802 | 1/1   | 0.81 | 0.18 | 31,31,31,31                 | 0     |
| 85  | OHX  | 6     | 1987 | 7/7   | 0.81 | 0.17 | 156,156,156,156             | 0     |
| 86  | MG   | 6     | 2160 | 1/1   | 0.81 | 0.29 | 71,71,71,71                 | 0     |
| 85  | OHX  | 5     | 3675 | 7/7   | 0.81 | 0.18 | 149,149,149,149             | 0     |
| 85  | OHX  | 6     | 2024 | 7/7   | 0.81 | 0.17 | 142,142,142,142             | 0     |
| 86  | MG   | S8    | 302  | 1/1   | 0.81 | 0.17 | 69,69,69,69                 | 0     |
| 86  | MG   | 1     | 4069 | 1/1   | 0.81 | 0.34 | 69,69,69,69                 | 0     |
| 86  | MG   | 4     | 229  | 1/1   | 0.81 | 0.15 | 51,51,51,51                 | 0     |
| 86  | MG   | 5     | 3827 | 1/1   | 0.81 | 0.11 | 45,45,45,45                 | 0     |
| 86  | MG   | 2     | 2090 | 1/1   | 0.81 | 0.29 | 72,72,72,72                 | 0     |
| 86  | MG   | 5     | 4068 | 1/1   | 0.81 | 0.25 | 36,36,36,36                 | 0     |
| 86  | MG   | 1     | 3909 | 1/1   | 0.81 | 0.35 | 36,36,36,36                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 5     | 3974 | 1/1   | 0.81 | 0.17 | 58,58,58,58                 | 0     |
| 86  | MG   | 1     | 3788 | 1/1   | 0.81 | 0.22 | 32,32,32,32                 | 0     |
| 86  | MG   | 1     | 3790 | 1/1   | 0.81 | 0.13 | 41,41,41,41                 | 0     |
| 86  | MG   | 5     | 4081 | 1/1   | 0.81 | 0.22 | 49,49,49,49                 | 0     |
| 86  | MG   | 6     | 2082 | 1/1   | 0.81 | 0.27 | 70,70,70,70                 | 0     |
| 86  | MG   | 6     | 2084 | 1/1   | 0.81 | 0.23 | 48,48,48,48                 | 0     |
| 86  | MG   | 8     | 223  | 1/1   | 0.81 | 0.28 | 50,50,50,50                 | 0     |
| 86  | MG   | 1     | 4077 | 1/1   | 0.81 | 0.20 | 88,88,88,88                 | 0     |
| 86  | MG   | 2     | 2112 | 1/1   | 0.81 | 0.25 | 80,80,80,80                 | 0     |
| 86  | MG   | 1     | 3837 | 1/1   | 0.81 | 0.28 | 37,37,37,37                 | 0     |
| 85  | OHX  | 6     | 2045 | 7/7   | 0.81 | 0.18 | 154,154,154,154             | 0     |
| 86  | MG   | 5     | 3991 | 1/1   | 0.81 | 0.15 | 47,47,47,47                 | 0     |
| 86  | MG   | 6     | 2138 | 1/1   | 0.81 | 0.32 | 67,67,67,67                 | 0     |
| 86  | MG   | 5     | 4102 | 1/1   | 0.81 | 0.25 | 42,42,42,42                 | 0     |
| 86  | MG   | 1     | 3980 | 1/1   | 0.81 | 0.24 | 58,58,58,58                 | 0     |
| 86  | MG   | 1     | 3840 | 1/1   | 0.81 | 0.22 | 34,34,34,34                 | 0     |
| 86  | MG   | 6     | 2096 | 1/1   | 0.81 | 0.43 | 73,73,73,73                 | 0     |
| 85  | OHX  | 1     | 3669 | 7/7   | 0.81 | 0.16 | 161,161,161,161             | 0     |
| 86  | MG   | 5     | 4004 | 1/1   | 0.81 | 0.14 | 53,53,53,53                 | 0     |
| 86  | MG   | 1     | 3749 | 1/1   | 0.81 | 0.34 | 66,66,66,66                 | 0     |
| 86  | MG   | 5     | 4120 | 1/1   | 0.81 | 0.13 | 52,52,52,52                 | 0     |
| 85  | OHX  | s1    | 302  | 7/7   | 0.81 | 0.17 | 154,154,154,154             | 0     |
| 86  | MG   | 5     | 3777 | 1/1   | 0.81 | 0.21 | 44,44,44,44                 | 0     |
| 86  | MG   | 2     | 2127 | 1/1   | 0.81 | 0.46 | 60,60,60,60                 | 0     |
| 86  | MG   | 5     | 3908 | 1/1   | 0.81 | 0.51 | 41,41,41,41                 | 0     |
| 86  | MG   | 6     | 2052 | 1/1   | 0.81 | 0.38 | 49,49,49,49                 | 0     |
| 86  | MG   | 1     | 3759 | 1/1   | 0.81 | 0.30 | 47,47,47,47                 | 0     |
| 86  | MG   | 5     | 3924 | 1/1   | 0.81 | 0.29 | 49,49,49,49                 | 0     |
| 86  | MG   | 1     | 4046 | 1/1   | 0.81 | 0.30 | 55,55,55,55                 | 0     |
| 86  | MG   | 2     | 2086 | 1/1   | 0.81 | 0.18 | 65,65,65,65                 | 0     |
| 85  | OHX  | 2     | 2028 | 7/7   | 0.82 | 0.13 | 175,175,175,175             | 0     |
| 86  | MG   | 5     | 3874 | 1/1   | 0.82 | 0.39 | 43,43,43,43                 | 0     |
| 86  | MG   | 2     | 2051 | 1/1   | 0.82 | 0.30 | 80,80,80,80                 | 0     |
| 85  | OHX  | 5     | 3740 | 7/7   | 0.82 | 0.34 | 134,134,134,134             | 0     |
| 86  | MG   | 5     | 3750 | 1/1   | 0.82 | 0.28 | 34,34,34,34                 | 0     |
| 86  | MG   | 6     | 2083 | 1/1   | 0.82 | 0.32 | 43,43,43,43                 | 0     |
| 86  | MG   | 1     | 4099 | 1/1   | 0.82 | 0.12 | 52,52,52,52                 | 0     |
| 85  | OHX  | 4     | 213  | 7/7   | 0.82 | 0.34 | 137,137,137,137             | 0     |
| 86  | MG   | 2     | 2121 | 1/1   | 0.82 | 0.21 | 88,88,88,88                 | 0     |
| 86  | MG   | 5     | 3907 | 1/1   | 0.82 | 0.30 | 33,33,33,33                 | 0     |
| 86  | MG   | 5     | 3774 | 1/1   | 0.82 | 0.13 | 31,31,31,31                 | 0     |
| 85  | OHX  | 6     | 2033 | 7/7   | 0.82 | 0.17 | 156,156,156,156             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 5     | 3916 | 1/1   | 0.82 | 0.40 | 52,52,52,52                 | 0     |
| 86  | MG   | 5     | 3917 | 1/1   | 0.82 | 0.39 | 41,41,41,41                 | 0     |
| 86  | MG   | 6     | 2092 | 1/1   | 0.82 | 0.24 | 58,58,58,58                 | 0     |
| 86  | MG   | 2     | 2076 | 1/1   | 0.82 | 0.29 | 75,75,75,75                 | 0     |
| 86  | MG   | 5     | 4168 | 1/1   | 0.82 | 0.40 | 38,38,38,38                 | 0     |
| 86  | MG   | 1     | 3950 | 1/1   | 0.82 | 0.31 | 71,71,71,71                 | 0     |
| 86  | MG   | 1     | 4064 | 1/1   | 0.82 | 0.16 | 81,81,81,81                 | 0     |
| 86  | MG   | M7    | 207  | 1/1   | 0.82 | 0.24 | 56,56,56,56                 | 0     |
| 86  | MG   | 5     | 4173 | 1/1   | 0.82 | 0.23 | 43,43,43,43                 | 0     |
| 86  | MG   | 1     | 3953 | 1/1   | 0.82 | 0.12 | 57,57,57,57                 | 0     |
| 86  | MG   | 5     | 3795 | 1/1   | 0.82 | 0.23 | 36,36,36,36                 | 0     |
| 86  | MG   | 1     | 3883 | 1/1   | 0.82 | 0.41 | 51,51,51,51                 | 0     |
| 85  | OHX  | l3    | 402  | 7/7   | 0.82 | 0.17 | 145,145,145,145             | 0     |
| 86  | MG   | 1     | 4113 | 1/1   | 0.82 | 0.24 | 34,34,34,34                 | 0     |
| 86  | MG   | 1     | 4114 | 1/1   | 0.82 | 0.28 | 41,41,41,41                 | 0     |
| 86  | MG   | 1     | 4009 | 1/1   | 0.82 | 0.26 | 65,65,65,65                 | 0     |
| 86  | MG   | 5     | 3811 | 1/1   | 0.82 | 0.14 | 39,39,39,39                 | 0     |
| 86  | MG   | 1     | 3763 | 1/1   | 0.82 | 0.37 | 44,44,44,44                 | 0     |
| 85  | OHX  | 1     | 3709 | 7/7   | 0.82 | 0.17 | 166,166,166,166             | 0     |
| 86  | MG   | 5     | 3819 | 1/1   | 0.82 | 0.12 | 49,49,49,49                 | 0     |
| 86  | MG   | 5     | 4091 | 1/1   | 0.82 | 0.25 | 73,73,73,73                 | 0     |
| 86  | MG   | 1     | 3961 | 1/1   | 0.82 | 0.21 | 36,36,36,36                 | 0     |
| 86  | MG   | 1     | 3773 | 1/1   | 0.82 | 0.37 | 64,64,64,64                 | 0     |
| 85  | OHX  | 5     | 3711 | 7/7   | 0.82 | 0.35 | 134,134,134,134             | 0     |
| 86  | MG   | 1     | 3967 | 1/1   | 0.82 | 0.19 | 42,42,42,42                 | 0     |
| 86  | MG   | m6    | 201  | 1/1   | 0.82 | 0.18 | 40,40,40,40                 | 0     |
| 86  | MG   | 6     | 2174 | 1/1   | 0.82 | 0.43 | 62,62,62,62                 | 0     |
| 86  | MG   | 5     | 4099 | 1/1   | 0.82 | 0.32 | 63,63,63,63                 | 0     |
| 85  | OHX  | 5     | 3717 | 7/7   | 0.82 | 0.18 | 143,143,143,143             | 0     |
| 86  | MG   | 6     | 2176 | 1/1   | 0.82 | 0.20 | 54,54,54,54                 | 0     |
| 86  | MG   | 2     | 2047 | 1/1   | 0.82 | 0.32 | 65,65,65,65                 | 0     |
| 86  | MG   | 2     | 2131 | 1/1   | 0.82 | 0.24 | 80,80,80,80                 | 0     |
| 86  | MG   | 5     | 3848 | 1/1   | 0.82 | 0.17 | 38,38,38,38                 | 0     |
| 86  | MG   | 5     | 3993 | 1/1   | 0.82 | 0.22 | 39,39,39,39                 | 0     |
| 86  | MG   | 5     | 4114 | 1/1   | 0.82 | 0.12 | 59,59,59,59                 | 0     |
| 85  | OHX  | O4    | 201  | 7/7   | 0.82 | 0.40 | 135,135,135,135             | 0     |
| 85  | OHX  | 1     | 3688 | 7/7   | 0.82 | 0.16 | 146,146,146,146             | 0     |
| 86  | MG   | 3     | 218  | 1/1   | 0.82 | 0.41 | 81,81,81,81                 | 0     |
| 86  | MG   | 1     | 3925 | 1/1   | 0.82 | 0.26 | 73,73,73,73                 | 0     |
| 86  | MG   | 5     | 4122 | 1/1   | 0.82 | 0.12 | 53,53,53,53                 | 0     |
| 86  | MG   | 1     | 4041 | 1/1   | 0.82 | 0.28 | 45,45,45,45                 | 0     |
| 87  | ZN   | q2    | 501  | 1/1   | 0.82 | 0.31 | 83,83,83,83                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 1     | 3862 | 1/1   | 0.83 | 0.18 | 40,40,40,40                 | 0     |
| 85  | OHX  | 5     | 3745 | 7/7   | 0.83 | 0.17 | 139,139,139,139             | 0     |
| 86  | MG   | 5     | 4164 | 1/1   | 0.83 | 0.29 | 45,45,45,45                 | 0     |
| 85  | OHX  | 2     | 2039 | 7/7   | 0.83 | 0.20 | 153,153,153,153             | 0     |
| 86  | MG   | 5     | 4167 | 1/1   | 0.83 | 0.13 | 65,65,65,65                 | 0     |
| 86  | MG   | 5     | 4074 | 1/1   | 0.83 | 0.25 | 51,51,51,51                 | 0     |
| 86  | MG   | 1     | 4058 | 1/1   | 0.83 | 0.12 | 70,70,70,70                 | 0     |
| 86  | MG   | 1     | 3877 | 1/1   | 0.83 | 0.22 | 35,35,35,35                 | 0     |
| 86  | MG   | 4     | 225  | 1/1   | 0.83 | 0.31 | 41,41,41,41                 | 0     |
| 86  | MG   | 5     | 3899 | 1/1   | 0.83 | 0.36 | 33,33,33,33                 | 0     |
| 86  | MG   | 6     | 2076 | 1/1   | 0.83 | 0.19 | 58,58,58,58                 | 0     |
| 86  | MG   | 1     | 3812 | 1/1   | 0.83 | 0.39 | 40,40,40,40                 | 0     |
| 86  | MG   | 5     | 4094 | 1/1   | 0.83 | 0.14 | 35,35,35,35                 | 0     |
| 85  | OHX  | S9    | 201  | 7/7   | 0.83 | 0.43 | 127,127,127,127             | 0     |
| 85  | OHX  | 5     | 3654 | 7/7   | 0.83 | 0.39 | 134,134,134,134             | 0     |
| 85  | OHX  | 5     | 3657 | 7/7   | 0.83 | 0.48 | 113,113,113,113             | 0     |
| 85  | OHX  | 1     | 3735 | 7/7   | 0.83 | 0.17 | 153,153,153,153             | 0     |
| 86  | MG   | 2     | 2067 | 1/1   | 0.83 | 0.43 | 71,71,71,71                 | 0     |
| 86  | MG   | 5     | 3816 | 1/1   | 0.83 | 0.18 | 37,37,37,37                 | 0     |
| 86  | MG   | 5     | 3923 | 1/1   | 0.83 | 0.37 | 36,36,36,36                 | 0     |
| 85  | OHX  | 5     | 3673 | 7/7   | 0.83 | 0.21 | 130,130,130,130             | 0     |
| 86  | MG   | 1     | 3831 | 1/1   | 0.83 | 0.28 | 30,30,30,30                 | 0     |
| 85  | OHX  | 1     | 3698 | 7/7   | 0.83 | 0.16 | 148,148,148,148             | 0     |
| 85  | OHX  | 1     | 3723 | 7/7   | 0.83 | 0.41 | 115,115,115,115             | 0     |
| 86  | MG   | 5     | 3826 | 1/1   | 0.83 | 0.33 | 51,51,51,51                 | 0     |
| 86  | MG   | 6     | 2184 | 1/1   | 0.83 | 0.37 | 58,58,58,58                 | 0     |
| 85  | OHX  | 6     | 2037 | 7/7   | 0.83 | 0.19 | 146,146,146,146             | 0     |
| 86  | MG   | 2     | 2129 | 1/1   | 0.83 | 0.44 | 80,80,80,80                 | 0     |
| 86  | MG   | 1     | 4037 | 1/1   | 0.83 | 0.14 | 104,104,104,104             | 0     |
| 85  | OHX  | 5     | 3724 | 7/7   | 0.83 | 0.13 | 175,175,175,175             | 0     |
| 85  | OHX  | 1     | 3599 | 7/7   | 0.83 | 0.35 | 126,126,126,126             | 0     |
| 86  | MG   | 1     | 3799 | 1/1   | 0.83 | 0.23 | 50,50,50,50                 | 0     |
| 85  | OHX  | 6     | 2041 | 7/7   | 0.83 | 0.15 | 153,153,153,153             | 0     |
| 86  | MG   | 5     | 4049 | 1/1   | 0.83 | 0.23 | 54,54,54,54                 | 0     |
| 86  | MG   | 1     | 3856 | 1/1   | 0.83 | 0.31 | 32,32,32,32                 | 0     |
| 85  | OHX  | 1     | 3619 | 7/7   | 0.83 | 0.16 | 146,146,146,146             | 0     |
| 86  | MG   | 5     | 3771 | 1/1   | 0.83 | 0.25 | 50,50,50,50                 | 0     |
| 86  | MG   | 5     | 4057 | 1/1   | 0.83 | 0.11 | 115,115,115,115             | 0     |
| 86  | MG   | 5     | 3975 | 1/1   | 0.83 | 0.09 | 40,40,40,40                 | 0     |
| 86  | MG   | 6     | 2057 | 1/1   | 0.83 | 0.29 | 49,49,49,49                 | 0     |
| 86  | MG   | 5     | 4067 | 1/1   | 0.83 | 0.36 | 39,39,39,39                 | 0     |
| 86  | MG   | 3     | 217  | 1/1   | 0.83 | 0.39 | 66,66,66,66                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | OHX  | 6     | 2047 | 7/7   | 0.83 | 0.14 | 168,168,168,168             | 0     |
| 86  | MG   | 1     | 3844 | 1/1   | 0.84 | 0.37 | 33,33,33,33                 | 0     |
| 86  | MG   | 5     | 3995 | 1/1   | 0.84 | 0.16 | 47,47,47,47                 | 0     |
| 86  | MG   | 5     | 3860 | 1/1   | 0.84 | 0.24 | 37,37,37,37                 | 0     |
| 86  | MG   | 1     | 3947 | 1/1   | 0.84 | 0.19 | 34,34,34,34                 | 0     |
| 86  | MG   | 5     | 3862 | 1/1   | 0.84 | 0.43 | 54,54,54,54                 | 0     |
| 86  | MG   | 1     | 4010 | 1/1   | 0.84 | 0.20 | 35,35,35,35                 | 0     |
| 86  | MG   | 5     | 4002 | 1/1   | 0.84 | 0.23 | 38,38,38,38                 | 0     |
| 86  | MG   | 5     | 4131 | 1/1   | 0.84 | 0.32 | 86,86,86,86                 | 0     |
| 86  | MG   | 5     | 3755 | 1/1   | 0.84 | 0.24 | 52,52,52,52                 | 0     |
| 85  | OHX  | 5     | 3735 | 7/7   | 0.84 | 0.14 | 158,158,158,158             | 0     |
| 86  | MG   | 5     | 4136 | 1/1   | 0.84 | 0.33 | 55,55,55,55                 | 0     |
| 86  | MG   | 5     | 4137 | 1/1   | 0.84 | 0.31 | 36,36,36,36                 | 0     |
| 86  | MG   | 5     | 3762 | 1/1   | 0.84 | 0.12 | 34,34,34,34                 | 0     |
| 86  | MG   | 5     | 4141 | 1/1   | 0.84 | 0.23 | 28,28,28,28                 | 0     |
| 86  | MG   | 5     | 3878 | 1/1   | 0.84 | 0.23 | 37,37,37,37                 | 0     |
| 86  | MG   | 6     | 2067 | 1/1   | 0.84 | 0.29 | 42,42,42,42                 | 0     |
| 86  | MG   | 3     | 213  | 1/1   | 0.84 | 0.28 | 44,44,44,44                 | 0     |
| 86  | MG   | 1     | 3800 | 1/1   | 0.84 | 0.22 | 51,51,51,51                 | 0     |
| 86  | MG   | 5     | 4020 | 1/1   | 0.84 | 0.25 | 62,62,62,62                 | 0     |
| 85  | OHX  | 5     | 3736 | 7/7   | 0.84 | 0.17 | 141,141,141,141             | 0     |
| 86  | MG   | 5     | 3894 | 1/1   | 0.84 | 0.35 | 36,36,36,36                 | 0     |
| 86  | MG   | 5     | 4026 | 1/1   | 0.84 | 0.12 | 54,54,54,54                 | 0     |
| 86  | MG   | 5     | 4154 | 1/1   | 0.84 | 0.17 | 40,40,40,40                 | 0     |
| 86  | MG   | 1     | 3746 | 1/1   | 0.84 | 0.24 | 53,53,53,53                 | 0     |
| 85  | OHX  | 5     | 3738 | 7/7   | 0.84 | 0.17 | 160,160,160,160             | 0     |
| 86  | MG   | 5     | 4037 | 1/1   | 0.84 | 0.28 | 39,39,39,39                 | 0     |
| 86  | MG   | 1     | 4023 | 1/1   | 0.84 | 0.45 | 47,47,47,47                 | 0     |
| 86  | MG   | 1     | 3864 | 1/1   | 0.84 | 0.28 | 53,53,53,53                 | 0     |
| 86  | MG   | 5     | 4041 | 1/1   | 0.84 | 0.32 | 47,47,47,47                 | 0     |
| 85  | OHX  | 2     | 2038 | 7/7   | 0.84 | 0.18 | 143,143,143,143             | 0     |
| 86  | MG   | 5     | 3787 | 1/1   | 0.84 | 0.18 | 34,34,34,34                 | 0     |
| 86  | MG   | 1     | 3960 | 1/1   | 0.84 | 0.31 | 46,46,46,46                 | 0     |
| 86  | MG   | 1     | 4029 | 1/1   | 0.84 | 0.20 | 73,73,73,73                 | 0     |
| 86  | MG   | 5     | 3793 | 1/1   | 0.84 | 0.20 | 46,46,46,46                 | 0     |
| 86  | MG   | 5     | 4052 | 1/1   | 0.84 | 0.30 | 75,75,75,75                 | 0     |
| 86  | MG   | 7     | 214  | 1/1   | 0.84 | 0.13 | 27,27,27,27                 | 0     |
| 85  | OHX  | 1     | 3683 | 7/7   | 0.84 | 0.17 | 153,153,153,153             | 0     |
| 85  | OHX  | 5     | 3692 | 7/7   | 0.84 | 0.15 | 148,148,148,148             | 0     |
| 85  | OHX  | 5     | 3710 | 7/7   | 0.84 | 0.35 | 137,137,137,137             | 0     |
| 86  | MG   | L3    | 403  | 1/1   | 0.84 | 0.18 | 38,38,38,38                 | 0     |
| 85  | OHX  | 2     | 2010 | 7/7   | 0.84 | 0.37 | 134,134,134,134             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 8     | 219  | 1/1   | 0.84 | 0.16 | 42,42,42,42                 | 0     |
| 86  | MG   | 2     | 2062 | 1/1   | 0.84 | 0.25 | 74,74,74,74                 | 0     |
| 85  | OHX  | 6     | 2032 | 7/7   | 0.84 | 0.17 | 140,140,140,140             | 0     |
| 85  | OHX  | 15    | 303  | 7/7   | 0.84 | 0.36 | 136,136,136,136             | 0     |
| 86  | MG   | 5     | 3954 | 1/1   | 0.84 | 0.15 | 46,46,46,46                 | 0     |
| 86  | MG   | 13    | 404  | 1/1   | 0.84 | 0.36 | 49,49,49,49                 | 0     |
| 86  | MG   | 1     | 3823 | 1/1   | 0.84 | 0.15 | 40,40,40,40                 | 0     |
| 86  | MG   | M7    | 204  | 1/1   | 0.84 | 0.29 | 43,43,43,43                 | 0     |
| 86  | MG   | 1     | 3905 | 1/1   | 0.84 | 0.39 | 33,33,33,33                 | 0     |
| 86  | MG   | 5     | 3818 | 1/1   | 0.84 | 0.25 | 51,51,51,51                 | 0     |
| 86  | MG   | 1     | 3825 | 1/1   | 0.84 | 0.33 | 38,38,38,38                 | 0     |
| 86  | MG   | N3    | 201  | 1/1   | 0.84 | 0.25 | 38,38,38,38                 | 0     |
| 86  | MG   | 5     | 4084 | 1/1   | 0.84 | 0.14 | 143,143,143,143             | 0     |
| 86  | MG   | 5     | 3968 | 1/1   | 0.84 | 0.20 | 42,42,42,42                 | 0     |
| 86  | MG   | 1     | 3828 | 1/1   | 0.84 | 0.32 | 35,35,35,35                 | 0     |
| 86  | MG   | 5     | 3823 | 1/1   | 0.84 | 0.25 | 50,50,50,50                 | 0     |
| 85  | OHX  | 15    | 304  | 7/7   | 0.84 | 0.33 | 134,134,134,134             | 0     |
| 86  | MG   | 1     | 4052 | 1/1   | 0.84 | 0.18 | 49,49,49,49                 | 0     |
| 85  | OHX  | 1     | 3649 | 7/7   | 0.84 | 0.41 | 118,118,118,118             | 0     |
| 86  | MG   | 1     | 3783 | 1/1   | 0.84 | 0.46 | 65,65,65,65                 | 0     |
| 85  | OHX  | o4    | 201  | 7/7   | 0.84 | 0.41 | 126,126,126,126             | 0     |
| 86  | MG   | D9    | 104  | 1/1   | 0.84 | 0.24 | 89,89,89,89                 | 0     |
| 85  | OHX  | 1     | 3664 | 7/7   | 0.84 | 0.32 | 137,137,137,137             | 0     |
| 86  | MG   | 5     | 3986 | 1/1   | 0.84 | 0.28 | 35,35,35,35                 | 0     |
| 86  | MG   | 5     | 3845 | 1/1   | 0.84 | 0.29 | 44,44,44,44                 | 0     |
| 86  | MG   | 1     | 3793 | 1/1   | 0.84 | 0.25 | 46,46,46,46                 | 0     |
| 85  | OHX  | 1     | 3668 | 7/7   | 0.84 | 0.19 | 148,148,148,148             | 0     |
| 86  | MG   | 1     | 4124 | 1/1   | 0.84 | 0.34 | 59,59,59,59                 | 0     |
| 85  | OHX  | 1     | 3729 | 7/7   | 0.84 | 0.17 | 134,134,134,134             | 0     |
| 86  | MG   | 6     | 2172 | 1/1   | 0.85 | 0.16 | 74,74,74,74                 | 0     |
| 86  | MG   | 5     | 4110 | 1/1   | 0.85 | 0.22 | 34,34,34,34                 | 0     |
| 85  | OHX  | s9    | 201  | 7/7   | 0.85 | 0.38 | 126,126,126,126             | 0     |
| 85  | OHX  | 6     | 2023 | 7/7   | 0.85 | 0.16 | 155,155,155,155             | 0     |
| 85  | OHX  | 2     | 2034 | 7/7   | 0.85 | 0.17 | 135,135,135,135             | 0     |
| 86  | MG   | 5     | 3832 | 1/1   | 0.85 | 0.33 | 54,54,54,54                 | 0     |
| 85  | OHX  | 1     | 3696 | 7/7   | 0.85 | 0.17 | 139,139,139,139             | 0     |
| 86  | MG   | 5     | 4117 | 1/1   | 0.85 | 0.29 | 48,48,48,48                 | 0     |
| 86  | MG   | 5     | 3835 | 1/1   | 0.85 | 0.22 | 37,37,37,37                 | 0     |
| 86  | MG   | 2     | 2094 | 1/1   | 0.85 | 0.30 | 75,75,75,75                 | 0     |
| 86  | MG   | 6     | 2104 | 1/1   | 0.85 | 0.36 | 63,63,63,63                 | 0     |
| 86  | MG   | 5     | 4126 | 1/1   | 0.85 | 0.27 | 49,49,49,49                 | 0     |
| 86  | MG   | 5     | 4127 | 1/1   | 0.85 | 0.25 | 61,61,61,61                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | OHX  | 8     | 213  | 7/7   | 0.85 | 0.26 | 124,124,124,124             | 0     |
| 86  | MG   | 1     | 3875 | 1/1   | 0.85 | 0.33 | 54,54,54,54                 | 0     |
| 85  | OHX  | 2     | 2035 | 7/7   | 0.85 | 0.12 | 223,223,223,223             | 0     |
| 85  | OHX  | 5     | 3674 | 7/7   | 0.85 | 0.13 | 178,178,178,178             | 0     |
| 86  | MG   | 1     | 3811 | 1/1   | 0.85 | 0.26 | 53,53,53,53                 | 0     |
| 86  | MG   | 5     | 3996 | 1/1   | 0.85 | 0.41 | 56,56,56,56                 | 0     |
| 85  | OHX  | 2     | 2037 | 7/7   | 0.85 | 0.11 | 242,242,242,242             | 0     |
| 86  | MG   | 1     | 3890 | 1/1   | 0.85 | 0.34 | 26,26,26,26                 | 0     |
| 86  | MG   | c1    | 202  | 1/1   | 0.85 | 0.23 | 52,52,52,52                 | 0     |
| 85  | OHX  | 5     | 3682 | 7/7   | 0.85 | 0.52 | 103,103,103,103             | 0     |
| 86  | MG   | 1     | 3751 | 1/1   | 0.85 | 0.11 | 59,59,59,59                 | 0     |
| 85  | OHX  | 5     | 3691 | 7/7   | 0.85 | 0.40 | 110,110,110,110             | 0     |
| 86  | MG   | 1     | 3755 | 1/1   | 0.85 | 0.27 | 40,40,40,40                 | 0     |
| 86  | MG   | 1     | 3903 | 1/1   | 0.85 | 0.33 | 43,43,43,43                 | 0     |
| 86  | MG   | 5     | 3759 | 1/1   | 0.85 | 0.29 | 36,36,36,36                 | 0     |
| 86  | MG   | 6     | 2124 | 1/1   | 0.85 | 0.24 | 54,54,54,54                 | 0     |
| 86  | MG   | 5     | 3880 | 1/1   | 0.85 | 0.44 | 54,54,54,54                 | 0     |
| 86  | MG   | 5     | 4153 | 1/1   | 0.85 | 0.21 | 38,38,38,38                 | 0     |
| 86  | MG   | 1     | 3758 | 1/1   | 0.85 | 0.23 | 57,57,57,57                 | 0     |
| 86  | MG   | 1     | 4053 | 1/1   | 0.85 | 0.28 | 45,45,45,45                 | 0     |
| 85  | OHX  | n5    | 201  | 7/7   | 0.85 | 0.13 | 193,193,193,193             | 0     |
| 86  | MG   | 5     | 4161 | 1/1   | 0.85 | 0.25 | 113,113,113,113             | 0     |
| 86  | MG   | 5     | 3887 | 1/1   | 0.85 | 0.16 | 49,49,49,49                 | 0     |
| 86  | MG   | 1     | 3911 | 1/1   | 0.85 | 0.23 | 46,46,46,46                 | 0     |
| 85  | OHX  | 1     | 3659 | 7/7   | 0.85 | 0.16 | 145,145,145,145             | 0     |
| 86  | MG   | 5     | 3898 | 1/1   | 0.85 | 0.35 | 30,30,30,30                 | 0     |
| 86  | MG   | 5     | 4033 | 1/1   | 0.85 | 0.29 | 41,41,41,41                 | 0     |
| 86  | MG   | 1     | 4060 | 1/1   | 0.85 | 0.18 | 35,35,35,35                 | 0     |
| 86  | MG   | 5     | 3902 | 1/1   | 0.85 | 0.21 | 33,33,33,33                 | 0     |
| 85  | OHX  | 1     | 3713 | 7/7   | 0.85 | 0.16 | 140,140,140,140             | 0     |
| 86  | MG   | 1     | 3988 | 1/1   | 0.85 | 0.38 | 58,58,58,58                 | 0     |
| 86  | MG   | 1     | 3989 | 1/1   | 0.85 | 0.15 | 47,47,47,47                 | 0     |
| 86  | MG   | 5     | 3781 | 1/1   | 0.85 | 0.21 | 30,30,30,30                 | 0     |
| 86  | MG   | 5     | 3911 | 1/1   | 0.85 | 0.16 | 30,30,30,30                 | 0     |
| 86  | MG   | 5     | 3783 | 1/1   | 0.85 | 0.31 | 57,57,57,57                 | 0     |
| 86  | MG   | 5     | 3785 | 1/1   | 0.85 | 0.19 | 39,39,39,39                 | 0     |
| 85  | OHX  | 6     | 2038 | 7/7   | 0.85 | 0.37 | 127,127,127,127             | 0     |
| 86  | MG   | 5     | 3788 | 1/1   | 0.85 | 0.19 | 31,31,31,31                 | 0     |
| 86  | MG   | 5     | 3922 | 1/1   | 0.85 | 0.30 | 23,23,23,23                 | 0     |
| 86  | MG   | 8     | 220  | 1/1   | 0.85 | 0.24 | 41,41,41,41                 | 0     |
| 85  | OHX  | 2     | 1978 | 7/7   | 0.85 | 0.16 | 153,153,153,153             | 0     |
| 85  | OHX  | 2     | 2026 | 7/7   | 0.85 | 0.14 | 168,168,168,168             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 5     | 3925 | 1/1   | 0.85 | 0.22 | 26,26,26,26                 | 0     |
| 86  | MG   | 5     | 3926 | 1/1   | 0.85 | 0.34 | 30,30,30,30                 | 0     |
| 86  | MG   | 5     | 3927 | 1/1   | 0.85 | 0.37 | 46,46,46,46                 | 0     |
| 86  | MG   | 5     | 3931 | 1/1   | 0.85 | 0.27 | 48,48,48,48                 | 0     |
| 86  | MG   | 1     | 4074 | 1/1   | 0.85 | 0.20 | 48,48,48,48                 | 0     |
| 86  | MG   | 6     | 2078 | 1/1   | 0.85 | 0.44 | 70,70,70,70                 | 0     |
| 86  | MG   | 5     | 3935 | 1/1   | 0.85 | 0.21 | 37,37,37,37                 | 0     |
| 86  | MG   | 5     | 3936 | 1/1   | 0.85 | 0.31 | 55,55,55,55                 | 0     |
| 86  | MG   | 5     | 3937 | 1/1   | 0.85 | 0.27 | 34,34,34,34                 | 0     |
| 86  | MG   | 5     | 4076 | 1/1   | 0.85 | 0.12 | 36,36,36,36                 | 0     |
| 86  | MG   | 5     | 4077 | 1/1   | 0.85 | 0.26 | 79,79,79,79                 | 0     |
| 85  | OHX  | 6     | 2042 | 7/7   | 0.85 | 0.17 | 139,139,139,139             | 0     |
| 85  | OHX  | 2     | 2023 | 7/7   | 0.85 | 0.14 | 166,166,166,166             | 0     |
| 86  | MG   | 1     | 4006 | 1/1   | 0.85 | 0.19 | 48,48,48,48                 | 0     |
| 86  | MG   | 5     | 3803 | 1/1   | 0.85 | 0.12 | 44,44,44,44                 | 0     |
| 85  | OHX  | 2     | 2032 | 7/7   | 0.85 | 0.14 | 168,168,168,168             | 0     |
| 85  | OHX  | 5     | 3733 | 7/7   | 0.85 | 0.16 | 148,148,148,148             | 0     |
| 85  | OHX  | 1     | 3724 | 7/7   | 0.85 | 0.34 | 136,136,136,136             | 0     |
| 86  | MG   | 6     | 2157 | 1/1   | 0.85 | 0.23 | 49,49,49,49                 | 0     |
| 86  | MG   | 1     | 3941 | 1/1   | 0.85 | 0.35 | 34,34,34,34                 | 0     |
| 86  | MG   | 1     | 3942 | 1/1   | 0.85 | 0.19 | 38,38,38,38                 | 0     |
| 86  | MG   | 4     | 228  | 1/1   | 0.85 | 0.13 | 36,36,36,36                 | 0     |
| 86  | MG   | 1     | 4088 | 1/1   | 0.85 | 0.23 | 52,52,52,52                 | 0     |
| 85  | OHX  | 6     | 2050 | 7/7   | 0.85 | 0.14 | 173,173,173,173             | 0     |
| 85  | OHX  | 6     | 2021 | 7/7   | 0.85 | 0.13 | 169,169,169,169             | 0     |
| 86  | MG   | 2     | 2061 | 1/1   | 0.85 | 0.42 | 59,59,59,59                 | 0     |
| 85  | OHX  | 2     | 2018 | 7/7   | 0.86 | 0.18 | 151,151,151,151             | 0     |
| 85  | OHX  | 5     | 3664 | 7/7   | 0.86 | 0.30 | 125,125,125,125             | 0     |
| 86  | MG   | 6     | 2101 | 1/1   | 0.86 | 0.44 | 53,53,53,53                 | 0     |
| 86  | MG   | 5     | 3885 | 1/1   | 0.86 | 0.36 | 49,49,49,49                 | 0     |
| 86  | MG   | 5     | 4158 | 1/1   | 0.86 | 0.29 | 52,52,52,52                 | 0     |
| 86  | MG   | 2     | 2073 | 1/1   | 0.86 | 0.29 | 60,60,60,60                 | 0     |
| 85  | OHX  | 1     | 3631 | 7/7   | 0.86 | 0.25 | 135,135,135,135             | 0     |
| 86  | MG   | 1     | 4030 | 1/1   | 0.86 | 0.24 | 43,43,43,43                 | 0     |
| 86  | MG   | 1     | 3854 | 1/1   | 0.86 | 0.26 | 43,43,43,43                 | 0     |
| 86  | MG   | 6     | 2165 | 1/1   | 0.86 | 0.27 | 70,70,70,70                 | 0     |
| 86  | MG   | 6     | 2107 | 1/1   | 0.86 | 0.15 | 48,48,48,48                 | 0     |
| 85  | OHX  | 3     | 211  | 7/7   | 0.86 | 0.16 | 165,165,165,165             | 0     |
| 85  | OHX  | 1     | 3686 | 7/7   | 0.86 | 0.15 | 141,141,141,141             | 0     |
| 85  | OHX  | 2     | 2043 | 7/7   | 0.86 | 0.13 | 179,179,179,179             | 0     |
| 86  | MG   | 1     | 4038 | 1/1   | 0.86 | 0.17 | 60,60,60,60                 | 0     |
| 86  | MG   | 5     | 3909 | 1/1   | 0.86 | 0.32 | 25,25,25,25                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | OHX  | S6    | 301  | 7/7   | 0.86 | 0.14 | 167,167,167,167             | 0     |
| 86  | MG   | 1     | 3764 | 1/1   | 0.86 | 0.16 | 37,37,37,37                 | 0     |
| 85  | OHX  | 2     | 2003 | 7/7   | 0.86 | 0.17 | 144,144,144,144             | 0     |
| 86  | MG   | 1     | 3771 | 1/1   | 0.86 | 0.28 | 37,37,37,37                 | 0     |
| 86  | MG   | 1     | 3990 | 1/1   | 0.86 | 0.27 | 47,47,47,47                 | 0     |
| 86  | MG   | 1     | 3946 | 1/1   | 0.86 | 0.18 | 52,52,52,52                 | 0     |
| 86  | MG   | 6     | 2182 | 1/1   | 0.86 | 0.27 | 76,76,76,76                 | 0     |
| 86  | MG   | 1     | 3772 | 1/1   | 0.86 | 0.21 | 32,32,32,32                 | 0     |
| 85  | OHX  | 6     | 1979 | 7/7   | 0.86 | 0.33 | 134,134,134,134             | 0     |
| 86  | MG   | 1     | 3998 | 1/1   | 0.86 | 0.22 | 60,60,60,60                 | 0     |
| 86  | MG   | s4    | 302  | 1/1   | 0.86 | 0.35 | 62,62,62,62                 | 0     |
| 86  | MG   | 4     | 226  | 1/1   | 0.86 | 0.20 | 56,56,56,56                 | 0     |
| 86  | MG   | 1     | 3819 | 1/1   | 0.86 | 0.25 | 33,33,33,33                 | 0     |
| 86  | MG   | l3    | 405  | 1/1   | 0.86 | 0.14 | 39,39,39,39                 | 0     |
| 86  | MG   | 1     | 4104 | 1/1   | 0.86 | 0.34 | 46,46,46,46                 | 0     |
| 85  | OHX  | 5     | 3707 | 7/7   | 0.86 | 0.30 | 135,135,135,135             | 0     |
| 85  | OHX  | 1     | 3699 | 7/7   | 0.86 | 0.15 | 147,147,147,147             | 0     |
| 86  | MG   | 6     | 2133 | 1/1   | 0.86 | 0.13 | 84,84,84,84                 | 0     |
| 85  | OHX  | 6     | 1990 | 7/7   | 0.86 | 0.26 | 129,129,129,129             | 0     |
| 86  | MG   | 5     | 3946 | 1/1   | 0.86 | 0.12 | 39,39,39,39                 | 0     |
| 85  | OHX  | 6     | 2010 | 7/7   | 0.86 | 0.15 | 146,146,146,146             | 0     |
| 86  | MG   | M0    | 302  | 1/1   | 0.86 | 0.16 | 40,40,40,40                 | 0     |
| 86  | MG   | n6    | 201  | 1/1   | 0.86 | 0.37 | 58,58,58,58                 | 0     |
| 86  | MG   | 1     | 3787 | 1/1   | 0.86 | 0.24 | 35,35,35,35                 | 0     |
| 85  | OHX  | 1     | 3667 | 7/7   | 0.86 | 0.16 | 154,154,154,154             | 0     |
| 86  | MG   | n9    | 102  | 1/1   | 0.86 | 0.12 | 34,34,34,34                 | 0     |
| 86  | MG   | 5     | 3955 | 1/1   | 0.86 | 0.12 | 46,46,46,46                 | 0     |
| 85  | OHX  | 1     | 3708 | 7/7   | 0.86 | 0.15 | 152,152,152,152             | 0     |
| 86  | MG   | 5     | 3852 | 1/1   | 0.86 | 0.22 | 32,32,32,32                 | 0     |
| 86  | MG   | 6     | 2091 | 1/1   | 0.86 | 0.42 | 77,77,77,77                 | 0     |
| 86  | MG   | 5     | 3772 | 1/1   | 0.86 | 0.25 | 39,39,39,39                 | 0     |
| 86  | MG   | 1     | 3791 | 1/1   | 0.86 | 0.21 | 37,37,37,37                 | 0     |
| 86  | MG   | M7    | 206  | 1/1   | 0.86 | 0.15 | 37,37,37,37                 | 0     |
| 86  | MG   | 1     | 4115 | 1/1   | 0.86 | 0.29 | 29,29,29,29                 | 0     |
| 85  | OHX  | 1     | 3730 | 7/7   | 0.86 | 0.15 | 150,150,150,150             | 0     |
| 85  | OHX  | 5     | 3603 | 7/7   | 0.86 | 0.33 | 134,134,134,134             | 0     |
| 85  | OHX  | 2     | 2029 | 7/7   | 0.86 | 0.14 | 167,167,167,167             | 0     |
| 86  | MG   | 6     | 2098 | 1/1   | 0.86 | 0.35 | 69,69,69,69                 | 0     |
| 86  | MG   | 6     | 2156 | 1/1   | 0.86 | 0.09 | 81,81,81,81                 | 0     |
| 86  | MG   | 1     | 4049 | 1/1   | 0.87 | 0.21 | 41,41,41,41                 | 0     |
| 86  | MG   | 1     | 3895 | 1/1   | 0.87 | 0.19 | 29,29,29,29                 | 0     |
| 86  | MG   | 1     | 4051 | 1/1   | 0.87 | 0.26 | 44,44,44,44                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 1     | 3976 | 1/1   | 0.87 | 0.25 | 41,41,41,41                 | 0     |
| 86  | MG   | 5     | 4138 | 1/1   | 0.87 | 0.63 | 62,62,62,62                 | 0     |
| 86  | MG   | 2     | 2091 | 1/1   | 0.87 | 0.21 | 74,74,74,74                 | 0     |
| 86  | MG   | 5     | 4140 | 1/1   | 0.87 | 0.14 | 34,34,34,34                 | 0     |
| 86  | MG   | 6     | 2075 | 1/1   | 0.87 | 0.30 | 61,61,61,61                 | 0     |
| 86  | MG   | 1     | 3897 | 1/1   | 0.87 | 0.39 | 57,57,57,57                 | 0     |
| 86  | MG   | 1     | 3821 | 1/1   | 0.87 | 0.25 | 33,33,33,33                 | 0     |
| 86  | MG   | 5     | 4146 | 1/1   | 0.87 | 0.29 | 31,31,31,31                 | 0     |
| 86  | MG   | 1     | 4057 | 1/1   | 0.87 | 0.46 | 39,39,39,39                 | 0     |
| 85  | OHX  | 5     | 3600 | 7/7   | 0.87 | 0.16 | 147,147,147,147             | 0     |
| 85  | OHX  | 2     | 1994 | 7/7   | 0.87 | 0.15 | 152,152,152,152             | 0     |
| 86  | MG   | 1     | 3824 | 1/1   | 0.87 | 0.32 | 40,40,40,40                 | 0     |
| 85  | OHX  | 5     | 3646 | 7/7   | 0.87 | 0.38 | 123,123,123,123             | 0     |
| 86  | MG   | 1     | 4068 | 1/1   | 0.87 | 0.26 | 34,34,34,34                 | 0     |
| 86  | MG   | 1     | 3779 | 1/1   | 0.87 | 0.26 | 53,53,53,53                 | 0     |
| 86  | MG   | 1     | 3829 | 1/1   | 0.87 | 0.36 | 43,43,43,43                 | 0     |
| 86  | MG   | 2     | 2044 | 1/1   | 0.87 | 0.21 | 38,38,38,38                 | 0     |
| 85  | OHX  | 5     | 3727 | 7/7   | 0.87 | 0.15 | 136,136,136,136             | 0     |
| 86  | MG   | 1     | 3922 | 1/1   | 0.87 | 0.39 | 55,55,55,55                 | 0     |
| 85  | OHX  | 1     | 3679 | 7/7   | 0.87 | 0.36 | 122,122,122,122             | 0     |
| 86  | MG   | 6     | 2166 | 1/1   | 0.87 | 0.30 | 72,72,72,72                 | 0     |
| 86  | MG   | 5     | 4163 | 1/1   | 0.87 | 0.31 | 54,54,54,54                 | 0     |
| 86  | MG   | 1     | 3739 | 1/1   | 0.87 | 0.24 | 52,52,52,52                 | 0     |
| 86  | MG   | 1     | 3835 | 1/1   | 0.87 | 0.41 | 38,38,38,38                 | 0     |
| 85  | OHX  | 1     | 3680 | 7/7   | 0.87 | 0.31 | 114,114,114,114             | 0     |
| 86  | MG   | 1     | 3935 | 1/1   | 0.87 | 0.17 | 36,36,36,36                 | 0     |
| 86  | MG   | 5     | 4064 | 1/1   | 0.87 | 0.13 | 47,47,47,47                 | 0     |
| 86  | MG   | 5     | 3828 | 1/1   | 0.87 | 0.22 | 49,49,49,49                 | 0     |
| 86  | MG   | 5     | 3830 | 1/1   | 0.87 | 0.29 | 32,32,32,32                 | 0     |
| 86  | MG   | 1     | 3937 | 1/1   | 0.87 | 0.19 | 57,57,57,57                 | 0     |
| 85  | OHX  | 6     | 1971 | 7/7   | 0.87 | 0.17 | 138,138,138,138             | 0     |
| 86  | MG   | 1     | 3743 | 1/1   | 0.87 | 0.24 | 47,47,47,47                 | 0     |
| 86  | MG   | 7     | 215  | 1/1   | 0.87 | 0.30 | 61,61,61,61                 | 0     |
| 85  | OHX  | 1     | 3657 | 7/7   | 0.87 | 0.37 | 110,110,110,110             | 0     |
| 86  | MG   | 5     | 3837 | 1/1   | 0.87 | 0.21 | 35,35,35,35                 | 0     |
| 85  | OHX  | 1     | 3710 | 7/7   | 0.87 | 0.45 | 123,123,123,123             | 0     |
| 86  | MG   | 1     | 4019 | 1/1   | 0.87 | 0.12 | 51,51,51,51                 | 0     |
| 86  | MG   | 1     | 4092 | 1/1   | 0.87 | 0.37 | 44,44,44,44                 | 0     |
| 86  | MG   | 5     | 3842 | 1/1   | 0.87 | 0.24 | 33,33,33,33                 | 0     |
| 86  | MG   | M6    | 201  | 1/1   | 0.87 | 0.13 | 39,39,39,39                 | 0     |
| 85  | OHX  | 2     | 1946 | 7/7   | 0.87 | 0.13 | 170,170,170,170             | 0     |
| 86  | MG   | 1     | 3798 | 1/1   | 0.87 | 0.17 | 41,41,41,41                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | OHX  | 2     | 2031 | 7/7   | 0.87 | 0.17 | 147,147,147,147             | 0     |
| 86  | MG   | 5     | 3977 | 1/1   | 0.87 | 0.23 | 45,45,45,45                 | 0     |
| 85  | OHX  | 5     | 3741 | 7/7   | 0.87 | 0.36 | 127,127,127,127             | 0     |
| 85  | OHX  | 1     | 3691 | 7/7   | 0.87 | 0.35 | 129,129,129,129             | 0     |
| 86  | MG   | 6     | 2112 | 1/1   | 0.87 | 0.36 | 71,71,71,71                 | 0     |
| 86  | MG   | 1     | 3804 | 1/1   | 0.87 | 0.15 | 38,38,38,38                 | 0     |
| 86  | MG   | 1     | 3754 | 1/1   | 0.87 | 0.08 | 89,89,89,89                 | 0     |
| 86  | MG   | 2     | 2058 | 1/1   | 0.87 | 0.29 | 58,58,58,58                 | 0     |
| 86  | MG   | 5     | 4100 | 1/1   | 0.87 | 0.10 | 40,40,40,40                 | 0     |
| 85  | OHX  | 5     | 3687 | 7/7   | 0.87 | 0.35 | 130,130,130,130             | 0     |
| 85  | OHX  | 1     | 3736 | 7/7   | 0.87 | 0.32 | 119,119,119,119             | 0     |
| 86  | MG   | m6    | 204  | 1/1   | 0.87 | 0.14 | 43,43,43,43                 | 0     |
| 86  | MG   | n0    | 203  | 1/1   | 0.87 | 0.11 | 40,40,40,40                 | 0     |
| 86  | MG   | 1     | 4035 | 1/1   | 0.87 | 0.15 | 49,49,49,49                 | 0     |
| 85  | OHX  | S8    | 301  | 7/7   | 0.87 | 0.13 | 165,165,165,165             | 0     |
| 85  | OHX  | 5     | 3700 | 7/7   | 0.87 | 0.26 | 136,136,136,136             | 0     |
| 86  | MG   | Q2    | 504  | 1/1   | 0.87 | 0.10 | 52,52,52,52                 | 0     |
| 86  | MG   | 1     | 3814 | 1/1   | 0.87 | 0.20 | 50,50,50,50                 | 0     |
| 86  | MG   | 1     | 3885 | 1/1   | 0.87 | 0.31 | 30,30,30,30                 | 0     |
| 85  | OHX  | 6     | 2026 | 7/7   | 0.87 | 0.15 | 158,158,158,158             | 0     |
| 85  | OHX  | 6     | 2027 | 7/7   | 0.87 | 0.18 | 143,143,143,143             | 0     |
| 86  | MG   | 1     | 3970 | 1/1   | 0.87 | 0.21 | 44,44,44,44                 | 0     |
| 86  | MG   | 1     | 3766 | 1/1   | 0.87 | 0.15 | 39,39,39,39                 | 0     |
| 86  | MG   | 1     | 3892 | 1/1   | 0.87 | 0.31 | 44,44,44,44                 | 0     |
| 86  | MG   | 5     | 3896 | 1/1   | 0.87 | 0.32 | 29,29,29,29                 | 0     |
| 86  | MG   | 5     | 4008 | 1/1   | 0.87 | 0.20 | 42,42,42,42                 | 0     |
| 86  | MG   | 5     | 4011 | 1/1   | 0.87 | 0.28 | 42,42,42,42                 | 0     |
| 86  | MG   | 6     | 2063 | 1/1   | 0.87 | 0.30 | 42,42,42,42                 | 0     |
| 85  | OHX  | 1     | 3648 | 7/7   | 0.87 | 0.16 | 137,137,137,137             | 0     |
| 86  | MG   | 6     | 2140 | 1/1   | 0.87 | 0.15 | 61,61,61,61                 | 0     |
| 86  | MG   | 5     | 4132 | 1/1   | 0.87 | 0.39 | 35,35,35,35                 | 0     |
| 85  | OHX  | 6     | 1995 | 7/7   | 0.88 | 0.12 | 162,162,162,162             | 0     |
| 86  | MG   | 1     | 3756 | 1/1   | 0.88 | 0.17 | 37,37,37,37                 | 0     |
| 85  | OHX  | 6     | 2002 | 7/7   | 0.88 | 0.24 | 125,125,125,125             | 0     |
| 86  | MG   | 2     | 2132 | 1/1   | 0.88 | 0.17 | 70,70,70,70                 | 0     |
| 85  | OHX  | 6     | 2006 | 7/7   | 0.88 | 0.16 | 141,141,141,141             | 0     |
| 85  | OHX  | 5     | 3685 | 7/7   | 0.88 | 0.32 | 133,133,133,133             | 0     |
| 85  | OHX  | 8     | 216  | 7/7   | 0.88 | 0.25 | 134,134,134,134             | 0     |
| 85  | OHX  | 1     | 3598 | 7/7   | 0.88 | 0.14 | 142,142,142,142             | 0     |
| 85  | OHX  | 1     | 3716 | 7/7   | 0.88 | 0.37 | 113,113,113,113             | 0     |
| 86  | MG   | 1     | 3820 | 1/1   | 0.88 | 0.45 | 54,54,54,54                 | 0     |
| 86  | MG   | 1     | 3978 | 1/1   | 0.88 | 0.33 | 51,51,51,51                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 6     | 2072 | 1/1   | 0.88 | 0.37 | 42,42,42,42                 | 0     |
| 86  | MG   | 5     | 3791 | 1/1   | 0.88 | 0.15 | 29,29,29,29                 | 0     |
| 86  | MG   | 1     | 4130 | 1/1   | 0.88 | 0.20 | 52,52,52,52                 | 0     |
| 86  | MG   | 1     | 3899 | 1/1   | 0.88 | 0.36 | 43,43,43,43                 | 0     |
| 86  | MG   | 5     | 4034 | 1/1   | 0.88 | 0.22 | 51,51,51,51                 | 0     |
| 86  | MG   | 5     | 4036 | 1/1   | 0.88 | 0.17 | 41,41,41,41                 | 0     |
| 86  | MG   | 1     | 3768 | 1/1   | 0.88 | 0.26 | 37,37,37,37                 | 0     |
| 86  | MG   | 5     | 4038 | 1/1   | 0.88 | 0.25 | 37,37,37,37                 | 0     |
| 86  | MG   | 2     | 2104 | 1/1   | 0.88 | 0.32 | 68,68,68,68                 | 0     |
| 86  | MG   | 5     | 3797 | 1/1   | 0.88 | 0.33 | 52,52,52,52                 | 0     |
| 85  | OHX  | 6     | 2022 | 7/7   | 0.88 | 0.32 | 116,116,116,116             | 0     |
| 86  | MG   | 6     | 2152 | 1/1   | 0.88 | 0.12 | 70,70,70,70                 | 0     |
| 86  | MG   | 6     | 2153 | 1/1   | 0.88 | 0.14 | 97,97,97,97                 | 0     |
| 85  | OHX  | 1     | 3717 | 7/7   | 0.88 | 0.28 | 132,132,132,132             | 0     |
| 85  | OHX  | 5     | 3701 | 7/7   | 0.88 | 0.27 | 126,126,126,126             | 0     |
| 86  | MG   | 1     | 4066 | 1/1   | 0.88 | 0.17 | 41,41,41,41                 | 0     |
| 86  | MG   | 1     | 3777 | 1/1   | 0.88 | 0.20 | 44,44,44,44                 | 0     |
| 86  | MG   | 5     | 4165 | 1/1   | 0.88 | 0.46 | 33,33,33,33                 | 0     |
| 86  | MG   | 6     | 2158 | 1/1   | 0.88 | 0.13 | 46,46,46,46                 | 0     |
| 85  | OHX  | 2     | 1995 | 7/7   | 0.88 | 0.16 | 139,139,139,139             | 0     |
| 85  | OHX  | 5     | 3709 | 7/7   | 0.88 | 0.30 | 128,128,128,128             | 0     |
| 86  | MG   | 1     | 3993 | 1/1   | 0.88 | 0.25 | 49,49,49,49                 | 0     |
| 86  | MG   | 5     | 4058 | 1/1   | 0.88 | 0.06 | 35,35,35,35                 | 0     |
| 86  | MG   | 4     | 219  | 1/1   | 0.88 | 0.37 | 38,38,38,38                 | 0     |
| 86  | MG   | 5     | 3820 | 1/1   | 0.88 | 0.22 | 28,28,28,28                 | 0     |
| 85  | OHX  | 1     | 3650 | 7/7   | 0.88 | 0.13 | 158,158,158,158             | 0     |
| 85  | OHX  | 1     | 3653 | 7/7   | 0.88 | 0.35 | 119,119,119,119             | 0     |
| 86  | MG   | 5     | 3950 | 1/1   | 0.88 | 0.20 | 38,38,38,38                 | 0     |
| 86  | MG   | 1     | 3924 | 1/1   | 0.88 | 0.20 | 79,79,79,79                 | 0     |
| 86  | MG   | 5     | 3825 | 1/1   | 0.88 | 0.25 | 30,30,30,30                 | 0     |
| 86  | MG   | 1     | 3999 | 1/1   | 0.88 | 0.28 | 66,66,66,66                 | 0     |
| 86  | MG   | 1     | 3784 | 1/1   | 0.88 | 0.15 | 32,32,32,32                 | 0     |
| 85  | OHX  | 5     | 3714 | 7/7   | 0.88 | 0.18 | 144,144,144,144             | 0     |
| 85  | OHX  | 1     | 3701 | 7/7   | 0.88 | 0.13 | 144,144,144,144             | 0     |
| 85  | OHX  | 5     | 3720 | 7/7   | 0.88 | 0.32 | 128,128,128,128             | 0     |
| 85  | OHX  | 5     | 3607 | 7/7   | 0.88 | 0.14 | 144,144,144,144             | 0     |
| 85  | OHX  | 5     | 3725 | 7/7   | 0.88 | 0.30 | 125,125,125,125             | 0     |
| 85  | OHX  | 5     | 3633 | 7/7   | 0.88 | 0.14 | 141,141,141,141             | 0     |
| 86  | MG   | 5     | 4085 | 1/1   | 0.88 | 0.12 | 36,36,36,36                 | 0     |
| 86  | MG   | 1     | 3842 | 1/1   | 0.88 | 0.25 | 33,33,33,33                 | 0     |
| 86  | MG   | 5     | 3838 | 1/1   | 0.88 | 0.20 | 35,35,35,35                 | 0     |
| 86  | MG   | 1     | 3940 | 1/1   | 0.88 | 0.18 | 65,65,65,65                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 1     | 3794 | 1/1   | 0.88 | 0.16 | 29,29,29,29                 | 0     |
| 86  | MG   | 17    | 301  | 1/1   | 0.88 | 0.16 | 35,35,35,35                 | 0     |
| 86  | MG   | 6     | 2105 | 1/1   | 0.88 | 0.30 | 42,42,42,42                 | 0     |
| 85  | OHX  | 5     | 3642 | 7/7   | 0.88 | 0.33 | 126,126,126,126             | 0     |
| 86  | MG   | 1     | 3943 | 1/1   | 0.88 | 0.26 | 73,73,73,73                 | 0     |
| 85  | OHX  | 1     | 3608 | 7/7   | 0.88 | 0.25 | 135,135,135,135             | 0     |
| 86  | MG   | 1     | 3945 | 1/1   | 0.88 | 0.20 | 43,43,43,43                 | 0     |
| 85  | OHX  | 2     | 2000 | 7/7   | 0.88 | 0.15 | 140,140,140,140             | 0     |
| 86  | MG   | n0    | 202  | 1/1   | 0.88 | 0.14 | 36,36,36,36                 | 0     |
| 86  | MG   | 1     | 3745 | 1/1   | 0.88 | 0.36 | 32,32,32,32                 | 0     |
| 85  | OHX  | 5     | 3656 | 7/7   | 0.88 | 0.16 | 151,151,151,151             | 0     |
| 86  | MG   | n3    | 202  | 1/1   | 0.88 | 0.36 | 27,27,27,27                 | 0     |
| 86  | MG   | 5     | 3987 | 1/1   | 0.88 | 0.32 | 53,53,53,53                 | 0     |
| 86  | MG   | 5     | 4107 | 1/1   | 0.88 | 0.20 | 40,40,40,40                 | 0     |
| 86  | MG   | 1     | 3801 | 1/1   | 0.88 | 0.34 | 43,43,43,43                 | 0     |
| 86  | MG   | 5     | 3747 | 1/1   | 0.88 | 0.17 | 34,34,34,34                 | 0     |
| 85  | OHX  | 6     | 2034 | 7/7   | 0.88 | 0.34 | 129,129,129,129             | 0     |
| 86  | MG   | N9    | 101  | 1/1   | 0.88 | 0.24 | 38,38,38,38                 | 0     |
| 86  | MG   | 1     | 3865 | 1/1   | 0.88 | 0.40 | 39,39,39,39                 | 0     |
| 85  | OHX  | 1     | 3684 | 7/7   | 0.88 | 0.16 | 139,139,139,139             | 0     |
| 86  | MG   | 1     | 3869 | 1/1   | 0.88 | 0.26 | 31,31,31,31                 | 0     |
| 86  | MG   | 5     | 3760 | 1/1   | 0.88 | 0.29 | 56,56,56,56                 | 0     |
| 86  | MG   | MG    | 2207 | 1/1   | 0.88 | 0.22 | 109,109,109,109             | 0     |
| 85  | OHX  | 1     | 3661 | 7/7   | 0.88 | 0.23 | 132,132,132,132             | 0     |
| 86  | MG   | Q2    | 503  | 1/1   | 0.88 | 0.24 | 68,68,68,68                 | 0     |
| 86  | MG   | 5     | 3999 | 1/1   | 0.88 | 0.14 | 42,42,42,42                 | 0     |
| 85  | OHX  | 5     | 3670 | 7/7   | 0.88 | 0.34 | 126,126,126,126             | 0     |
| 85  | OHX  | 2     | 2001 | 7/7   | 0.88 | 0.15 | 141,141,141,141             | 0     |
| 86  | MG   | 5     | 3883 | 1/1   | 0.88 | 0.23 | 48,48,48,48                 | 0     |
| 86  | MG   | 1     | 3880 | 1/1   | 0.88 | 0.18 | 36,36,36,36                 | 0     |
| 86  | MG   | 1     | 3995 | 1/1   | 0.89 | 0.20 | 39,39,39,39                 | 0     |
| 86  | MG   | 1     | 3921 | 1/1   | 0.89 | 0.19 | 50,50,50,50                 | 0     |
| 86  | MG   | 5     | 3815 | 1/1   | 0.89 | 0.27 | 29,29,29,29                 | 0     |
| 85  | OHX  | s8    | 301  | 7/7   | 0.89 | 0.13 | 155,155,155,155             | 0     |
| 86  | MG   | 4     | 224  | 1/1   | 0.89 | 0.11 | 50,50,50,50                 | 0     |
| 85  | OHX  | 1     | 3617 | 7/7   | 0.89 | 0.28 | 129,129,129,129             | 0     |
| 85  | OHX  | 5     | 3579 | 7/7   | 0.89 | 0.32 | 122,122,122,122             | 0     |
| 85  | OHX  | 5     | 3712 | 7/7   | 0.89 | 0.13 | 148,148,148,148             | 0     |
| 86  | MG   | 1     | 4003 | 1/1   | 0.89 | 0.25 | 34,34,34,34                 | 0     |
| 86  | MG   | 5     | 4047 | 1/1   | 0.89 | 0.10 | 35,35,35,35                 | 0     |
| 86  | MG   | 1     | 3782 | 1/1   | 0.89 | 0.21 | 35,35,35,35                 | 0     |
| 86  | MG   | 1     | 4083 | 1/1   | 0.89 | 0.12 | 46,46,46,46                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 5     | 3943 | 1/1   | 0.89 | 0.17 | 65,65,65,65                 | 0     |
| 85  | OHX  | 1     | 3733 | 7/7   | 0.89 | 0.32 | 119,119,119,119             | 0     |
| 86  | MG   | 1     | 3838 | 1/1   | 0.89 | 0.12 | 38,38,38,38                 | 0     |
| 86  | MG   | 5     | 4159 | 1/1   | 0.89 | 0.25 | 52,52,52,52                 | 0     |
| 85  | OHX  | 2     | 1996 | 7/7   | 0.89 | 0.14 | 144,144,144,144             | 0     |
| 85  | OHX  | 5     | 3719 | 7/7   | 0.89 | 0.11 | 181,181,181,181             | 0     |
| 86  | MG   | 2     | 2100 | 1/1   | 0.89 | 0.49 | 69,69,69,69                 | 0     |
| 85  | OHX  | 1     | 3630 | 7/7   | 0.89 | 0.26 | 126,126,126,126             | 0     |
| 85  | OHX  | 5     | 3723 | 7/7   | 0.89 | 0.32 | 128,128,128,128             | 0     |
| 86  | MG   | D3    | 201  | 1/1   | 0.89 | 0.13 | 64,64,64,64                 | 0     |
| 85  | OHX  | 5     | 3625 | 7/7   | 0.89 | 0.14 | 146,146,146,146             | 0     |
| 85  | OHX  | 1     | 3672 | 7/7   | 0.89 | 0.28 | 113,113,113,113             | 0     |
| 85  | OHX  | 1     | 3673 | 7/7   | 0.89 | 0.29 | 116,116,116,116             | 0     |
| 85  | OHX  | 4     | 211  | 7/7   | 0.89 | 0.30 | 111,111,111,111             | 0     |
| 85  | OHX  | 5     | 3647 | 7/7   | 0.89 | 0.31 | 117,117,117,117             | 0     |
| 85  | OHX  | 2     | 1997 | 7/7   | 0.89 | 0.13 | 138,138,138,138             | 0     |
| 85  | OHX  | 2     | 2012 | 7/7   | 0.89 | 0.13 | 153,153,153,153             | 0     |
| 85  | OHX  | M7    | 201  | 7/7   | 0.89 | 0.41 | 100,100,100,100             | 0     |
| 86  | MG   | 6     | 2116 | 1/1   | 0.89 | 0.22 | 57,57,57,57                 | 0     |
| 86  | MG   | 5     | 3847 | 1/1   | 0.89 | 0.36 | 27,27,27,27                 | 0     |
| 85  | OHX  | 5     | 3660 | 7/7   | 0.89 | 0.31 | 127,127,127,127             | 0     |
| 85  | OHX  | 5     | 3737 | 7/7   | 0.89 | 0.36 | 118,118,118,118             | 0     |
| 85  | OHX  | 2     | 2013 | 7/7   | 0.89 | 0.22 | 136,136,136,136             | 0     |
| 85  | OHX  | 5     | 3666 | 7/7   | 0.89 | 0.42 | 104,104,104,104             | 0     |
| 86  | MG   | 5     | 4087 | 1/1   | 0.89 | 0.41 | 50,50,50,50                 | 0     |
| 86  | MG   | 6     | 2123 | 1/1   | 0.89 | 0.40 | 83,83,83,83                 | 0     |
| 85  | OHX  | 6     | 2036 | 7/7   | 0.89 | 0.26 | 128,128,128,128             | 0     |
| 85  | OHX  | 2     | 2017 | 7/7   | 0.89 | 0.14 | 139,139,139,139             | 0     |
| 86  | MG   | 1     | 4110 | 1/1   | 0.89 | 0.12 | 32,32,32,32                 | 0     |
| 86  | MG   | 5     | 3865 | 1/1   | 0.89 | 0.21 | 30,30,30,30                 | 0     |
| 86  | MG   | 5     | 3869 | 1/1   | 0.89 | 0.22 | 52,52,52,52                 | 0     |
| 86  | MG   | 6     | 2053 | 1/1   | 0.89 | 0.18 | 79,79,79,79                 | 0     |
| 86  | MG   | 1     | 3810 | 1/1   | 0.89 | 0.17 | 41,41,41,41                 | 0     |
| 86  | MG   | 5     | 3767 | 1/1   | 0.89 | 0.22 | 39,39,39,39                 | 0     |
| 86  | MG   | 1     | 3965 | 1/1   | 0.89 | 0.15 | 44,44,44,44                 | 0     |
| 86  | MG   | 1     | 3886 | 1/1   | 0.89 | 0.39 | 41,41,41,41                 | 0     |
| 85  | OHX  | 2     | 1998 | 7/7   | 0.89 | 0.16 | 138,138,138,138             | 0     |
| 86  | MG   | 1     | 3753 | 1/1   | 0.89 | 0.14 | 49,49,49,49                 | 0     |
| 85  | OHX  | D9    | 102  | 7/7   | 0.89 | 0.17 | 140,140,140,140             | 0     |
| 85  | OHX  | 2     | 1981 | 7/7   | 0.89 | 0.15 | 146,146,146,146             | 0     |
| 86  | MG   | m6    | 202  | 1/1   | 0.89 | 0.18 | 35,35,35,35                 | 0     |
| 85  | OHX  | 5     | 3679 | 7/7   | 0.89 | 0.32 | 136,136,136,136             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | OHX  | 8     | 217  | 7/7   | 0.89 | 0.40 | 113,113,113,113             | 0     |
| 86  | MG   | 5     | 3886 | 1/1   | 0.89 | 0.32 | 31,31,31,31                 | 0     |
| 85  | OHX  | 2     | 1990 | 7/7   | 0.89 | 0.11 | 169,169,169,169             | 0     |
| 86  | MG   | 5     | 4003 | 1/1   | 0.89 | 0.11 | 33,33,33,33                 | 0     |
| 85  | OHX  | 5     | 3683 | 7/7   | 0.89 | 0.28 | 133,133,133,133             | 0     |
| 86  | MG   | 5     | 3786 | 1/1   | 0.89 | 0.15 | 37,37,37,37                 | 0     |
| 86  | MG   | 1     | 3898 | 1/1   | 0.89 | 0.46 | 53,53,53,53                 | 0     |
| 85  | OHX  | 1     | 3663 | 7/7   | 0.89 | 0.35 | 107,107,107,107             | 0     |
| 86  | MG   | 5     | 4125 | 1/1   | 0.89 | 0.23 | 35,35,35,35                 | 0     |
| 85  | OHX  | 6     | 2046 | 7/7   | 0.89 | 0.14 | 142,142,142,142             | 0     |
| 85  | OHX  | 1     | 3727 | 7/7   | 0.89 | 0.34 | 119,119,119,119             | 0     |
| 86  | MG   | 6     | 2149 | 1/1   | 0.89 | 0.34 | 52,52,52,52                 | 0     |
| 85  | OHX  | 6     | 2048 | 7/7   | 0.89 | 0.14 | 171,171,171,171             | 0     |
| 86  | MG   | 1     | 4059 | 1/1   | 0.89 | 0.11 | 62,62,62,62                 | 0     |
| 85  | OHX  | 5     | 3694 | 7/7   | 0.89 | 0.26 | 135,135,135,135             | 0     |
| 85  | OHX  | 2     | 2002 | 7/7   | 0.89 | 0.16 | 149,149,149,149             | 0     |
| 86  | MG   | 1     | 3826 | 1/1   | 0.89 | 0.35 | 24,24,24,24                 | 0     |
| 85  | OHX  | 1     | 3665 | 7/7   | 0.89 | 0.28 | 138,138,138,138             | 0     |
| 86  | MG   | 4     | 215  | 1/1   | 0.89 | 0.28 | 51,51,51,51                 | 0     |
| 86  | MG   | 1     | 3918 | 1/1   | 0.89 | 0.35 | 47,47,47,47                 | 0     |
| 85  | OHX  | 6     | 2011 | 7/7   | 0.89 | 0.34 | 136,136,136,136             | 0     |
| 87  | ZN   | e1    | 501  | 1/1   | 0.89 | 0.08 | 173,173,173,173             | 0     |
| 85  | OHX  | 5     | 3708 | 7/7   | 0.89 | 0.35 | 122,122,122,122             | 0     |
| 86  | MG   | sM    | 402  | 1/1   | 0.90 | 0.23 | 44,44,44,44                 | 0     |
| 85  | OHX  | 5     | 3631 | 7/7   | 0.90 | 0.36 | 113,113,113,113             | 0     |
| 85  | OHX  | 5     | 3632 | 7/7   | 0.90 | 0.36 | 132,132,132,132             | 0     |
| 85  | OHX  | 6     | 2028 | 7/7   | 0.90 | 0.31 | 116,116,116,116             | 0     |
| 85  | OHX  | 2     | 2004 | 7/7   | 0.90 | 0.27 | 126,126,126,126             | 0     |
| 85  | OHX  | 2     | 2006 | 7/7   | 0.90 | 0.26 | 135,135,135,135             | 0     |
| 86  | MG   | M6    | 202  | 1/1   | 0.90 | 0.19 | 42,42,42,42                 | 0     |
| 86  | MG   | 1     | 3917 | 1/1   | 0.90 | 0.09 | 63,63,63,63                 | 0     |
| 86  | MG   | 5     | 3761 | 1/1   | 0.90 | 0.17 | 36,36,36,36                 | 0     |
| 86  | MG   | 5     | 4135 | 1/1   | 0.90 | 0.11 | 83,83,83,83                 | 0     |
| 86  | MG   | 5     | 3877 | 1/1   | 0.90 | 0.35 | 36,36,36,36                 | 0     |
| 85  | OHX  | 2     | 1992 | 7/7   | 0.90 | 0.14 | 153,153,153,153             | 0     |
| 85  | OHX  | 5     | 3649 | 7/7   | 0.90 | 0.22 | 129,129,129,129             | 0     |
| 86  | MG   | 1     | 3761 | 1/1   | 0.90 | 0.18 | 47,47,47,47                 | 0     |
| 86  | MG   | 5     | 4009 | 1/1   | 0.90 | 0.24 | 49,49,49,49                 | 0     |
| 85  | OHX  | 5     | 3652 | 7/7   | 0.90 | 0.23 | 126,126,126,126             | 0     |
| 85  | OHX  | 5     | 3729 | 7/7   | 0.90 | 0.24 | 135,135,135,135             | 0     |
| 85  | OHX  | 6     | 1976 | 7/7   | 0.90 | 0.13 | 147,147,147,147             | 0     |
| 85  | OHX  | 1     | 3702 | 7/7   | 0.90 | 0.12 | 157,157,157,157             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 1     | 3767 | 1/1   | 0.90 | 0.34 | 61,61,61,61                 | 0     |
| 86  | MG   | 5     | 3775 | 1/1   | 0.90 | 0.17 | 34,34,34,34                 | 0     |
| 86  | MG   | 5     | 3888 | 1/1   | 0.90 | 0.34 | 43,43,43,43                 | 0     |
| 85  | OHX  | 5     | 3732 | 7/7   | 0.90 | 0.27 | 127,127,127,127             | 0     |
| 85  | OHX  | 6     | 1985 | 7/7   | 0.90 | 0.14 | 143,143,143,143             | 0     |
| 85  | OHX  | 5     | 3658 | 7/7   | 0.90 | 0.37 | 97,97,97,97                 | 0     |
| 86  | MG   | 1     | 3936 | 1/1   | 0.90 | 0.15 | 66,66,66,66                 | 0     |
| 85  | OHX  | 1     | 3728 | 7/7   | 0.90 | 0.33 | 111,111,111,111             | 0     |
| 86  | MG   | 5     | 3901 | 1/1   | 0.90 | 0.30 | 40,40,40,40                 | 0     |
| 85  | OHX  | 2     | 2019 | 7/7   | 0.90 | 0.14 | 156,156,156,156             | 0     |
| 86  | MG   | 1     | 3774 | 1/1   | 0.90 | 0.14 | 53,53,53,53                 | 0     |
| 85  | OHX  | 5     | 3665 | 7/7   | 0.90 | 0.28 | 114,114,114,114             | 0     |
| 86  | MG   | 5     | 3906 | 1/1   | 0.90 | 0.30 | 45,45,45,45                 | 0     |
| 86  | MG   | 1     | 4025 | 1/1   | 0.90 | 0.20 | 55,55,55,55                 | 0     |
| 86  | MG   | 6     | 2054 | 1/1   | 0.90 | 0.34 | 58,58,58,58                 | 0     |
| 85  | OHX  | 1     | 3636 | 7/7   | 0.90 | 0.13 | 147,147,147,147             | 0     |
| 85  | OHX  | 5     | 3668 | 7/7   | 0.90 | 0.16 | 138,138,138,138             | 0     |
| 86  | MG   | 5     | 3912 | 1/1   | 0.90 | 0.41 | 43,43,43,43                 | 0     |
| 86  | MG   | 5     | 4043 | 1/1   | 0.90 | 0.15 | 40,40,40,40                 | 0     |
| 85  | OHX  | 5     | 3742 | 7/7   | 0.90 | 0.28 | 127,127,127,127             | 0     |
| 85  | OHX  | 6     | 1997 | 7/7   | 0.90 | 0.14 | 142,142,142,142             | 0     |
| 86  | MG   | 2     | 2135 | 1/1   | 0.90 | 0.10 | 101,101,101,101             | 0     |
| 86  | MG   | 1     | 3847 | 1/1   | 0.90 | 0.28 | 71,71,71,71                 | 0     |
| 85  | OHX  | C3    | 201  | 7/7   | 0.90 | 0.12 | 150,150,150,150             | 0     |
| 86  | MG   | 1     | 3855 | 1/1   | 0.90 | 0.29 | 29,29,29,29                 | 0     |
| 86  | MG   | 1     | 3785 | 1/1   | 0.90 | 0.29 | 46,46,46,46                 | 0     |
| 85  | OHX  | 6     | 2043 | 7/7   | 0.90 | 0.22 | 138,138,138,138             | 0     |
| 86  | MG   | 7     | 216  | 1/1   | 0.90 | 0.17 | 68,68,68,68                 | 0     |
| 86  | MG   | 1     | 4117 | 1/1   | 0.90 | 0.28 | 36,36,36,36                 | 0     |
| 85  | OHX  | 6     | 2044 | 7/7   | 0.90 | 0.28 | 123,123,123,123             | 0     |
| 86  | MG   | 5     | 3929 | 1/1   | 0.90 | 0.48 | 40,40,40,40                 | 0     |
| 85  | OHX  | 6     | 2004 | 7/7   | 0.90 | 0.14 | 141,141,141,141             | 0     |
| 86  | MG   | 6     | 2073 | 1/1   | 0.90 | 0.37 | 53,53,53,53                 | 0     |
| 85  | OHX  | 6     | 2005 | 7/7   | 0.90 | 0.28 | 117,117,117,117             | 0     |
| 86  | MG   | 5     | 3814 | 1/1   | 0.90 | 0.40 | 45,45,45,45                 | 0     |
| 85  | OHX  | 8     | 218  | 7/7   | 0.90 | 0.32 | 123,123,123,123             | 0     |
| 85  | OHX  | 5     | 3680 | 7/7   | 0.90 | 0.25 | 132,132,132,132             | 0     |
| 85  | OHX  | 2     | 2020 | 7/7   | 0.90 | 0.12 | 172,172,172,172             | 0     |
| 86  | MG   | 1     | 3962 | 1/1   | 0.90 | 0.10 | 46,46,46,46                 | 0     |
| 86  | MG   | 8     | 228  | 1/1   | 0.90 | 0.33 | 44,44,44,44                 | 0     |
| 86  | MG   | 5     | 3945 | 1/1   | 0.90 | 0.08 | 32,32,32,32                 | 0     |
| 86  | MG   | 1     | 3870 | 1/1   | 0.90 | 0.28 | 43,43,43,43                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 1     | 3874 | 1/1   | 0.90 | 0.27 | 29,29,29,29                 | 0     |
| 86  | MG   | 5     | 3949 | 1/1   | 0.90 | 0.38 | 41,41,41,41                 | 0     |
| 85  | OHX  | 1     | 3712 | 7/7   | 0.90 | 0.11 | 170,170,170,170             | 0     |
| 85  | OHX  | SR    | 401  | 7/7   | 0.90 | 0.12 | 168,168,168,168             | 0     |
| 85  | OHX  | 6     | 2012 | 7/7   | 0.90 | 0.15 | 139,139,139,139             | 0     |
| 85  | OHX  | 5     | 3690 | 7/7   | 0.90 | 0.30 | 120,120,120,120             | 0     |
| 86  | MG   | m3    | 201  | 1/1   | 0.90 | 0.10 | 35,35,35,35                 | 0     |
| 85  | OHX  | 6     | 2018 | 7/7   | 0.90 | 0.11 | 174,174,174,174             | 0     |
| 86  | MG   | 5     | 3956 | 1/1   | 0.90 | 0.11 | 34,34,34,34                 | 0     |
| 86  | MG   | 6     | 2088 | 1/1   | 0.90 | 0.33 | 45,45,45,45                 | 0     |
| 86  | MG   | m6    | 203  | 1/1   | 0.90 | 0.16 | 37,37,37,37                 | 0     |
| 86  | MG   | 6     | 2169 | 1/1   | 0.90 | 0.21 | 70,70,70,70                 | 0     |
| 86  | MG   | 6     | 2170 | 1/1   | 0.90 | 0.11 | 62,62,62,62                 | 0     |
| 85  | OHX  | 6     | 2020 | 7/7   | 0.90 | 0.15 | 146,146,146,146             | 0     |
| 85  | OHX  | 1     | 3559 | 7/7   | 0.90 | 0.13 | 143,143,143,143             | 0     |
| 86  | MG   | 5     | 4096 | 1/1   | 0.90 | 0.12 | 36,36,36,36                 | 0     |
| 85  | OHX  | 5     | 3696 | 7/7   | 0.90 | 0.29 | 114,114,114,114             | 0     |
| 85  | OHX  | 5     | 3698 | 7/7   | 0.90 | 0.12 | 164,164,164,164             | 0     |
| 86  | MG   | 5     | 3836 | 1/1   | 0.90 | 0.31 | 40,40,40,40                 | 0     |
| 86  | MG   | 1     | 4062 | 1/1   | 0.90 | 0.44 | 37,37,37,37                 | 0     |
| 86  | MG   | 5     | 3971 | 1/1   | 0.90 | 0.22 | 38,38,38,38                 | 0     |
| 85  | OHX  | 5     | 3555 | 7/7   | 0.90 | 0.37 | 104,104,104,104             | 0     |
| 85  | OHX  | 1     | 3564 | 7/7   | 0.90 | 0.31 | 107,107,107,107             | 0     |
| 86  | MG   | q0    | 202  | 1/1   | 0.90 | 0.16 | 43,43,43,43                 | 0     |
| 85  | OHX  | 5     | 3598 | 7/7   | 0.90 | 0.28 | 130,130,130,130             | 0     |
| 86  | MG   | 1     | 4067 | 1/1   | 0.90 | 0.38 | 58,58,58,58                 | 0     |
| 85  | OHX  | 1     | 3565 | 7/7   | 0.90 | 0.15 | 138,138,138,138             | 0     |
| 86  | MG   | 2     | 2054 | 1/1   | 0.90 | 0.33 | 70,70,70,70                 | 0     |
| 85  | OHX  | 2     | 2030 | 7/7   | 0.90 | 0.12 | 179,179,179,179             | 0     |
| 85  | OHX  | 2     | 1971 | 7/7   | 0.90 | 0.12 | 151,151,151,151             | 0     |
| 86  | MG   | 1     | 4072 | 1/1   | 0.90 | 0.11 | 44,44,44,44                 | 0     |
| 86  | MG   | 5     | 3849 | 1/1   | 0.90 | 0.24 | 62,62,62,62                 | 0     |
| 85  | OHX  | 5     | 3615 | 7/7   | 0.90 | 0.28 | 130,130,130,130             | 0     |
| 85  | OHX  | 2     | 2042 | 7/7   | 0.90 | 0.31 | 130,130,130,130             | 0     |
| 86  | MG   | L3    | 404  | 1/1   | 0.90 | 0.14 | 71,71,71,71                 | 0     |
| 85  | OHX  | 5     | 3630 | 7/7   | 0.90 | 0.30 | 132,132,132,132             | 0     |
| 86  | MG   | 1     | 3867 | 1/1   | 0.91 | 0.21 | 54,54,54,54                 | 0     |
| 85  | OHX  | 1     | 3676 | 7/7   | 0.91 | 0.26 | 128,128,128,128             | 0     |
| 86  | MG   | 6     | 2137 | 1/1   | 0.91 | 0.37 | 66,66,66,66                 | 0     |
| 86  | MG   | 1     | 4112 | 1/1   | 0.91 | 0.21 | 54,54,54,54                 | 0     |
| 86  | MG   | 2     | 2053 | 1/1   | 0.91 | 0.10 | 72,72,72,72                 | 0     |
| 85  | OHX  | 1     | 3537 | 7/7   | 0.91 | 0.29 | 108,108,108,108             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 1     | 3803 | 1/1   | 0.91 | 0.29 | 47,47,47,47                 | 0     |
| 86  | MG   | 5     | 3889 | 1/1   | 0.91 | 0.21 | 33,33,33,33                 | 0     |
| 86  | MG   | 5     | 3891 | 1/1   | 0.91 | 0.22 | 31,31,31,31                 | 0     |
| 86  | MG   | 5     | 3892 | 1/1   | 0.91 | 0.27 | 29,29,29,29                 | 0     |
| 86  | MG   | 5     | 4005 | 1/1   | 0.91 | 0.21 | 61,61,61,61                 | 0     |
| 86  | MG   | 6     | 2142 | 1/1   | 0.91 | 0.15 | 57,57,57,57                 | 0     |
| 86  | MG   | 6     | 2060 | 1/1   | 0.91 | 0.28 | 54,54,54,54                 | 0     |
| 85  | OHX  | 1     | 3633 | 7/7   | 0.91 | 0.25 | 138,138,138,138             | 0     |
| 85  | OHX  | 5     | 3653 | 7/7   | 0.91 | 0.31 | 126,126,126,126             | 0     |
| 85  | OHX  | 1     | 3681 | 7/7   | 0.91 | 0.27 | 131,131,131,131             | 0     |
| 86  | MG   | 1     | 4047 | 1/1   | 0.91 | 0.26 | 75,75,75,75                 | 0     |
| 86  | MG   | 5     | 4015 | 1/1   | 0.91 | 0.21 | 51,51,51,51                 | 0     |
| 86  | MG   | 1     | 3748 | 1/1   | 0.91 | 0.21 | 40,40,40,40                 | 0     |
| 86  | MG   | 6     | 2068 | 1/1   | 0.91 | 0.25 | 45,45,45,45                 | 0     |
| 86  | MG   | 1     | 3808 | 1/1   | 0.91 | 0.18 | 54,54,54,54                 | 0     |
| 86  | MG   | 1     | 3968 | 1/1   | 0.91 | 0.24 | 47,47,47,47                 | 0     |
| 86  | MG   | 5     | 4021 | 1/1   | 0.91 | 0.23 | 54,54,54,54                 | 0     |
| 86  | MG   | 5     | 3798 | 1/1   | 0.91 | 0.33 | 27,27,27,27                 | 0     |
| 85  | OHX  | 5     | 3722 | 7/7   | 0.91 | 0.25 | 131,131,131,131             | 0     |
| 85  | OHX  | 5     | 3655 | 7/7   | 0.91 | 0.34 | 100,100,100,100             | 0     |
| 86  | MG   | 5     | 3910 | 1/1   | 0.91 | 0.23 | 40,40,40,40                 | 0     |
| 85  | OHX  | 1     | 3555 | 7/7   | 0.91 | 0.19 | 135,135,135,135             | 0     |
| 86  | MG   | 5     | 4157 | 1/1   | 0.91 | 0.13 | 48,48,48,48                 | 0     |
| 85  | OHX  | 1     | 3647 | 7/7   | 0.91 | 0.33 | 101,101,101,101             | 0     |
| 85  | OHX  | 1     | 3557 | 7/7   | 0.91 | 0.26 | 113,113,113,113             | 0     |
| 86  | MG   | 5     | 4035 | 1/1   | 0.91 | 0.19 | 66,66,66,66                 | 0     |
| 85  | OHX  | 2     | 1976 | 7/7   | 0.91 | 0.13 | 148,148,148,148             | 0     |
| 85  | OHX  | 5     | 3662 | 7/7   | 0.91 | 0.31 | 129,129,129,129             | 0     |
| 86  | MG   | 5     | 3918 | 1/1   | 0.91 | 0.33 | 29,29,29,29                 | 0     |
| 85  | OHX  | 5     | 3663 | 7/7   | 0.91 | 0.29 | 99,99,99,99                 | 0     |
| 85  | OHX  | 1     | 3560 | 7/7   | 0.91 | 0.12 | 145,145,145,145             | 0     |
| 86  | MG   | 1     | 4061 | 1/1   | 0.91 | 0.22 | 43,43,43,43                 | 0     |
| 85  | OHX  | 1     | 3651 | 7/7   | 0.91 | 0.33 | 119,119,119,119             | 0     |
| 86  | MG   | 5     | 4169 | 1/1   | 0.91 | 0.24 | 34,34,34,34                 | 0     |
| 85  | OHX  | 2     | 1958 | 7/7   | 0.91 | 0.12 | 170,170,170,170             | 0     |
| 85  | OHX  | 1     | 3655 | 7/7   | 0.91 | 0.29 | 115,115,115,115             | 0     |
| 85  | OHX  | s4    | 301  | 7/7   | 0.91 | 0.18 | 139,139,139,139             | 0     |
| 85  | OHX  | 1     | 3700 | 7/7   | 0.91 | 0.17 | 136,136,136,136             | 0     |
| 86  | MG   | 5     | 3930 | 1/1   | 0.91 | 0.24 | 32,32,32,32                 | 0     |
| 85  | OHX  | 5     | 3672 | 7/7   | 0.91 | 0.13 | 143,143,143,143             | 0     |
| 85  | OHX  | 2     | 2027 | 7/7   | 0.91 | 0.25 | 117,117,117,117             | 0     |
| 86  | MG   | 5     | 3933 | 1/1   | 0.91 | 0.14 | 61,61,61,61                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | OHX  | c5    | 201  | 7/7   | 0.91 | 0.12 | 151,151,151,151             | 0     |
| 86  | MG   | 5     | 3824 | 1/1   | 0.91 | 0.24 | 51,51,51,51                 | 0     |
| 85  | OHX  | d4    | 201  | 7/7   | 0.91 | 0.12 | 142,142,142,142             | 0     |
| 86  | MG   | 1     | 3915 | 1/1   | 0.91 | 0.19 | 45,45,45,45                 | 0     |
| 86  | MG   | 5     | 3940 | 1/1   | 0.91 | 0.25 | 48,48,48,48                 | 0     |
| 86  | MG   | 5     | 4062 | 1/1   | 0.91 | 0.43 | 51,51,51,51                 | 0     |
| 85  | OHX  | 5     | 3676 | 7/7   | 0.91 | 0.31 | 90,90,90,90                 | 0     |
| 86  | MG   | 1     | 3770 | 1/1   | 0.91 | 0.24 | 36,36,36,36                 | 0     |
| 85  | OHX  | 5     | 3546 | 7/7   | 0.91 | 0.25 | 122,122,122,122             | 0     |
| 85  | OHX  | 2     | 2036 | 7/7   | 0.91 | 0.34 | 112,112,112,112             | 0     |
| 85  | OHX  | 7     | 212  | 7/7   | 0.91 | 0.19 | 138,138,138,138             | 0     |
| 85  | OHX  | 2     | 2011 | 7/7   | 0.91 | 0.12 | 161,161,161,161             | 0     |
| 86  | MG   | L4    | 402  | 1/1   | 0.91 | 0.09 | 35,35,35,35                 | 0     |
| 85  | OHX  | 8     | 215  | 7/7   | 0.91 | 0.31 | 112,112,112,112             | 0     |
| 86  | MG   | 2     | 2084 | 1/1   | 0.91 | 0.34 | 59,59,59,59                 | 0     |
| 85  | OHX  | 5     | 3590 | 7/7   | 0.91 | 0.27 | 124,124,124,124             | 0     |
| 85  | OHX  | 1     | 3662 | 7/7   | 0.91 | 0.13 | 146,146,146,146             | 0     |
| 85  | OHX  | 1     | 3605 | 7/7   | 0.91 | 0.23 | 117,117,117,117             | 0     |
| 86  | MG   | M4    | 201  | 1/1   | 0.91 | 0.18 | 49,49,49,49                 | 0     |
| 86  | MG   | 5     | 3958 | 1/1   | 0.91 | 0.24 | 56,56,56,56                 | 0     |
| 86  | MG   | M5    | 301  | 1/1   | 0.91 | 0.16 | 42,42,42,42                 | 0     |
| 86  | MG   | 5     | 3963 | 1/1   | 0.91 | 0.22 | 52,52,52,52                 | 0     |
| 86  | MG   | 1     | 3933 | 1/1   | 0.91 | 0.13 | 43,43,43,43                 | 0     |
| 85  | OHX  | 5     | 3688 | 7/7   | 0.91 | 0.33 | 111,111,111,111             | 0     |
| 86  | MG   | 1     | 4012 | 1/1   | 0.91 | 0.19 | 45,45,45,45                 | 0     |
| 86  | MG   | 1     | 4091 | 1/1   | 0.91 | 0.16 | 41,41,41,41                 | 0     |
| 86  | MG   | 5     | 3748 | 1/1   | 0.91 | 0.31 | 43,43,43,43                 | 0     |
| 85  | OHX  | 4     | 214  | 7/7   | 0.91 | 0.23 | 130,130,130,130             | 0     |
| 85  | OHX  | M5    | 303  | 7/7   | 0.91 | 0.29 | 114,114,114,114             | 0     |
| 85  | OHX  | 5     | 3611 | 7/7   | 0.91 | 0.28 | 110,110,110,110             | 0     |
| 86  | MG   | 5     | 3855 | 1/1   | 0.91 | 0.21 | 28,28,28,28                 | 0     |
| 85  | OHX  | 2     | 1956 | 7/7   | 0.91 | 0.15 | 138,138,138,138             | 0     |
| 86  | MG   | 1     | 3848 | 1/1   | 0.91 | 0.21 | 32,32,32,32                 | 0     |
| 86  | MG   | 5     | 3978 | 1/1   | 0.91 | 0.27 | 30,30,30,30                 | 0     |
| 86  | MG   | 1     | 3850 | 1/1   | 0.91 | 0.28 | 35,35,35,35                 | 0     |
| 85  | OHX  | M7    | 202  | 7/7   | 0.91 | 0.26 | 127,127,127,127             | 0     |
| 85  | OHX  | 1     | 3609 | 7/7   | 0.91 | 0.34 | 91,91,91,91                 | 0     |
| 86  | MG   | 5     | 3868 | 1/1   | 0.91 | 0.30 | 31,31,31,31                 | 0     |
| 85  | OHX  | 1     | 3614 | 7/7   | 0.91 | 0.37 | 110,110,110,110             | 0     |
| 86  | MG   | 5     | 3985 | 1/1   | 0.91 | 0.25 | 44,44,44,44                 | 0     |
| 85  | OHX  | 1     | 3616 | 7/7   | 0.91 | 0.35 | 111,111,111,111             | 0     |
| 85  | OHX  | 2     | 1986 | 7/7   | 0.91 | 0.24 | 131,131,131,131             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | OHX  | 2     | 2015 | 7/7   | 0.91 | 0.28 | 128,128,128,128             | 0     |
| 86  | MG   | 5     | 3769 | 1/1   | 0.91 | 0.19 | 59,59,59,59                 | 0     |
| 86  | MG   | 1     | 3863 | 1/1   | 0.91 | 0.11 | 30,30,30,30                 | 0     |
| 85  | OHX  | 5     | 3643 | 7/7   | 0.91 | 0.17 | 133,133,133,133             | 0     |
| 86  | MG   | 5     | 3992 | 1/1   | 0.91 | 0.13 | 29,29,29,29                 | 0     |
| 85  | OHX  | 5     | 3645 | 7/7   | 0.91 | 0.23 | 119,119,119,119             | 0     |
| 86  | MG   | 5     | 4124 | 1/1   | 0.91 | 0.18 | 86,86,86,86                 | 0     |
| 85  | OHX  | 1     | 3490 | 7/7   | 0.91 | 0.21 | 94,94,94,94                 | 0     |
| 85  | OHX  | 2     | 2016 | 7/7   | 0.92 | 0.12 | 149,149,149,149             | 0     |
| 85  | OHX  | 1     | 3719 | 7/7   | 0.92 | 0.26 | 127,127,127,127             | 0     |
| 85  | OHX  | 6     | 2019 | 7/7   | 0.92 | 0.21 | 139,139,139,139             | 0     |
| 85  | OHX  | 5     | 3744 | 7/7   | 0.92 | 0.13 | 134,134,134,134             | 0     |
| 86  | MG   | 5     | 4104 | 1/1   | 0.92 | 0.34 | 32,32,32,32                 | 0     |
| 85  | OHX  | 1     | 3666 | 7/7   | 0.92 | 0.23 | 115,115,115,115             | 0     |
| 85  | OHX  | 5     | 3650 | 7/7   | 0.92 | 0.30 | 117,117,117,117             | 0     |
| 85  | OHX  | 1     | 3722 | 7/7   | 0.92 | 0.13 | 139,139,139,139             | 0     |
| 85  | OHX  | 2     | 1935 | 7/7   | 0.92 | 0.24 | 134,134,134,134             | 0     |
| 85  | OHX  | 1     | 3542 | 7/7   | 0.92 | 0.28 | 120,120,120,120             | 0     |
| 85  | OHX  | 8     | 214  | 7/7   | 0.92 | 0.12 | 142,142,142,142             | 0     |
| 86  | MG   | 5     | 3976 | 1/1   | 0.92 | 0.13 | 42,42,42,42                 | 0     |
| 85  | OHX  | 1     | 3549 | 7/7   | 0.92 | 0.13 | 139,139,139,139             | 0     |
| 86  | MG   | 5     | 3843 | 1/1   | 0.92 | 0.45 | 37,37,37,37                 | 0     |
| 86  | MG   | 5     | 4118 | 1/1   | 0.92 | 0.27 | 52,52,52,52                 | 0     |
| 86  | MG   | 5     | 4119 | 1/1   | 0.92 | 0.14 | 33,33,33,33                 | 0     |
| 86  | MG   | 1     | 3881 | 1/1   | 0.92 | 0.33 | 31,31,31,31                 | 0     |
| 86  | MG   | 6     | 2171 | 1/1   | 0.92 | 0.15 | 92,92,92,92                 | 0     |
| 86  | MG   | 6     | 2070 | 1/1   | 0.92 | 0.17 | 59,59,59,59                 | 0     |
| 85  | OHX  | 6     | 2025 | 7/7   | 0.92 | 0.33 | 107,107,107,107             | 0     |
| 86  | MG   | 1     | 3884 | 1/1   | 0.92 | 0.26 | 37,37,37,37                 | 0     |
| 85  | OHX  | 1     | 3671 | 7/7   | 0.92 | 0.22 | 128,128,128,128             | 0     |
| 85  | OHX  | 2     | 2005 | 7/7   | 0.92 | 0.14 | 136,136,136,136             | 0     |
| 85  | OHX  | 1     | 3622 | 7/7   | 0.92 | 0.26 | 119,119,119,119             | 0     |
| 86  | MG   | 5     | 3853 | 1/1   | 0.92 | 0.23 | 43,43,43,43                 | 0     |
| 85  | OHX  | 14    | 401  | 7/7   | 0.92 | 0.17 | 127,127,127,127             | 0     |
| 86  | MG   | 5     | 3857 | 1/1   | 0.92 | 0.33 | 37,37,37,37                 | 0     |
| 85  | OHX  | 1     | 3626 | 7/7   | 0.92 | 0.11 | 152,152,152,152             | 0     |
| 85  | OHX  | 15    | 302  | 7/7   | 0.92 | 0.21 | 134,134,134,134             | 0     |
| 85  | OHX  | 6     | 2031 | 7/7   | 0.92 | 0.31 | 106,106,106,106             | 0     |
| 85  | OHX  | 1     | 3627 | 7/7   | 0.92 | 0.28 | 108,108,108,108             | 0     |
| 86  | MG   | 5     | 3864 | 1/1   | 0.92 | 0.13 | 34,34,34,34                 | 0     |
| 85  | OHX  | 1     | 3628 | 7/7   | 0.92 | 0.12 | 146,146,146,146             | 0     |
| 85  | OHX  | 2     | 1991 | 7/7   | 0.92 | 0.21 | 136,136,136,136             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 85  | OHX  | 1     | 3682 | 7/7   | 0.92 | 0.19 | 109,109,109,109            | 0     |
| 86  | MG   | 1     | 4014 | 1/1   | 0.92 | 0.15 | 32,32,32,32                | 0     |
| 86  | MG   | 1     | 4015 | 1/1   | 0.92 | 0.13 | 41,41,41,41                | 0     |
| 85  | OHX  | 2     | 1999 | 7/7   | 0.92 | 0.13 | 144,144,144,144            | 0     |
| 85  | OHX  | 1     | 3632 | 7/7   | 0.92 | 0.12 | 136,136,136,136            | 0     |
| 85  | OHX  | 3     | 210  | 7/7   | 0.92 | 0.29 | 107,107,107,107            | 0     |
| 86  | MG   | 1     | 4122 | 1/1   | 0.92 | 0.14 | 46,46,46,46                | 0     |
| 86  | MG   | 1     | 3904 | 1/1   | 0.92 | 0.35 | 51,51,51,51                | 0     |
| 86  | MG   | 5     | 4006 | 1/1   | 0.92 | 0.08 | 44,44,44,44                | 0     |
| 86  | MG   | 5     | 4007 | 1/1   | 0.92 | 0.24 | 61,61,61,61                | 0     |
| 85  | OHX  | 1     | 3685 | 7/7   | 0.92 | 0.23 | 128,128,128,128            | 0     |
| 86  | MG   | 1     | 3908 | 1/1   | 0.92 | 0.31 | 30,30,30,30                | 0     |
| 85  | OHX  | 6     | 2040 | 7/7   | 0.92 | 0.22 | 137,137,137,137            | 0     |
| 85  | OHX  | 4     | 207  | 7/7   | 0.92 | 0.21 | 117,117,117,117            | 0     |
| 86  | MG   | 5     | 3757 | 1/1   | 0.92 | 0.24 | 29,29,29,29                | 0     |
| 85  | OHX  | 2     | 2021 | 7/7   | 0.92 | 0.16 | 133,133,133,133            | 0     |
| 85  | OHX  | 1     | 3687 | 7/7   | 0.92 | 0.12 | 140,140,140,140            | 0     |
| 85  | OHX  | 2     | 2033 | 7/7   | 0.92 | 0.20 | 138,138,138,138            | 0     |
| 86  | MG   | 5     | 4160 | 1/1   | 0.92 | 0.24 | 70,70,70,70                | 0     |
| 85  | OHX  | 1     | 3644 | 7/7   | 0.92 | 0.22 | 126,126,126,126            | 0     |
| 85  | OHX  | 1     | 3692 | 7/7   | 0.92 | 0.25 | 125,125,125,125            | 0     |
| 85  | OHX  | 1     | 3693 | 7/7   | 0.92 | 0.26 | 123,123,123,123            | 0     |
| 85  | OHX  | 1     | 3646 | 7/7   | 0.92 | 0.31 | 129,129,129,129            | 0     |
| 85  | OHX  | 2     | 1979 | 7/7   | 0.92 | 0.12 | 156,156,156,156            | 0     |
| 86  | MG   | 5     | 4024 | 1/1   | 0.92 | 0.07 | 33,33,33,33                | 0     |
| 86  | MG   | 5     | 3895 | 1/1   | 0.92 | 0.34 | 36,36,36,36                | 0     |
| 86  | MG   | 2     | 2059 | 1/1   | 0.92 | 0.31 | 70,70,70,70                | 0     |
| 85  | OHX  | 1     | 3567 | 7/7   | 0.92 | 0.30 | 104,104,104,104            | 0     |
| 86  | MG   | 5     | 4030 | 1/1   | 0.92 | 0.10 | 47,47,47,47                | 0     |
| 85  | OHX  | 6     | 1970 | 7/7   | 0.92 | 0.27 | 130,130,130,130            | 0     |
| 86  | MG   | 1     | 4040 | 1/1   | 0.92 | 0.10 | 61,61,61,61                | 0     |
| 85  | OHX  | 1     | 3575 | 7/7   | 0.92 | 0.28 | 110,110,110,110            | 0     |
| 86  | MG   | 4     | 221  | 1/1   | 0.92 | 0.25 | 41,41,41,41                | 0     |
| 85  | OHX  | 5     | 3693 | 7/7   | 0.92 | 0.34 | 116,116,116,116            | 0     |
| 86  | MG   | 5     | 3778 | 1/1   | 0.92 | 0.30 | 53,53,53,53                | 0     |
| 85  | OHX  | 6     | 1973 | 7/7   | 0.92 | 0.14 | 138,138,138,138            | 0     |
| 86  | MG   | 7     | 217  | 1/1   | 0.92 | 0.44 | 28,28,28,28                | 0     |
| 85  | OHX  | 5     | 3695 | 7/7   | 0.92 | 0.28 | 117,117,117,117            | 0     |
| 85  | OHX  | 6     | 1975 | 7/7   | 0.92 | 0.36 | 109,109,109,109            | 0     |
| 85  | OHX  | c3    | 201  | 7/7   | 0.92 | 0.11 | 144,144,144,144            | 0     |
| 86  | MG   | 6     | 2117 | 1/1   | 0.92 | 0.16 | 50,50,50,50                | 0     |
| 85  | OHX  | 5     | 3699 | 7/7   | 0.92 | 0.29 | 115,115,115,115            | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | OHX  | 1     | 3588 | 7/7   | 0.92 | 0.21 | 135,135,135,135             | 0     |
| 85  | OHX  | 1     | 3596 | 7/7   | 0.92 | 0.21 | 120,120,120,120             | 0     |
| 85  | OHX  | 1     | 3597 | 7/7   | 0.92 | 0.11 | 144,144,144,144             | 0     |
| 85  | OHX  | 6     | 1986 | 7/7   | 0.92 | 0.29 | 127,127,127,127             | 0     |
| 85  | OHX  | 5     | 3566 | 7/7   | 0.92 | 0.26 | 121,121,121,121             | 0     |
| 86  | MG   | 1     | 3741 | 1/1   | 0.92 | 0.28 | 60,60,60,60                 | 0     |
| 85  | OHX  | 1     | 3705 | 7/7   | 0.92 | 0.28 | 109,109,109,109             | 0     |
| 85  | OHX  | 5     | 3580 | 7/7   | 0.92 | 0.29 | 119,119,119,119             | 0     |
| 85  | OHX  | 6     | 1988 | 7/7   | 0.92 | 0.22 | 124,124,124,124             | 0     |
| 86  | MG   | 5     | 4056 | 1/1   | 0.92 | 0.19 | 57,57,57,57                 | 0     |
| 85  | OHX  | 5     | 3593 | 7/7   | 0.92 | 0.33 | 106,106,106,106             | 0     |
| 86  | MG   | 1     | 3948 | 1/1   | 0.92 | 0.20 | 41,41,41,41                 | 0     |
| 86  | MG   | 5     | 3801 | 1/1   | 0.92 | 0.13 | 35,35,35,35                 | 0     |
| 86  | MG   | 5     | 4060 | 1/1   | 0.92 | 0.08 | 44,44,44,44                 | 0     |
| 86  | MG   | m0    | 305  | 1/1   | 0.92 | 0.19 | 39,39,39,39                 | 0     |
| 86  | MG   | 5     | 4061 | 1/1   | 0.92 | 0.23 | 62,62,62,62                 | 0     |
| 85  | OHX  | 5     | 3716 | 7/7   | 0.92 | 0.21 | 131,131,131,131             | 0     |
| 85  | OHX  | 6     | 1989 | 7/7   | 0.92 | 0.14 | 137,137,137,137             | 0     |
| 85  | OHX  | 1     | 3706 | 7/7   | 0.92 | 0.23 | 110,110,110,110             | 0     |
| 85  | OHX  | 6     | 1993 | 7/7   | 0.92 | 0.14 | 142,142,142,142             | 0     |
| 85  | OHX  | 5     | 3604 | 7/7   | 0.92 | 0.24 | 128,128,128,128             | 0     |
| 86  | MG   | 5     | 3810 | 1/1   | 0.92 | 0.29 | 39,39,39,39                 | 0     |
| 86  | MG   | n0    | 201  | 1/1   | 0.92 | 0.15 | 38,38,38,38                 | 0     |
| 85  | OHX  | 2     | 1953 | 7/7   | 0.92 | 0.14 | 141,141,141,141             | 0     |
| 85  | OHX  | 5     | 3608 | 7/7   | 0.92 | 0.21 | 127,127,127,127             | 0     |
| 86  | MG   | 5     | 3939 | 1/1   | 0.92 | 0.16 | 41,41,41,41                 | 0     |
| 85  | OHX  | 6     | 1996 | 7/7   | 0.92 | 0.30 | 125,125,125,125             | 0     |
| 86  | MG   | 5     | 4075 | 1/1   | 0.92 | 0.23 | 37,37,37,37                 | 0     |
| 85  | OHX  | 1     | 3656 | 7/7   | 0.92 | 0.32 | 99,99,99,99                 | 0     |
| 85  | OHX  | 5     | 3624 | 7/7   | 0.92 | 0.25 | 119,119,119,119             | 0     |
| 85  | OHX  | 5     | 3728 | 7/7   | 0.92 | 0.27 | 115,115,115,115             | 0     |
| 85  | OHX  | 6     | 2000 | 7/7   | 0.92 | 0.23 | 131,131,131,131             | 0     |
| 86  | MG   | 5     | 4083 | 1/1   | 0.92 | 0.11 | 44,44,44,44                 | 0     |
| 85  | OHX  | C5    | 201  | 7/7   | 0.92 | 0.10 | 153,153,153,153             | 0     |
| 86  | MG   | 1     | 3851 | 1/1   | 0.92 | 0.25 | 48,48,48,48                 | 0     |
| 86  | MG   | 1     | 3853 | 1/1   | 0.92 | 0.47 | 38,38,38,38                 | 0     |
| 85  | OHX  | 1     | 3600 | 7/7   | 0.92 | 0.28 | 118,118,118,118             | 0     |
| 86  | MG   | 5     | 4089 | 1/1   | 0.92 | 0.20 | 67,67,67,67                 | 0     |
| 85  | OHX  | 1     | 3604 | 7/7   | 0.92 | 0.26 | 129,129,129,129             | 0     |
| 85  | OHX  | 2     | 1984 | 7/7   | 0.92 | 0.20 | 133,133,133,133             | 0     |
| 86  | MG   | 1     | 3857 | 1/1   | 0.92 | 0.25 | 36,36,36,36                 | 0     |
| 85  | OHX  | 5     | 3636 | 7/7   | 0.92 | 0.12 | 162,162,162,162             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | OHX  | 5     | 3639 | 7/7   | 0.92 | 0.32 | 106,106,106,106             | 0     |
| 85  | OHX  | 1     | 3607 | 7/7   | 0.92 | 0.21 | 130,130,130,130             | 0     |
| 86  | MG   | 5     | 3960 | 1/1   | 0.92 | 0.24 | 45,45,45,45                 | 0     |
| 86  | MG   | 5     | 3829 | 1/1   | 0.92 | 0.24 | 54,54,54,54                 | 0     |
| 85  | OHX  | 2     | 1945 | 7/7   | 0.92 | 0.12 | 144,144,144,144             | 0     |
| 86  | MG   | 5     | 4106 | 1/1   | 0.93 | 0.13 | 64,64,64,64                 | 0     |
| 86  | MG   | 5     | 3972 | 1/1   | 0.93 | 0.14 | 41,41,41,41                 | 0     |
| 85  | OHX  | 6     | 1998 | 7/7   | 0.93 | 0.25 | 127,127,127,127             | 0     |
| 85  | OHX  | 3     | 209  | 7/7   | 0.93 | 0.21 | 132,132,132,132             | 0     |
| 85  | OHX  | 1     | 3635 | 7/7   | 0.93 | 0.25 | 111,111,111,111             | 0     |
| 86  | MG   | 2     | 2074 | 1/1   | 0.93 | 0.32 | 66,66,66,66                 | 0     |
| 86  | MG   | 6     | 2062 | 1/1   | 0.93 | 0.40 | 46,46,46,46                 | 0     |
| 86  | MG   | 5     | 3979 | 1/1   | 0.93 | 0.24 | 36,36,36,36                 | 0     |
| 85  | OHX  | 1     | 3601 | 7/7   | 0.93 | 0.24 | 97,97,97,97                 | 0     |
| 85  | OHX  | 1     | 3707 | 7/7   | 0.93 | 0.25 | 113,113,113,113             | 0     |
| 85  | OHX  | 4     | 208  | 7/7   | 0.93 | 0.31 | 99,99,99,99                 | 0     |
| 86  | MG   | 6     | 2066 | 1/1   | 0.93 | 0.37 | 66,66,66,66                 | 0     |
| 86  | MG   | 1     | 4100 | 1/1   | 0.93 | 0.13 | 45,45,45,45                 | 0     |
| 85  | OHX  | 1     | 3637 | 7/7   | 0.93 | 0.20 | 132,132,132,132             | 0     |
| 85  | OHX  | 1     | 3603 | 7/7   | 0.93 | 0.30 | 103,103,103,103             | 0     |
| 85  | OHX  | c1    | 201  | 7/7   | 0.93 | 0.23 | 137,137,137,137             | 0     |
| 86  | MG   | 1     | 4001 | 1/1   | 0.93 | 0.15 | 51,51,51,51                 | 0     |
| 85  | OHX  | 1     | 3645 | 7/7   | 0.93 | 0.23 | 119,119,119,119             | 0     |
| 85  | OHX  | 5     | 3661 | 7/7   | 0.93 | 0.21 | 122,122,122,122             | 0     |
| 85  | OHX  | 6     | 2015 | 7/7   | 0.93 | 0.25 | 119,119,119,119             | 0     |
| 85  | OHX  | 6     | 2017 | 7/7   | 0.93 | 0.22 | 122,122,122,122             | 0     |
| 85  | OHX  | d9    | 102  | 7/7   | 0.93 | 0.12 | 153,153,153,153             | 0     |
| 85  | OHX  | 5     | 3502 | 7/7   | 0.93 | 0.13 | 112,112,112,112             | 0     |
| 86  | MG   | 1     | 3910 | 1/1   | 0.93 | 0.35 | 17,17,17,17                 | 0     |
| 86  | MG   | 6     | 2079 | 1/1   | 0.93 | 0.20 | 48,48,48,48                 | 0     |
| 85  | OHX  | 5     | 3523 | 7/7   | 0.93 | 0.28 | 116,116,116,116             | 0     |
| 86  | MG   | 5     | 3867 | 1/1   | 0.93 | 0.13 | 45,45,45,45                 | 0     |
| 85  | OHX  | 5     | 3539 | 7/7   | 0.93 | 0.24 | 117,117,117,117             | 0     |
| 85  | OHX  | 5     | 3541 | 7/7   | 0.93 | 0.16 | 114,114,114,114             | 0     |
| 86  | MG   | 1     | 3914 | 1/1   | 0.93 | 0.20 | 43,43,43,43                 | 0     |
| 85  | OHX  | 1     | 3677 | 7/7   | 0.93 | 0.31 | 104,104,104,104             | 0     |
| 86  | MG   | 1     | 4018 | 1/1   | 0.93 | 0.11 | 40,40,40,40                 | 0     |
| 86  | MG   | 5     | 3875 | 1/1   | 0.93 | 0.22 | 20,20,20,20                 | 0     |
| 85  | OHX  | 7     | 211  | 7/7   | 0.93 | 0.22 | 104,104,104,104             | 0     |
| 86  | MG   | 1     | 4119 | 1/1   | 0.93 | 0.28 | 31,31,31,31                 | 0     |
| 85  | OHX  | 5     | 3671 | 7/7   | 0.93 | 0.22 | 114,114,114,114             | 0     |
| 85  | OHX  | L3    | 401  | 7/7   | 0.93 | 0.33 | 117,117,117,117             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 5     | 3752 | 1/1   | 0.93 | 0.09 | 46,46,46,46                 | 0     |
| 86  | MG   | 5     | 3753 | 1/1   | 0.93 | 0.15 | 35,35,35,35                 | 0     |
| 85  | OHX  | M0    | 301  | 7/7   | 0.93 | 0.14 | 104,104,104,104             | 0     |
| 85  | OHX  | 5     | 3568 | 7/7   | 0.93 | 0.11 | 146,146,146,146             | 0     |
| 85  | OHX  | 5     | 3573 | 7/7   | 0.93 | 0.19 | 131,131,131,131             | 0     |
| 85  | OHX  | 2     | 1942 | 7/7   | 0.93 | 0.32 | 115,115,115,115             | 0     |
| 85  | OHX  | 1     | 3562 | 7/7   | 0.93 | 0.19 | 122,122,122,122             | 0     |
| 86  | MG   | 1     | 3927 | 1/1   | 0.93 | 0.23 | 52,52,52,52                 | 0     |
| 85  | OHX  | 2     | 1982 | 7/7   | 0.93 | 0.10 | 193,193,193,193             | 0     |
| 85  | OHX  | 2     | 1983 | 7/7   | 0.93 | 0.23 | 116,116,116,116             | 0     |
| 86  | MG   | 1     | 4033 | 1/1   | 0.93 | 0.14 | 42,42,42,42                 | 0     |
| 86  | MG   | 1     | 3930 | 1/1   | 0.93 | 0.32 | 51,51,51,51                 | 0     |
| 86  | MG   | 1     | 3832 | 1/1   | 0.93 | 0.31 | 40,40,40,40                 | 0     |
| 86  | MG   | 5     | 3768 | 1/1   | 0.93 | 0.10 | 43,43,43,43                 | 0     |
| 85  | OHX  | 5     | 3596 | 7/7   | 0.93 | 0.29 | 102,102,102,102             | 0     |
| 86  | MG   | 5     | 4027 | 1/1   | 0.93 | 0.07 | 45,45,45,45                 | 0     |
| 86  | MG   | 1     | 3934 | 1/1   | 0.93 | 0.14 | 44,44,44,44                 | 0     |
| 86  | MG   | 1     | 3757 | 1/1   | 0.93 | 0.23 | 42,42,42,42                 | 0     |
| 85  | OHX  | 2     | 1959 | 7/7   | 0.93 | 0.16 | 133,133,133,133             | 0     |
| 85  | OHX  | 6     | 1949 | 7/7   | 0.93 | 0.14 | 122,122,122,122             | 0     |
| 85  | OHX  | 6     | 1954 | 7/7   | 0.93 | 0.12 | 164,164,164,164             | 0     |
| 85  | OHX  | 6     | 1961 | 7/7   | 0.93 | 0.22 | 125,125,125,125             | 0     |
| 85  | OHX  | 5     | 3605 | 7/7   | 0.93 | 0.11 | 141,141,141,141             | 0     |
| 86  | MG   | 4     | 220  | 1/1   | 0.93 | 0.23 | 36,36,36,36                 | 0     |
| 85  | OHX  | 1     | 3611 | 7/7   | 0.93 | 0.28 | 113,113,113,113             | 0     |
| 85  | OHX  | o7    | 502  | 7/7   | 0.93 | 0.31 | 116,116,116,116             | 0     |
| 86  | MG   | 5     | 3782 | 1/1   | 0.93 | 0.20 | 41,41,41,41                 | 0     |
| 85  | OHX  | 1     | 3652 | 7/7   | 0.93 | 0.25 | 111,111,111,111             | 0     |
| 86  | MG   | 2     | 2110 | 1/1   | 0.93 | 0.25 | 91,91,91,91                 | 0     |
| 86  | MG   | 5     | 3914 | 1/1   | 0.93 | 0.23 | 31,31,31,31                 | 0     |
| 85  | OHX  | 1     | 3568 | 7/7   | 0.93 | 0.22 | 131,131,131,131             | 0     |
| 85  | OHX  | 5     | 3613 | 7/7   | 0.93 | 0.27 | 113,113,113,113             | 0     |
| 85  | OHX  | 1     | 3539 | 7/7   | 0.93 | 0.18 | 119,119,119,119             | 0     |
| 86  | MG   | 1     | 3849 | 1/1   | 0.93 | 0.32 | 42,42,42,42                 | 0     |
| 85  | OHX  | 5     | 3697 | 7/7   | 0.93 | 0.28 | 111,111,111,111             | 0     |
| 86  | MG   | 2     | 2115 | 1/1   | 0.93 | 0.27 | 79,79,79,79                 | 0     |
| 86  | MG   | 1     | 3852 | 1/1   | 0.93 | 0.31 | 37,37,37,37                 | 0     |
| 85  | OHX  | 5     | 3616 | 7/7   | 0.93 | 0.24 | 111,111,111,111             | 0     |
| 86  | MG   | 6     | 2125 | 1/1   | 0.93 | 0.19 | 51,51,51,51                 | 0     |
| 85  | OHX  | 5     | 3620 | 7/7   | 0.93 | 0.11 | 138,138,138,138             | 0     |
| 86  | MG   | 1     | 3775 | 1/1   | 0.93 | 0.23 | 39,39,39,39                 | 0     |
| 86  | MG   | 5     | 3928 | 1/1   | 0.93 | 0.27 | 24,24,24,24                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | OHX  | 5     | 3623 | 7/7   | 0.93 | 0.24 | 110,110,110,110             | 0     |
| 86  | MG   | 6     | 2129 | 1/1   | 0.93 | 0.20 | 54,54,54,54                 | 0     |
| 85  | OHX  | 1     | 3583 | 7/7   | 0.93 | 0.31 | 107,107,107,107             | 0     |
| 85  | OHX  | 5     | 3702 | 7/7   | 0.93 | 0.30 | 107,107,107,107             | 0     |
| 86  | MG   | 5     | 3804 | 1/1   | 0.93 | 0.30 | 39,39,39,39                 | 0     |
| 86  | MG   | 5     | 3805 | 1/1   | 0.93 | 0.22 | 41,41,41,41                 | 0     |
| 86  | MG   | 5     | 4066 | 1/1   | 0.93 | 0.14 | 64,64,64,64                 | 0     |
| 86  | MG   | 1     | 3859 | 1/1   | 0.93 | 0.27 | 48,48,48,48                 | 0     |
| 85  | OHX  | 5     | 3705 | 7/7   | 0.93 | 0.30 | 114,114,114,114             | 0     |
| 86  | MG   | 1     | 3781 | 1/1   | 0.93 | 0.09 | 45,45,45,45                 | 0     |
| 86  | MG   | 6     | 2135 | 1/1   | 0.93 | 0.12 | 76,76,76,76                 | 0     |
| 85  | OHX  | 1     | 3584 | 7/7   | 0.93 | 0.26 | 127,127,127,127             | 0     |
| 85  | OHX  | 5     | 3626 | 7/7   | 0.93 | 0.19 | 136,136,136,136             | 0     |
| 86  | MG   | 5     | 3813 | 1/1   | 0.93 | 0.24 | 48,48,48,48                 | 0     |
| 85  | OHX  | 1     | 3541 | 7/7   | 0.93 | 0.22 | 119,119,119,119             | 0     |
| 85  | OHX  | 1     | 3625 | 7/7   | 0.93 | 0.17 | 125,125,125,125             | 0     |
| 85  | OHX  | 1     | 3594 | 7/7   | 0.93 | 0.30 | 109,109,109,109             | 0     |
| 86  | MG   | 5     | 4080 | 1/1   | 0.93 | 0.15 | 33,33,33,33                 | 0     |
| 86  | MG   | M7    | 208  | 1/1   | 0.93 | 0.08 | 50,50,50,50                 | 0     |
| 85  | OHX  | 1     | 3697 | 7/7   | 0.93 | 0.23 | 126,126,126,126             | 0     |
| 85  | OHX  | 1     | 3595 | 7/7   | 0.93 | 0.12 | 159,159,159,159             | 0     |
| 86  | MG   | 1     | 3789 | 1/1   | 0.93 | 0.20 | 30,30,30,30                 | 0     |
| 85  | OHX  | 5     | 3638 | 7/7   | 0.93 | 0.23 | 130,130,130,130             | 0     |
| 86  | MG   | 1     | 3975 | 1/1   | 0.93 | 0.23 | 58,58,58,58                 | 0     |
| 86  | MG   | 1     | 4078 | 1/1   | 0.93 | 0.07 | 84,84,84,84                 | 0     |
| 86  | MG   | o1    | 201  | 1/1   | 0.93 | 0.21 | 51,51,51,51                 | 0     |
| 85  | OHX  | 2     | 1961 | 7/7   | 0.93 | 0.18 | 135,135,135,135             | 0     |
| 86  | MG   | 1     | 3792 | 1/1   | 0.93 | 0.26 | 60,60,60,60                 | 0     |
| 86  | MG   | 5     | 3959 | 1/1   | 0.93 | 0.22 | 54,54,54,54                 | 0     |
| 86  | MG   | 1     | 4081 | 1/1   | 0.93 | 0.32 | 53,53,53,53                 | 0     |
| 86  | MG   | 5     | 3961 | 1/1   | 0.93 | 0.15 | 38,38,38,38                 | 0     |
| 86  | MG   | 1     | 3878 | 1/1   | 0.93 | 0.37 | 31,31,31,31                 | 0     |
| 86  | MG   | 1     | 3979 | 1/1   | 0.93 | 0.20 | 43,43,43,43                 | 0     |
| 85  | OHX  | 5     | 3640 | 7/7   | 0.93 | 0.22 | 123,123,123,123             | 0     |
| 86  | MG   | 6     | 2051 | 1/1   | 0.93 | 0.28 | 52,52,52,52                 | 0     |
| 86  | MG   | 1     | 3981 | 1/1   | 0.93 | 0.20 | 41,41,41,41                 | 0     |
| 85  | OHX  | 6     | 1991 | 7/7   | 0.93 | 0.25 | 118,118,118,118             | 0     |
| 85  | OHX  | 2     | 1968 | 7/7   | 0.93 | 0.28 | 130,130,130,130             | 0     |
| 87  | ZN   | Q2    | 501  | 1/1   | 0.93 | 0.27 | 83,83,83,83                 | 0     |
| 85  | OHX  | 2     | 1980 | 7/7   | 0.93 | 0.13 | 141,141,141,141             | 0     |
| 85  | OHX  | 2     | 2007 | 7/7   | 0.93 | 0.12 | 150,150,150,150             | 0     |
| 85  | OHX  | 2     | 2008 | 7/7   | 0.93 | 0.11 | 185,185,185,185             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | OHX  | 5     | 3589 | 7/7   | 0.94 | 0.17 | 115,115,115,115             | 0     |
| 86  | MG   | 1     | 3882 | 1/1   | 0.94 | 0.24 | 31,31,31,31                 | 0     |
| 86  | MG   | 1     | 4096 | 1/1   | 0.94 | 0.07 | 56,56,56,56                 | 0     |
| 85  | OHX  | 1     | 3640 | 7/7   | 0.94 | 0.19 | 122,122,122,122             | 0     |
| 85  | OHX  | 1     | 3678 | 7/7   | 0.94 | 0.25 | 116,116,116,116             | 0     |
| 86  | MG   | 1     | 3991 | 1/1   | 0.94 | 0.08 | 48,48,48,48                 | 0     |
| 85  | OHX  | 5     | 3595 | 7/7   | 0.94 | 0.29 | 99,99,99,99                 | 0     |
| 85  | OHX  | 5     | 3684 | 7/7   | 0.94 | 0.10 | 150,150,150,150             | 0     |
| 86  | MG   | 5     | 3854 | 1/1   | 0.94 | 0.31 | 25,25,25,25                 | 0     |
| 86  | MG   | 1     | 3887 | 1/1   | 0.94 | 0.23 | 27,27,27,27                 | 0     |
| 86  | MG   | 2     | 2045 | 1/1   | 0.94 | 0.31 | 53,53,53,53                 | 0     |
| 85  | OHX  | 6     | 1965 | 7/7   | 0.94 | 0.17 | 125,125,125,125             | 0     |
| 85  | OHX  | 6     | 1966 | 7/7   | 0.94 | 0.21 | 122,122,122,122             | 0     |
| 85  | OHX  | 6     | 1969 | 7/7   | 0.94 | 0.23 | 120,120,120,120             | 0     |
| 85  | OHX  | 5     | 3689 | 7/7   | 0.94 | 0.26 | 114,114,114,114             | 0     |
| 85  | OHX  | 5     | 3602 | 7/7   | 0.94 | 0.15 | 123,123,123,123             | 0     |
| 86  | MG   | 2     | 2130 | 1/1   | 0.94 | 0.29 | 70,70,70,70                 | 0     |
| 85  | OHX  | 1     | 3642 | 7/7   | 0.94 | 0.09 | 208,208,208,208             | 0     |
| 86  | MG   | 5     | 4130 | 1/1   | 0.94 | 0.13 | 46,46,46,46                 | 0     |
| 85  | OHX  | 1     | 3643 | 7/7   | 0.94 | 0.29 | 106,106,106,106             | 0     |
| 85  | OHX  | 1     | 3511 | 7/7   | 0.94 | 0.11 | 122,122,122,122             | 0     |
| 86  | MG   | 1     | 3901 | 1/1   | 0.94 | 0.21 | 34,34,34,34                 | 0     |
| 86  | MG   | 5     | 3872 | 1/1   | 0.94 | 0.29 | 30,30,30,30                 | 0     |
| 85  | OHX  | 1     | 3527 | 7/7   | 0.94 | 0.26 | 109,109,109,109             | 0     |
| 85  | OHX  | 2     | 1969 | 7/7   | 0.94 | 0.21 | 136,136,136,136             | 0     |
| 86  | MG   | 5     | 3751 | 1/1   | 0.94 | 0.12 | 44,44,44,44                 | 0     |
| 85  | OHX  | 1     | 3576 | 7/7   | 0.94 | 0.28 | 110,110,110,110             | 0     |
| 85  | OHX  | 5     | 3612 | 7/7   | 0.94 | 0.23 | 129,129,129,129             | 0     |
| 86  | MG   | 5     | 3754 | 1/1   | 0.94 | 0.28 | 47,47,47,47                 | 0     |
| 86  | MG   | 5     | 3879 | 1/1   | 0.94 | 0.18 | 37,37,37,37                 | 0     |
| 86  | MG   | 5     | 4142 | 1/1   | 0.94 | 0.17 | 53,53,53,53                 | 0     |
| 85  | OHX  | 6     | 1981 | 7/7   | 0.94 | 0.24 | 114,114,114,114             | 0     |
| 85  | OHX  | 1     | 3612 | 7/7   | 0.94 | 0.23 | 117,117,117,117             | 0     |
| 85  | OHX  | 1     | 3613 | 7/7   | 0.94 | 0.17 | 123,123,123,123             | 0     |
| 85  | OHX  | 5     | 3617 | 7/7   | 0.94 | 0.30 | 102,102,102,102             | 0     |
| 86  | MG   | 1     | 3813 | 1/1   | 0.94 | 0.20 | 33,33,33,33                 | 0     |
| 86  | MG   | 1     | 4020 | 1/1   | 0.94 | 0.22 | 39,39,39,39                 | 0     |
| 85  | OHX  | 5     | 3619 | 7/7   | 0.94 | 0.28 | 109,109,109,109             | 0     |
| 85  | OHX  | 5     | 3704 | 7/7   | 0.94 | 0.22 | 100,100,100,100             | 0     |
| 86  | MG   | 5     | 3764 | 1/1   | 0.94 | 0.33 | 38,38,38,38                 | 0     |
| 85  | OHX  | 1     | 3578 | 7/7   | 0.94 | 0.17 | 134,134,134,134             | 0     |
| 86  | MG   | 5     | 3890 | 1/1   | 0.94 | 0.30 | 49,49,49,49                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 1     | 3916 | 1/1   | 0.94 | 0.10 | 46,46,46,46                 | 0     |
| 86  | MG   | 1     | 4131 | 1/1   | 0.94 | 0.18 | 34,34,34,34                 | 0     |
| 85  | OHX  | 5     | 3622 | 7/7   | 0.94 | 0.20 | 132,132,132,132             | 0     |
| 85  | OHX  | 2     | 1952 | 7/7   | 0.94 | 0.25 | 119,119,119,119             | 0     |
| 85  | OHX  | 1     | 3689 | 7/7   | 0.94 | 0.28 | 108,108,108,108             | 0     |
| 85  | OHX  | 2     | 1934 | 7/7   | 0.94 | 0.14 | 124,124,124,124             | 0     |
| 86  | MG   | 5     | 3773 | 1/1   | 0.94 | 0.39 | 47,47,47,47                 | 0     |
| 85  | OHX  | 1     | 3732 | 7/7   | 0.94 | 0.10 | 158,158,158,158             | 0     |
| 86  | MG   | 3     | 215  | 1/1   | 0.94 | 0.20 | 39,39,39,39                 | 0     |
| 85  | OHX  | 5     | 3628 | 7/7   | 0.94 | 0.12 | 139,139,139,139             | 0     |
| 86  | MG   | 1     | 4032 | 1/1   | 0.94 | 0.22 | 70,70,70,70                 | 0     |
| 85  | OHX  | 6     | 1992 | 7/7   | 0.94 | 0.18 | 117,117,117,117             | 0     |
| 86  | MG   | 5     | 3905 | 1/1   | 0.94 | 0.31 | 27,27,27,27                 | 0     |
| 85  | OHX  | 5     | 3715 | 7/7   | 0.94 | 0.25 | 92,92,92,92                 | 0     |
| 86  | MG   | 1     | 3926 | 1/1   | 0.94 | 0.23 | 48,48,48,48                 | 0     |
| 85  | OHX  | 1     | 3618 | 7/7   | 0.94 | 0.21 | 125,125,125,125             | 0     |
| 85  | OHX  | 2     | 2014 | 7/7   | 0.94 | 0.22 | 125,125,125,125             | 0     |
| 85  | OHX  | 2     | 1947 | 7/7   | 0.94 | 0.22 | 111,111,111,111             | 0     |
| 86  | MG   | 5     | 3784 | 1/1   | 0.94 | 0.20 | 31,31,31,31                 | 0     |
| 85  | OHX  | 1     | 3623 | 7/7   | 0.94 | 0.20 | 120,120,120,120             | 0     |
| 85  | OHX  | 5     | 3637 | 7/7   | 0.94 | 0.28 | 111,111,111,111             | 0     |
| 85  | OHX  | 1     | 3550 | 7/7   | 0.94 | 0.19 | 119,119,119,119             | 0     |
| 85  | OHX  | 1     | 3660 | 7/7   | 0.94 | 0.27 | 98,98,98,98                 | 0     |
| 85  | OHX  | 1     | 3553 | 7/7   | 0.94 | 0.10 | 141,141,141,141             | 0     |
| 86  | MG   | 5     | 3790 | 1/1   | 0.94 | 0.18 | 37,37,37,37                 | 0     |
| 85  | OHX  | 4     | 206  | 7/7   | 0.94 | 0.25 | 103,103,103,103             | 0     |
| 86  | MG   | 5     | 4050 | 1/1   | 0.94 | 0.39 | 52,52,52,52                 | 0     |
| 85  | OHX  | 2     | 1964 | 7/7   | 0.94 | 0.23 | 120,120,120,120             | 0     |
| 85  | OHX  | 5     | 3644 | 7/7   | 0.94 | 0.30 | 90,90,90,90                 | 0     |
| 85  | OHX  | 2     | 2040 | 7/7   | 0.94 | 0.10 | 147,147,147,147             | 0     |
| 86  | MG   | L2    | 301  | 1/1   | 0.94 | 0.10 | 41,41,41,41                 | 0     |
| 86  | MG   | 5     | 3796 | 1/1   | 0.94 | 0.25 | 38,38,38,38                 | 0     |
| 85  | OHX  | 6     | 2008 | 7/7   | 0.94 | 0.13 | 133,133,133,133             | 0     |
| 85  | OHX  | 1     | 3629 | 7/7   | 0.94 | 0.10 | 144,144,144,144             | 0     |
| 85  | OHX  | 2     | 1957 | 7/7   | 0.94 | 0.27 | 117,117,117,117             | 0     |
| 85  | OHX  | 1     | 3456 | 7/7   | 0.94 | 0.12 | 112,112,112,112             | 0     |
| 86  | MG   | L4    | 403  | 1/1   | 0.94 | 0.41 | 39,39,39,39                 | 0     |
| 85  | OHX  | 5     | 3651 | 7/7   | 0.94 | 0.23 | 100,100,100,100             | 0     |
| 86  | MG   | 1     | 3843 | 1/1   | 0.94 | 0.17 | 30,30,30,30                 | 0     |
| 85  | OHX  | 5     | 3496 | 7/7   | 0.94 | 0.29 | 100,100,100,100             | 0     |
| 85  | OHX  | 6     | 2014 | 7/7   | 0.94 | 0.27 | 119,119,119,119             | 0     |
| 85  | OHX  | 5     | 3504 | 7/7   | 0.94 | 0.31 | 98,98,98,98                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | OHX  | 5     | 3517 | 7/7   | 0.94 | 0.23 | 90,90,90,90                 | 0     |
| 85  | OHX  | 5     | 3520 | 7/7   | 0.94 | 0.12 | 131,131,131,131             | 0     |
| 85  | OHX  | 1     | 3482 | 7/7   | 0.94 | 0.12 | 114,114,114,114             | 0     |
| 85  | OHX  | 6     | 2016 | 7/7   | 0.94 | 0.22 | 117,117,117,117             | 0     |
| 86  | MG   | 1     | 3765 | 1/1   | 0.94 | 0.10 | 51,51,51,51                 | 0     |
| 85  | OHX  | 1     | 3602 | 7/7   | 0.94 | 0.11 | 137,137,137,137             | 0     |
| 85  | OHX  | 1     | 3634 | 7/7   | 0.94 | 0.26 | 112,112,112,112             | 0     |
| 85  | OHX  | 7     | 208  | 7/7   | 0.94 | 0.12 | 125,125,125,125             | 0     |
| 85  | OHX  | 5     | 3551 | 7/7   | 0.94 | 0.19 | 117,117,117,117             | 0     |
| 85  | OHX  | 1     | 3487 | 7/7   | 0.94 | 0.12 | 118,118,118,118             | 0     |
| 86  | MG   | N0    | 201  | 1/1   | 0.94 | 0.14 | 47,47,47,47                 | 0     |
| 85  | OHX  | 5     | 3556 | 7/7   | 0.94 | 0.25 | 94,94,94,94                 | 0     |
| 85  | OHX  | 8     | 211  | 7/7   | 0.94 | 0.20 | 120,120,120,120             | 0     |
| 86  | MG   | 1     | 3860 | 1/1   | 0.94 | 0.17 | 45,45,45,45                 | 0     |
| 85  | OHX  | 8     | 212  | 7/7   | 0.94 | 0.21 | 125,125,125,125             | 0     |
| 85  | OHX  | 5     | 3558 | 7/7   | 0.94 | 0.24 | 107,107,107,107             | 0     |
| 86  | MG   | 1     | 4075 | 1/1   | 0.94 | 0.18 | 54,54,54,54                 | 0     |
| 85  | OHX  | 5     | 3560 | 7/7   | 0.94 | 0.23 | 101,101,101,101             | 0     |
| 86  | MG   | 5     | 4090 | 1/1   | 0.94 | 0.25 | 37,37,37,37                 | 0     |
| 85  | OHX  | 5     | 3667 | 7/7   | 0.94 | 0.26 | 100,100,100,100             | 0     |
| 85  | OHX  | 2     | 2025 | 7/7   | 0.94 | 0.22 | 126,126,126,126             | 0     |
| 85  | OHX  | 5     | 3567 | 7/7   | 0.94 | 0.14 | 119,119,119,119             | 0     |
| 85  | OHX  | 1     | 3566 | 7/7   | 0.94 | 0.18 | 133,133,133,133             | 0     |
| 85  | OHX  | 1     | 3714 | 7/7   | 0.94 | 0.32 | 95,95,95,95                 | 0     |
| 85  | OHX  | 5     | 3575 | 7/7   | 0.94 | 0.21 | 119,119,119,119             | 0     |
| 86  | MG   | 1     | 3871 | 1/1   | 0.94 | 0.26 | 31,31,31,31                 | 0     |
| 86  | MG   | 1     | 4084 | 1/1   | 0.94 | 0.22 | 35,35,35,35                 | 0     |
| 86  | MG   | 1     | 3872 | 1/1   | 0.94 | 0.26 | 42,42,42,42                 | 0     |
| 85  | OHX  | 5     | 3576 | 7/7   | 0.94 | 0.24 | 117,117,117,117             | 0     |
| 85  | OHX  | 1     | 3675 | 7/7   | 0.94 | 0.22 | 122,122,122,122             | 0     |
| 85  | OHX  | 1     | 3638 | 7/7   | 0.94 | 0.16 | 126,126,126,126             | 0     |
| 85  | OHX  | 5     | 3588 | 7/7   | 0.94 | 0.13 | 127,127,127,127             | 0     |
| 85  | OHX  | m0    | 303  | 7/7   | 0.94 | 0.22 | 119,119,119,119             | 0     |
| 86  | MG   | 1     | 3879 | 1/1   | 0.94 | 0.29 | 30,30,30,30                 | 0     |
| 85  | OHX  | m1    | 201  | 7/7   | 0.94 | 0.17 | 135,135,135,135             | 0     |
| 86  | MG   | 1     | 3986 | 1/1   | 0.94 | 0.16 | 42,42,42,42                 | 0     |
| 85  | OHX  | 2     | 1940 | 7/7   | 0.95 | 0.18 | 120,120,120,120             | 0     |
| 85  | OHX  | 2     | 1993 | 7/7   | 0.95 | 0.19 | 119,119,119,119             | 0     |
| 85  | OHX  | 1     | 3551 | 7/7   | 0.95 | 0.19 | 128,128,128,128             | 0     |
| 85  | OHX  | 6     | 1980 | 7/7   | 0.95 | 0.23 | 99,99,99,99                 | 0     |
| 85  | OHX  | o3    | 201  | 7/7   | 0.95 | 0.20 | 101,101,101,101             | 0     |
| 86  | MG   | 5     | 3951 | 1/1   | 0.95 | 0.11 | 41,41,41,41                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | OHX  | 2     | 1954 | 7/7   | 0.95 | 0.17 | 115,115,115,115             | 0     |
| 85  | OHX  | 6     | 1982 | 7/7   | 0.95 | 0.11 | 137,137,137,137             | 0     |
| 86  | MG   | 6     | 2121 | 1/1   | 0.95 | 0.10 | 68,68,68,68                 | 0     |
| 85  | OHX  | 6     | 1983 | 7/7   | 0.95 | 0.10 | 136,136,136,136             | 0     |
| 85  | OHX  | sR    | 401  | 7/7   | 0.95 | 0.09 | 156,156,156,156             | 0     |
| 86  | MG   | 1     | 3868 | 1/1   | 0.95 | 0.18 | 37,37,37,37                 | 0     |
| 85  | OHX  | 5     | 3476 | 7/7   | 0.95 | 0.10 | 104,104,104,104             | 0     |
| 85  | OHX  | 5     | 3486 | 7/7   | 0.95 | 0.20 | 99,99,99,99                 | 0     |
| 85  | OHX  | 5     | 3495 | 7/7   | 0.95 | 0.17 | 103,103,103,103             | 0     |
| 86  | MG   | 5     | 4105 | 1/1   | 0.95 | 0.08 | 47,47,47,47                 | 0     |
| 85  | OHX  | 2     | 1972 | 7/7   | 0.95 | 0.09 | 151,151,151,151             | 0     |
| 86  | MG   | 1     | 3873 | 1/1   | 0.95 | 0.31 | 32,32,32,32                 | 0     |
| 86  | MG   | 5     | 4108 | 1/1   | 0.95 | 0.30 | 29,29,29,29                 | 0     |
| 85  | OHX  | 5     | 3499 | 7/7   | 0.95 | 0.27 | 97,97,97,97                 | 0     |
| 85  | OHX  | 2     | 1974 | 7/7   | 0.95 | 0.22 | 140,140,140,140             | 0     |
| 86  | MG   | 5     | 4111 | 1/1   | 0.95 | 0.14 | 42,42,42,42                 | 0     |
| 85  | OHX  | 1     | 3558 | 7/7   | 0.95 | 0.21 | 111,111,111,111             | 0     |
| 85  | OHX  | 5     | 3509 | 7/7   | 0.95 | 0.12 | 107,107,107,107             | 0     |
| 85  | OHX  | 5     | 3514 | 7/7   | 0.95 | 0.23 | 102,102,102,102             | 0     |
| 85  | OHX  | 5     | 3515 | 7/7   | 0.95 | 0.23 | 102,102,102,102             | 0     |
| 85  | OHX  | 1     | 3720 | 7/7   | 0.95 | 0.23 | 96,96,96,96                 | 0     |
| 85  | OHX  | 2     | 1975 | 7/7   | 0.95 | 0.10 | 161,161,161,161             | 0     |
| 85  | OHX  | 5     | 3522 | 7/7   | 0.95 | 0.25 | 93,93,93,93                 | 0     |
| 85  | OHX  | 2     | 1929 | 7/7   | 0.95 | 0.23 | 116,116,116,116             | 0     |
| 86  | MG   | 5     | 3973 | 1/1   | 0.95 | 0.08 | 65,65,65,65                 | 0     |
| 85  | OHX  | 5     | 3527 | 7/7   | 0.95 | 0.22 | 102,102,102,102             | 0     |
| 85  | OHX  | 5     | 3530 | 7/7   | 0.95 | 0.24 | 92,92,92,92                 | 0     |
| 85  | OHX  | 5     | 3531 | 7/7   | 0.95 | 0.19 | 94,94,94,94                 | 0     |
| 85  | OHX  | 5     | 3533 | 7/7   | 0.95 | 0.22 | 84,84,84,84                 | 0     |
| 85  | OHX  | 5     | 3534 | 7/7   | 0.95 | 0.15 | 110,110,110,110             | 0     |
| 85  | OHX  | 5     | 3536 | 7/7   | 0.95 | 0.28 | 104,104,104,104             | 0     |
| 86  | MG   | 1     | 4028 | 1/1   | 0.95 | 0.09 | 87,87,87,87                 | 0     |
| 85  | OHX  | 5     | 3678 | 7/7   | 0.95 | 0.25 | 110,110,110,110             | 0     |
| 85  | OHX  | 2     | 1931 | 7/7   | 0.95 | 0.10 | 134,134,134,134             | 0     |
| 85  | OHX  | 1     | 3462 | 7/7   | 0.95 | 0.12 | 121,121,121,121             | 0     |
| 85  | OHX  | 5     | 3681 | 7/7   | 0.95 | 0.19 | 117,117,117,117             | 0     |
| 85  | OHX  | 5     | 3542 | 7/7   | 0.95 | 0.09 | 127,127,127,127             | 0     |
| 85  | OHX  | 1     | 3620 | 7/7   | 0.95 | 0.17 | 124,124,124,124             | 0     |
| 85  | OHX  | 5     | 3549 | 7/7   | 0.95 | 0.22 | 109,109,109,109             | 0     |
| 86  | MG   | 1     | 3776 | 1/1   | 0.95 | 0.16 | 34,34,34,34                 | 0     |
| 85  | OHX  | 6     | 1994 | 7/7   | 0.95 | 0.22 | 127,127,127,127             | 0     |
| 85  | OHX  | 5     | 3686 | 7/7   | 0.95 | 0.19 | 133,133,133,133             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | OHX  | 1     | 3464 | 7/7   | 0.95 | 0.12 | 102,102,102,102             | 0     |
| 85  | OHX  | 2     | 1932 | 7/7   | 0.95 | 0.16 | 128,128,128,128             | 0     |
| 85  | OHX  | 1     | 3484 | 7/7   | 0.95 | 0.15 | 114,114,114,114             | 0     |
| 85  | OHX  | 5     | 3559 | 7/7   | 0.95 | 0.19 | 98,98,98,98                 | 0     |
| 86  | MG   | M7    | 205  | 1/1   | 0.95 | 0.24 | 34,34,34,34                 | 0     |
| 85  | OHX  | 1     | 3486 | 7/7   | 0.95 | 0.11 | 117,117,117,117             | 0     |
| 85  | OHX  | 5     | 3562 | 7/7   | 0.95 | 0.15 | 130,130,130,130             | 0     |
| 85  | OHX  | 5     | 3564 | 7/7   | 0.95 | 0.11 | 137,137,137,137             | 0     |
| 86  | MG   | M8    | 201  | 1/1   | 0.95 | 0.13 | 43,43,43,43                 | 0     |
| 85  | OHX  | 1     | 3570 | 7/7   | 0.95 | 0.29 | 99,99,99,99                 | 0     |
| 85  | OHX  | 6     | 2001 | 7/7   | 0.95 | 0.20 | 101,101,101,101             | 0     |
| 85  | OHX  | 2     | 1921 | 7/7   | 0.95 | 0.13 | 112,112,112,112             | 0     |
| 85  | OHX  | 5     | 3571 | 7/7   | 0.95 | 0.12 | 113,113,113,113             | 0     |
| 85  | OHX  | 5     | 3572 | 7/7   | 0.95 | 0.25 | 99,99,99,99                 | 0     |
| 85  | OHX  | 2     | 1949 | 7/7   | 0.95 | 0.17 | 127,127,127,127             | 0     |
| 85  | OHX  | 5     | 3574 | 7/7   | 0.95 | 0.19 | 110,110,110,110             | 0     |
| 85  | OHX  | 1     | 3499 | 7/7   | 0.95 | 0.10 | 119,119,119,119             | 0     |
| 85  | OHX  | 1     | 3579 | 7/7   | 0.95 | 0.17 | 117,117,117,117             | 0     |
| 85  | OHX  | 6     | 2007 | 7/7   | 0.95 | 0.17 | 130,130,130,130             | 0     |
| 86  | MG   | 5     | 4010 | 1/1   | 0.95 | 0.35 | 40,40,40,40                 | 0     |
| 85  | OHX  | 1     | 3580 | 7/7   | 0.95 | 0.20 | 96,96,96,96                 | 0     |
| 86  | MG   | 1     | 3797 | 1/1   | 0.95 | 0.15 | 38,38,38,38                 | 0     |
| 85  | OHX  | 5     | 3583 | 7/7   | 0.95 | 0.21 | 113,113,113,113             | 0     |
| 85  | OHX  | 5     | 3586 | 7/7   | 0.95 | 0.29 | 105,105,105,105             | 0     |
| 85  | OHX  | 1     | 3582 | 7/7   | 0.95 | 0.26 | 101,101,101,101             | 0     |
| 85  | OHX  | 3     | 208  | 7/7   | 0.95 | 0.12 | 120,120,120,120             | 0     |
| 85  | OHX  | 1     | 3503 | 7/7   | 0.95 | 0.11 | 109,109,109,109             | 0     |
| 85  | OHX  | 1     | 3510 | 7/7   | 0.95 | 0.21 | 104,104,104,104             | 0     |
| 86  | MG   | 1     | 3931 | 1/1   | 0.95 | 0.20 | 49,49,49,49                 | 0     |
| 85  | OHX  | 5     | 3713 | 7/7   | 0.95 | 0.23 | 107,107,107,107             | 0     |
| 85  | OHX  | 5     | 3594 | 7/7   | 0.95 | 0.24 | 93,93,93,93                 | 0     |
| 86  | MG   | 5     | 4023 | 1/1   | 0.95 | 0.17 | 60,60,60,60                 | 0     |
| 85  | OHX  | 1     | 3586 | 7/7   | 0.95 | 0.21 | 98,98,98,98                 | 0     |
| 86  | MG   | sM    | 401  | 1/1   | 0.95 | 0.15 | 44,44,44,44                 | 0     |
| 85  | OHX  | 4     | 203  | 7/7   | 0.95 | 0.20 | 95,95,95,95                 | 0     |
| 85  | OHX  | 5     | 3597 | 7/7   | 0.95 | 0.26 | 107,107,107,107             | 0     |
| 85  | OHX  | 5     | 3718 | 7/7   | 0.95 | 0.26 | 109,109,109,109             | 0     |
| 85  | OHX  | 2     | 1963 | 7/7   | 0.95 | 0.11 | 142,142,142,142             | 0     |
| 85  | OHX  | 5     | 3599 | 7/7   | 0.95 | 0.21 | 123,123,123,123             | 0     |
| 85  | OHX  | 1     | 3590 | 7/7   | 0.95 | 0.14 | 131,131,131,131             | 0     |
| 85  | OHX  | 5     | 3601 | 7/7   | 0.95 | 0.25 | 112,112,112,112             | 0     |
| 85  | OHX  | 1     | 3591 | 7/7   | 0.95 | 0.24 | 100,100,100,100             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 85  | OHX  | 4     | 209  | 7/7   | 0.95 | 0.09 | 140,140,140,140            | 0     |
| 85  | OHX  | 1     | 3690 | 7/7   | 0.95 | 0.19 | 125,125,125,125            | 0     |
| 85  | OHX  | 1     | 3641 | 7/7   | 0.95 | 0.19 | 135,135,135,135            | 0     |
| 85  | OHX  | 5     | 3606 | 7/7   | 0.95 | 0.24 | 91,91,91,91                | 0     |
| 85  | OHX  | 1     | 3592 | 7/7   | 0.95 | 0.10 | 144,144,144,144            | 0     |
| 85  | OHX  | 1     | 3593 | 7/7   | 0.95 | 0.25 | 88,88,88,88                | 0     |
| 86  | MG   | 8     | 224  | 1/1   | 0.95 | 0.15 | 61,61,61,61                | 0     |
| 85  | OHX  | 1     | 3695 | 7/7   | 0.95 | 0.21 | 101,101,101,101            | 0     |
| 86  | MG   | 5     | 3900 | 1/1   | 0.95 | 0.21 | 29,29,29,29                | 0     |
| 85  | OHX  | L3    | 402  | 7/7   | 0.95 | 0.19 | 116,116,116,116            | 0     |
| 85  | OHX  | L4    | 401  | 7/7   | 0.95 | 0.17 | 121,121,121,121            | 0     |
| 85  | OHX  | 1     | 3516 | 7/7   | 0.95 | 0.17 | 106,106,106,106            | 0     |
| 85  | OHX  | 1     | 3522 | 7/7   | 0.95 | 0.28 | 98,98,98,98                | 0     |
| 85  | OHX  | 6     | 2030 | 7/7   | 0.95 | 0.20 | 98,98,98,98                | 0     |
| 85  | OHX  | 2     | 1951 | 7/7   | 0.95 | 0.09 | 148,148,148,148            | 0     |
| 86  | MG   | 5     | 4051 | 1/1   | 0.95 | 0.15 | 67,67,67,67                | 0     |
| 85  | OHX  | 1     | 3528 | 7/7   | 0.95 | 0.27 | 102,102,102,102            | 0     |
| 85  | OHX  | 5     | 3621 | 7/7   | 0.95 | 0.26 | 99,99,99,99                | 0     |
| 85  | OHX  | 1     | 3533 | 7/7   | 0.95 | 0.10 | 155,155,155,155            | 0     |
| 85  | OHX  | O3    | 201  | 7/7   | 0.95 | 0.27 | 105,105,105,105            | 0     |
| 86  | MG   | 1     | 3964 | 1/1   | 0.95 | 0.33 | 51,51,51,51                | 0     |
| 85  | OHX  | 2     | 1965 | 7/7   | 0.95 | 0.18 | 126,126,126,126            | 0     |
| 85  | OHX  | 6     | 1940 | 7/7   | 0.95 | 0.17 | 102,102,102,102            | 0     |
| 85  | OHX  | 2     | 1966 | 7/7   | 0.95 | 0.20 | 124,124,124,124            | 0     |
| 85  | OHX  | 7     | 209  | 7/7   | 0.95 | 0.24 | 102,102,102,102            | 0     |
| 86  | MG   | m7    | 201  | 1/1   | 0.95 | 0.24 | 32,32,32,32                | 0     |
| 85  | OHX  | 6     | 1951 | 7/7   | 0.95 | 0.08 | 161,161,161,161            | 0     |
| 85  | OHX  | 5     | 3629 | 7/7   | 0.95 | 0.13 | 135,135,135,135            | 0     |
| 86  | MG   | 5     | 4063 | 1/1   | 0.95 | 0.38 | 37,37,37,37                | 0     |
| 85  | OHX  | 6     | 1952 | 7/7   | 0.95 | 0.15 | 114,114,114,114            | 0     |
| 85  | OHX  | 8     | 207  | 7/7   | 0.95 | 0.12 | 114,114,114,114            | 0     |
| 85  | OHX  | 8     | 208  | 7/7   | 0.95 | 0.23 | 108,108,108,108            | 0     |
| 85  | OHX  | 8     | 209  | 7/7   | 0.95 | 0.14 | 114,114,114,114            | 0     |
| 85  | OHX  | 6     | 1953 | 7/7   | 0.95 | 0.09 | 155,155,155,155            | 0     |
| 85  | OHX  | 2     | 1967 | 7/7   | 0.95 | 0.18 | 113,113,113,113            | 0     |
| 85  | OHX  | 6     | 1959 | 7/7   | 0.95 | 0.14 | 110,110,110,110            | 0     |
| 86  | MG   | 1     | 3846 | 1/1   | 0.95 | 0.38 | 31,31,31,31                | 0     |
| 85  | OHX  | 6     | 1960 | 7/7   | 0.95 | 0.21 | 109,109,109,109            | 0     |
| 86  | MG   | o3    | 202  | 1/1   | 0.95 | 0.14 | 40,40,40,40                | 0     |
| 85  | OHX  | 2     | 1927 | 7/7   | 0.95 | 0.11 | 129,129,129,129            | 0     |
| 85  | OHX  | 1     | 3543 | 7/7   | 0.95 | 0.21 | 97,97,97,97                | 0     |
| 85  | OHX  | 1     | 3654 | 7/7   | 0.95 | 0.20 | 116,116,116,116            | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | OHX  | 6     | 1967 | 7/7   | 0.95 | 0.24 | 102,102,102,102             | 0     |
| 86  | MG   | 5     | 4078 | 1/1   | 0.95 | 0.07 | 32,32,32,32                 | 0     |
| 86  | MG   | 5     | 4079 | 1/1   | 0.95 | 0.15 | 41,41,41,41                 | 0     |
| 85  | OHX  | 5     | 3641 | 7/7   | 0.95 | 0.20 | 119,119,119,119             | 0     |
| 85  | OHX  | 1     | 3547 | 7/7   | 0.95 | 0.23 | 126,126,126,126             | 0     |
| 85  | OHX  | 1     | 3548 | 7/7   | 0.95 | 0.17 | 117,117,117,117             | 0     |
| 85  | OHX  | 15    | 301  | 7/7   | 0.95 | 0.12 | 127,127,127,127             | 0     |
| 85  | OHX  | 1     | 3606 | 7/7   | 0.95 | 0.27 | 106,106,106,106             | 0     |
| 87  | ZN   | E1    | 501  | 1/1   | 0.95 | 0.06 | 134,134,134,134             | 0     |
| 85  | OHX  | 1     | 3658 | 7/7   | 0.95 | 0.19 | 124,124,124,124             | 0     |
| 86  | MG   | 5     | 3941 | 1/1   | 0.95 | 0.19 | 40,40,40,40                 | 0     |
| 85  | OHX  | 6     | 1974 | 7/7   | 0.95 | 0.17 | 117,117,117,117             | 0     |
| 86  | MG   | 5     | 3800 | 1/1   | 0.95 | 0.24 | 27,27,27,27                 | 0     |
| 85  | OHX  | 6     | 2009 | 7/7   | 0.96 | 0.17 | 103,103,103,103             | 0     |
| 85  | OHX  | 1     | 3589 | 7/7   | 0.96 | 0.09 | 137,137,137,137             | 0     |
| 86  | MG   | 1     | 4063 | 1/1   | 0.96 | 0.08 | 33,33,33,33                 | 0     |
| 85  | OHX  | 5     | 3561 | 7/7   | 0.96 | 0.17 | 123,123,123,123             | 0     |
| 85  | OHX  | 1     | 3535 | 7/7   | 0.96 | 0.18 | 106,106,106,106             | 0     |
| 85  | OHX  | 5     | 3563 | 7/7   | 0.96 | 0.18 | 103,103,103,103             | 0     |
| 86  | MG   | 1     | 3923 | 1/1   | 0.96 | 0.24 | 40,40,40,40                 | 0     |
| 85  | OHX  | 2     | 1903 | 7/7   | 0.96 | 0.13 | 89,89,89,89                 | 0     |
| 85  | OHX  | 5     | 3565 | 7/7   | 0.96 | 0.20 | 97,97,97,97                 | 0     |
| 85  | OHX  | 1     | 3538 | 7/7   | 0.96 | 0.18 | 95,95,95,95                 | 0     |
| 85  | OHX  | 2     | 1933 | 7/7   | 0.96 | 0.14 | 112,112,112,112             | 0     |
| 85  | OHX  | 1     | 3540 | 7/7   | 0.96 | 0.22 | 101,101,101,101             | 0     |
| 85  | OHX  | 5     | 3569 | 7/7   | 0.96 | 0.22 | 106,106,106,106             | 0     |
| 85  | OHX  | 1     | 3471 | 7/7   | 0.96 | 0.12 | 97,97,97,97                 | 0     |
| 85  | OHX  | M5    | 302  | 7/7   | 0.96 | 0.20 | 107,107,107,107             | 0     |
| 85  | OHX  | 1     | 3473 | 7/7   | 0.96 | 0.11 | 89,89,89,89                 | 0     |
| 85  | OHX  | 2     | 1926 | 7/7   | 0.96 | 0.12 | 119,119,119,119             | 0     |
| 85  | OHX  | 1     | 3545 | 7/7   | 0.96 | 0.17 | 115,115,115,115             | 0     |
| 85  | OHX  | 1     | 3703 | 7/7   | 0.96 | 0.23 | 121,121,121,121             | 0     |
| 85  | OHX  | 5     | 3577 | 7/7   | 0.96 | 0.22 | 105,105,105,105             | 0     |
| 85  | OHX  | 1     | 3546 | 7/7   | 0.96 | 0.22 | 117,117,117,117             | 0     |
| 85  | OHX  | 2     | 1960 | 7/7   | 0.96 | 0.07 | 149,149,149,149             | 0     |
| 85  | OHX  | 5     | 3581 | 7/7   | 0.96 | 0.09 | 150,150,150,150             | 0     |
| 85  | OHX  | 5     | 3706 | 7/7   | 0.96 | 0.25 | 106,106,106,106             | 0     |
| 85  | OHX  | 6     | 1918 | 7/7   | 0.96 | 0.11 | 95,95,95,95                 | 0     |
| 85  | OHX  | 5     | 3584 | 7/7   | 0.96 | 0.14 | 116,116,116,116             | 0     |
| 86  | MG   | 6     | 2087 | 1/1   | 0.96 | 0.17 | 45,45,45,45                 | 0     |
| 85  | OHX  | 5     | 3585 | 7/7   | 0.96 | 0.20 | 96,96,96,96                 | 0     |
| 85  | OHX  | 6     | 1925 | 7/7   | 0.96 | 0.10 | 105,105,105,105             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | OHX  | 6     | 1927 | 7/7   | 0.96 | 0.10 | 128,128,128,128             | 0     |
| 85  | OHX  | 6     | 1931 | 7/7   | 0.96 | 0.12 | 109,109,109,109             | 0     |
| 85  | OHX  | 6     | 1938 | 7/7   | 0.96 | 0.09 | 110,110,110,110             | 0     |
| 85  | OHX  | 5     | 3591 | 7/7   | 0.96 | 0.18 | 118,118,118,118             | 0     |
| 85  | OHX  | 6     | 1939 | 7/7   | 0.96 | 0.09 | 135,135,135,135             | 0     |
| 85  | OHX  | 2     | 1973 | 7/7   | 0.96 | 0.09 | 146,146,146,146             | 0     |
| 86  | MG   | 1     | 3952 | 1/1   | 0.96 | 0.20 | 50,50,50,50                 | 0     |
| 85  | OHX  | 6     | 1942 | 7/7   | 0.96 | 0.11 | 112,112,112,112             | 0     |
| 85  | OHX  | 6     | 1943 | 7/7   | 0.96 | 0.13 | 125,125,125,125             | 0     |
| 85  | OHX  | 6     | 1945 | 7/7   | 0.96 | 0.14 | 110,110,110,110             | 0     |
| 85  | OHX  | 6     | 1948 | 7/7   | 0.96 | 0.09 | 131,131,131,131             | 0     |
| 86  | MG   | 1     | 3957 | 1/1   | 0.96 | 0.14 | 55,55,55,55                 | 0     |
| 86  | MG   | 5     | 4123 | 1/1   | 0.96 | 0.05 | 49,49,49,49                 | 0     |
| 86  | MG   | 1     | 3958 | 1/1   | 0.96 | 0.20 | 42,42,42,42                 | 0     |
| 85  | OHX  | 5     | 3721 | 7/7   | 0.96 | 0.26 | 95,95,95,95                 | 0     |
| 85  | OHX  | 2     | 1988 | 7/7   | 0.96 | 0.08 | 138,138,138,138             | 0     |
| 85  | OHX  | 1     | 3489 | 7/7   | 0.96 | 0.10 | 109,109,109,109             | 0     |
| 85  | OHX  | 2     | 1989 | 7/7   | 0.96 | 0.21 | 109,109,109,109             | 0     |
| 85  | OHX  | 1     | 3494 | 7/7   | 0.96 | 0.18 | 93,93,93,93                 | 0     |
| 86  | MG   | 1     | 3827 | 1/1   | 0.96 | 0.16 | 46,46,46,46                 | 0     |
| 85  | OHX  | 1     | 3711 | 7/7   | 0.96 | 0.20 | 100,100,100,100             | 0     |
| 85  | OHX  | 6     | 1955 | 7/7   | 0.96 | 0.09 | 167,167,167,167             | 0     |
| 85  | OHX  | 6     | 1956 | 7/7   | 0.96 | 0.13 | 112,112,112,112             | 0     |
| 85  | OHX  | 6     | 1957 | 7/7   | 0.96 | 0.18 | 104,104,104,104             | 0     |
| 85  | OHX  | 6     | 1958 | 7/7   | 0.96 | 0.14 | 120,120,120,120             | 0     |
| 85  | OHX  | 1     | 3554 | 7/7   | 0.96 | 0.17 | 109,109,109,109             | 0     |
| 85  | OHX  | 5     | 3609 | 7/7   | 0.96 | 0.24 | 99,99,99,99                 | 0     |
| 85  | OHX  | 2     | 1909 | 7/7   | 0.96 | 0.17 | 119,119,119,119             | 0     |
| 85  | OHX  | 1     | 3500 | 7/7   | 0.96 | 0.15 | 85,85,85,85                 | 0     |
| 85  | OHX  | 6     | 1963 | 7/7   | 0.96 | 0.17 | 116,116,116,116             | 0     |
| 85  | OHX  | 6     | 1964 | 7/7   | 0.96 | 0.20 | 110,110,110,110             | 0     |
| 85  | OHX  | 2     | 1936 | 7/7   | 0.96 | 0.12 | 107,107,107,107             | 0     |
| 85  | OHX  | 5     | 3739 | 7/7   | 0.96 | 0.19 | 97,97,97,97                 | 0     |
| 85  | OHX  | 1     | 3610 | 7/7   | 0.96 | 0.13 | 114,114,114,114             | 0     |
| 86  | MG   | 5     | 4145 | 1/1   | 0.96 | 0.10 | 38,38,38,38                 | 0     |
| 85  | OHX  | 5     | 3618 | 7/7   | 0.96 | 0.18 | 103,103,103,103             | 0     |
| 85  | OHX  | 1     | 3505 | 7/7   | 0.96 | 0.10 | 124,124,124,124             | 0     |
| 85  | OHX  | 5     | 3743 | 7/7   | 0.96 | 0.15 | 129,129,129,129             | 0     |
| 86  | MG   | 1     | 4125 | 1/1   | 0.96 | 0.31 | 64,64,64,64                 | 0     |
| 85  | OHX  | 1     | 3506 | 7/7   | 0.96 | 0.14 | 107,107,107,107             | 0     |
| 85  | OHX  | 2     | 1915 | 7/7   | 0.96 | 0.10 | 142,142,142,142             | 0     |
| 86  | MG   | 1     | 4128 | 1/1   | 0.96 | 0.08 | 41,41,41,41                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 5     | 3834 | 1/1   | 0.96 | 0.12 | 39,39,39,39                 | 0     |
| 86  | MG   | 1     | 4129 | 1/1   | 0.96 | 0.13 | 70,70,70,70                 | 0     |
| 85  | OHX  | 2     | 1930 | 7/7   | 0.96 | 0.17 | 118,118,118,118             | 0     |
| 85  | OHX  | 7     | 204  | 7/7   | 0.96 | 0.15 | 86,86,86,86                 | 0     |
| 85  | OHX  | 1     | 3615 | 7/7   | 0.96 | 0.21 | 119,119,119,119             | 0     |
| 85  | OHX  | 1     | 3514 | 7/7   | 0.96 | 0.18 | 83,83,83,83                 | 0     |
| 86  | MG   | 6     | 2136 | 1/1   | 0.96 | 0.15 | 76,76,76,76                 | 0     |
| 85  | OHX  | c8    | 201  | 7/7   | 0.96 | 0.10 | 132,132,132,132             | 0     |
| 85  | OHX  | 1     | 3515 | 7/7   | 0.96 | 0.26 | 86,86,86,86                 | 0     |
| 85  | OHX  | 5     | 3627 | 7/7   | 0.96 | 0.17 | 127,127,127,127             | 0     |
| 85  | OHX  | C8    | 201  | 7/7   | 0.96 | 0.10 | 112,112,112,112             | 0     |
| 85  | OHX  | 6     | 1977 | 7/7   | 0.96 | 0.13 | 138,138,138,138             | 0     |
| 85  | OHX  | 5     | 3459 | 7/7   | 0.96 | 0.13 | 80,80,80,80                 | 0     |
| 85  | OHX  | 5     | 3460 | 7/7   | 0.96 | 0.13 | 89,89,89,89                 | 0     |
| 85  | OHX  | 5     | 3468 | 7/7   | 0.96 | 0.10 | 99,99,99,99                 | 0     |
| 85  | OHX  | 1     | 3670 | 7/7   | 0.96 | 0.23 | 110,110,110,110             | 0     |
| 86  | MG   | D1    | 101  | 1/1   | 0.96 | 0.14 | 109,109,109,109             | 0     |
| 85  | OHX  | 5     | 3634 | 7/7   | 0.96 | 0.08 | 139,139,139,139             | 0     |
| 85  | OHX  | 5     | 3635 | 7/7   | 0.96 | 0.17 | 103,103,103,103             | 0     |
| 85  | OHX  | 5     | 3484 | 7/7   | 0.96 | 0.18 | 91,91,91,91                 | 0     |
| 85  | OHX  | 1     | 3517 | 7/7   | 0.96 | 0.13 | 95,95,95,95                 | 0     |
| 86  | MG   | 5     | 3856 | 1/1   | 0.96 | 0.28 | 38,38,38,38                 | 0     |
| 85  | OHX  | 5     | 3487 | 7/7   | 0.96 | 0.22 | 89,89,89,89                 | 0     |
| 85  | OHX  | 1     | 3569 | 7/7   | 0.96 | 0.24 | 98,98,98,98                 | 0     |
| 85  | OHX  | 1     | 3621 | 7/7   | 0.96 | 0.09 | 193,193,193,193             | 0     |
| 85  | OHX  | 5     | 3497 | 7/7   | 0.96 | 0.15 | 116,116,116,116             | 0     |
| 86  | MG   | 7     | 218  | 1/1   | 0.96 | 0.17 | 35,35,35,35                 | 0     |
| 85  | OHX  | 1     | 3674 | 7/7   | 0.96 | 0.11 | 102,102,102,102             | 0     |
| 85  | OHX  | 6     | 1984 | 7/7   | 0.96 | 0.17 | 110,110,110,110             | 0     |
| 85  | OHX  | 1     | 3519 | 7/7   | 0.96 | 0.12 | 120,120,120,120             | 0     |
| 86  | MG   | 4     | 230  | 1/1   | 0.96 | 0.06 | 51,51,51,51                 | 0     |
| 85  | OHX  | 5     | 3505 | 7/7   | 0.96 | 0.26 | 71,71,71,71                 | 0     |
| 85  | OHX  | 19    | 201  | 7/7   | 0.96 | 0.17 | 103,103,103,103             | 0     |
| 86  | MG   | 1     | 3747 | 1/1   | 0.96 | 0.26 | 40,40,40,40                 | 0     |
| 86  | MG   | 8     | 221  | 1/1   | 0.96 | 0.10 | 56,56,56,56                 | 0     |
| 86  | MG   | 5     | 3871 | 1/1   | 0.96 | 0.28 | 35,35,35,35                 | 0     |
| 85  | OHX  | 5     | 3506 | 7/7   | 0.96 | 0.12 | 104,104,104,104             | 0     |
| 86  | MG   | 5     | 4031 | 1/1   | 0.96 | 0.15 | 62,62,62,62                 | 0     |
| 85  | OHX  | 1     | 3571 | 7/7   | 0.96 | 0.08 | 143,143,143,143             | 0     |
| 85  | OHX  | 5     | 3648 | 7/7   | 0.96 | 0.24 | 102,102,102,102             | 0     |
| 85  | OHX  | m5    | 501  | 7/7   | 0.96 | 0.21 | 117,117,117,117             | 0     |
| 85  | OHX  | 1     | 3624 | 7/7   | 0.96 | 0.27 | 83,83,83,83                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 85  | OHX  | 1     | 3574 | 7/7   | 0.96 | 0.12 | 137,137,137,137            | 0     |
| 85  | OHX  | 1     | 3520 | 7/7   | 0.96 | 0.22 | 102,102,102,102            | 0     |
| 85  | OHX  | 5     | 3519 | 7/7   | 0.96 | 0.14 | 105,105,105,105            | 0     |
| 85  | OHX  | 2     | 1955 | 7/7   | 0.96 | 0.14 | 119,119,119,119            | 0     |
| 85  | OHX  | 1     | 3577 | 7/7   | 0.96 | 0.19 | 102,102,102,102            | 0     |
| 85  | OHX  | 1     | 3737 | 7/7   | 0.96 | 0.14 | 118,118,118,118            | 0     |
| 85  | OHX  | 5     | 3524 | 7/7   | 0.96 | 0.22 | 91,91,91,91                | 0     |
| 85  | OHX  | 5     | 3526 | 7/7   | 0.96 | 0.16 | 109,109,109,109            | 0     |
| 86  | MG   | 1     | 3888 | 1/1   | 0.96 | 0.21 | 31,31,31,31                | 0     |
| 85  | OHX  | 3     | 203  | 7/7   | 0.96 | 0.17 | 112,112,112,112            | 0     |
| 86  | MG   | 5     | 4046 | 1/1   | 0.96 | 0.10 | 33,33,33,33                | 0     |
| 85  | OHX  | 5     | 3659 | 7/7   | 0.96 | 0.20 | 112,112,112,112            | 0     |
| 85  | OHX  | 3     | 206  | 7/7   | 0.96 | 0.19 | 112,112,112,112            | 0     |
| 85  | OHX  | 3     | 207  | 7/7   | 0.96 | 0.17 | 118,118,118,118            | 0     |
| 85  | OHX  | 1     | 3523 | 7/7   | 0.96 | 0.21 | 117,117,117,117            | 0     |
| 86  | MG   | 1     | 3894 | 1/1   | 0.96 | 0.32 | 42,42,42,42                | 0     |
| 85  | OHX  | 1     | 3525 | 7/7   | 0.96 | 0.13 | 116,116,116,116            | 0     |
| 85  | OHX  | 5     | 3535 | 7/7   | 0.96 | 0.12 | 132,132,132,132            | 0     |
| 85  | OHX  | 1     | 3526 | 7/7   | 0.96 | 0.17 | 96,96,96,96                | 0     |
| 86  | MG   | 6     | 2186 | 1/1   | 0.96 | 0.05 | 87,87,87,87                | 0     |
| 85  | OHX  | 6     | 1999 | 7/7   | 0.96 | 0.18 | 125,125,125,125            | 0     |
| 86  | MG   | N6    | 201  | 1/1   | 0.96 | 0.27 | 45,45,45,45                | 0     |
| 85  | OHX  | 5     | 3540 | 7/7   | 0.96 | 0.11 | 123,123,123,123            | 0     |
| 85  | OHX  | 2     | 1918 | 7/7   | 0.96 | 0.10 | 99,99,99,99                | 0     |
| 86  | MG   | 1     | 4044 | 1/1   | 0.96 | 0.18 | 77,77,77,77                | 0     |
| 85  | OHX  | 1     | 3446 | 7/7   | 0.96 | 0.14 | 88,88,88,88                | 0     |
| 85  | OHX  | 5     | 3544 | 7/7   | 0.96 | 0.20 | 114,114,114,114            | 0     |
| 86  | MG   | O7    | 105  | 1/1   | 0.96 | 0.14 | 69,69,69,69                | 0     |
| 85  | OHX  | 5     | 3545 | 7/7   | 0.96 | 0.09 | 148,148,148,148            | 0     |
| 85  | OHX  | 1     | 3529 | 7/7   | 0.96 | 0.13 | 133,133,133,133            | 0     |
| 86  | MG   | 1     | 3906 | 1/1   | 0.96 | 0.18 | 24,24,24,24                | 0     |
| 85  | OHX  | 5     | 3547 | 7/7   | 0.96 | 0.14 | 101,101,101,101            | 0     |
| 85  | OHX  | 1     | 3585 | 7/7   | 0.96 | 0.14 | 129,129,129,129            | 0     |
| 85  | OHX  | 5     | 3550 | 7/7   | 0.96 | 0.23 | 94,94,94,94                | 0     |
| 85  | OHX  | 1     | 3530 | 7/7   | 0.96 | 0.14 | 124,124,124,124            | 0     |
| 85  | OHX  | 5     | 3552 | 7/7   | 0.96 | 0.16 | 108,108,108,108            | 0     |
| 86  | MG   | 5     | 3913 | 1/1   | 0.96 | 0.19 | 27,27,27,27                | 0     |
| 85  | OHX  | 5     | 3553 | 7/7   | 0.96 | 0.19 | 95,95,95,95                | 0     |
| 86  | MG   | 5     | 3758 | 1/1   | 0.96 | 0.23 | 37,37,37,37                | 0     |
| 85  | OHX  | 5     | 3554 | 7/7   | 0.96 | 0.10 | 130,130,130,130            | 0     |
| 85  | OHX  | 1     | 3587 | 7/7   | 0.96 | 0.23 | 104,104,104,104            | 0     |
| 85  | OHX  | 4     | 210  | 7/7   | 0.96 | 0.12 | 131,131,131,131            | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 5     | 3920 | 1/1   | 0.96 | 0.30 | 24,24,24,24                 | 0     |
| 85  | OHX  | 2     | 2009 | 7/7   | 0.96 | 0.18 | 112,112,112,112             | 0     |
| 85  | OHX  | 1     | 3481 | 7/7   | 0.97 | 0.13 | 89,89,89,89                 | 0     |
| 85  | OHX  | 2     | 1911 | 7/7   | 0.97 | 0.12 | 116,116,116,116             | 0     |
| 85  | OHX  | m0    | 302  | 7/7   | 0.97 | 0.16 | 116,116,116,116             | 0     |
| 85  | OHX  | 1     | 3483 | 7/7   | 0.97 | 0.17 | 89,89,89,89                 | 0     |
| 85  | OHX  | 2     | 1941 | 7/7   | 0.97 | 0.11 | 135,135,135,135             | 0     |
| 85  | OHX  | 1     | 3531 | 7/7   | 0.97 | 0.10 | 129,129,129,129             | 0     |
| 85  | OHX  | 5     | 3570 | 7/7   | 0.97 | 0.17 | 104,104,104,104             | 0     |
| 85  | OHX  | 1     | 3532 | 7/7   | 0.97 | 0.16 | 99,99,99,99                 | 0     |
| 85  | OHX  | 2     | 1950 | 7/7   | 0.97 | 0.16 | 115,115,115,115             | 0     |
| 85  | OHX  | 2     | 1928 | 7/7   | 0.97 | 0.11 | 114,114,114,114             | 0     |
| 85  | OHX  | 1     | 3536 | 7/7   | 0.97 | 0.18 | 83,83,83,83                 | 0     |
| 85  | OHX  | 2     | 1985 | 7/7   | 0.97 | 0.15 | 110,110,110,110             | 0     |
| 86  | MG   | 5     | 3859 | 1/1   | 0.97 | 0.35 | 37,37,37,37                 | 0     |
| 85  | OHX  | 1     | 3441 | 7/7   | 0.97 | 0.10 | 87,87,87,87                 | 0     |
| 85  | OHX  | 6     | 1905 | 7/7   | 0.97 | 0.10 | 80,80,80,80                 | 0     |
| 85  | OHX  | 5     | 3578 | 7/7   | 0.97 | 0.17 | 109,109,109,109             | 0     |
| 85  | OHX  | 1     | 3491 | 7/7   | 0.97 | 0.15 | 95,95,95,95                 | 0     |
| 85  | OHX  | 5     | 3442 | 7/7   | 0.97 | 0.11 | 82,82,82,82                 | 0     |
| 86  | MG   | 5     | 3866 | 1/1   | 0.97 | 0.32 | 22,22,22,22                 | 0     |
| 85  | OHX  | 5     | 3444 | 7/7   | 0.97 | 0.15 | 95,95,95,95                 | 0     |
| 85  | OHX  | 5     | 3453 | 7/7   | 0.97 | 0.12 | 111,111,111,111             | 0     |
| 85  | OHX  | 5     | 3457 | 7/7   | 0.97 | 0.10 | 88,88,88,88                 | 0     |
| 85  | OHX  | 6     | 1920 | 7/7   | 0.97 | 0.11 | 124,124,124,124             | 0     |
| 85  | OHX  | 6     | 1923 | 7/7   | 0.97 | 0.09 | 99,99,99,99                 | 0     |
| 85  | OHX  | 5     | 3587 | 7/7   | 0.97 | 0.20 | 108,108,108,108             | 0     |
| 85  | OHX  | 5     | 3461 | 7/7   | 0.97 | 0.10 | 74,74,74,74                 | 0     |
| 85  | OHX  | 5     | 3465 | 7/7   | 0.97 | 0.10 | 90,90,90,90                 | 0     |
| 85  | OHX  | 5     | 3466 | 7/7   | 0.97 | 0.14 | 84,84,84,84                 | 0     |
| 85  | OHX  | 1     | 3492 | 7/7   | 0.97 | 0.19 | 87,87,87,87                 | 0     |
| 85  | OHX  | 5     | 3592 | 7/7   | 0.97 | 0.20 | 96,96,96,96                 | 0     |
| 85  | OHX  | 5     | 3469 | 7/7   | 0.97 | 0.14 | 92,92,92,92                 | 0     |
| 85  | OHX  | 5     | 3474 | 7/7   | 0.97 | 0.15 | 80,80,80,80                 | 0     |
| 85  | OHX  | 1     | 3445 | 7/7   | 0.97 | 0.10 | 76,76,76,76                 | 0     |
| 85  | OHX  | 5     | 3480 | 7/7   | 0.97 | 0.15 | 84,84,84,84                 | 0     |
| 85  | OHX  | 5     | 3481 | 7/7   | 0.97 | 0.11 | 87,87,87,87                 | 0     |
| 85  | OHX  | 5     | 3482 | 7/7   | 0.97 | 0.12 | 93,93,93,93                 | 0     |
| 85  | OHX  | 5     | 3483 | 7/7   | 0.97 | 0.15 | 103,103,103,103             | 0     |
| 85  | OHX  | 6     | 1930 | 7/7   | 0.97 | 0.13 | 99,99,99,99                 | 0     |
| 85  | OHX  | 1     | 3495 | 7/7   | 0.97 | 0.17 | 71,71,71,71                 | 0     |
| 86  | MG   | 5     | 4016 | 1/1   | 0.97 | 0.13 | 40,40,40,40                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | OHX  | 6     | 1933 | 7/7   | 0.97 | 0.12 | 112,112,112,112             | 0     |
| 86  | MG   | 1     | 3994 | 1/1   | 0.97 | 0.08 | 43,43,43,43                 | 0     |
| 85  | OHX  | 5     | 3490 | 7/7   | 0.97 | 0.13 | 91,91,91,91                 | 0     |
| 86  | MG   | 6     | 2090 | 1/1   | 0.97 | 0.34 | 32,32,32,32                 | 0     |
| 85  | OHX  | 5     | 3493 | 7/7   | 0.97 | 0.11 | 99,99,99,99                 | 0     |
| 85  | OHX  | 6     | 1935 | 7/7   | 0.97 | 0.15 | 98,98,98,98                 | 0     |
| 85  | OHX  | 6     | 1936 | 7/7   | 0.97 | 0.09 | 112,112,112,112             | 0     |
| 85  | OHX  | 6     | 2003 | 7/7   | 0.97 | 0.18 | 103,103,103,103             | 0     |
| 85  | OHX  | 5     | 3498 | 7/7   | 0.97 | 0.15 | 104,104,104,104             | 0     |
| 85  | OHX  | 6     | 1937 | 7/7   | 0.97 | 0.08 | 113,113,113,113             | 0     |
| 85  | OHX  | 5     | 3610 | 7/7   | 0.97 | 0.20 | 103,103,103,103             | 0     |
| 86  | MG   | 5     | 4028 | 1/1   | 0.97 | 0.17 | 41,41,41,41                 | 0     |
| 85  | OHX  | 5     | 3500 | 7/7   | 0.97 | 0.09 | 117,117,117,117             | 0     |
| 85  | OHX  | 1     | 3497 | 7/7   | 0.97 | 0.15 | 102,102,102,102             | 0     |
| 86  | MG   | 1     | 4007 | 1/1   | 0.97 | 0.07 | 51,51,51,51                 | 0     |
| 85  | OHX  | 1     | 3544 | 7/7   | 0.97 | 0.20 | 101,101,101,101             | 0     |
| 85  | OHX  | 2     | 1944 | 7/7   | 0.97 | 0.08 | 142,142,142,142             | 0     |
| 85  | OHX  | 6     | 1941 | 7/7   | 0.97 | 0.16 | 111,111,111,111             | 0     |
| 85  | OHX  | 1     | 3451 | 7/7   | 0.97 | 0.09 | 99,99,99,99                 | 0     |
| 85  | OHX  | 5     | 3512 | 7/7   | 0.97 | 0.14 | 90,90,90,90                 | 0     |
| 85  | OHX  | 1     | 3502 | 7/7   | 0.97 | 0.15 | 98,98,98,98                 | 0     |
| 85  | OHX  | 6     | 1944 | 7/7   | 0.97 | 0.17 | 108,108,108,108             | 0     |
| 85  | OHX  | 5     | 3516 | 7/7   | 0.97 | 0.08 | 141,141,141,141             | 0     |
| 85  | OHX  | 1     | 3452 | 7/7   | 0.97 | 0.13 | 87,87,87,87                 | 0     |
| 85  | OHX  | 5     | 3518 | 7/7   | 0.97 | 0.18 | 103,103,103,103             | 0     |
| 85  | OHX  | 6     | 2013 | 7/7   | 0.97 | 0.19 | 103,103,103,103             | 0     |
| 86  | MG   | 1     | 3900 | 1/1   | 0.97 | 0.31 | 27,27,27,27                 | 0     |
| 85  | OHX  | 6     | 1946 | 7/7   | 0.97 | 0.10 | 113,113,113,113             | 0     |
| 85  | OHX  | 5     | 3521 | 7/7   | 0.97 | 0.08 | 119,119,119,119             | 0     |
| 85  | OHX  | 6     | 1947 | 7/7   | 0.97 | 0.13 | 102,102,102,102             | 0     |
| 85  | OHX  | 1     | 3504 | 7/7   | 0.97 | 0.17 | 88,88,88,88                 | 0     |
| 85  | OHX  | 1     | 3454 | 7/7   | 0.97 | 0.10 | 99,99,99,99                 | 0     |
| 86  | MG   | 5     | 3919 | 1/1   | 0.97 | 0.36 | 33,33,33,33                 | 0     |
| 85  | OHX  | 5     | 3525 | 7/7   | 0.97 | 0.14 | 108,108,108,108             | 0     |
| 86  | MG   | 1     | 3907 | 1/1   | 0.97 | 0.41 | 28,28,28,28                 | 0     |
| 85  | OHX  | 6     | 1950 | 7/7   | 0.97 | 0.10 | 123,123,123,123             | 0     |
| 85  | OHX  | 5     | 3734 | 7/7   | 0.97 | 0.23 | 97,97,97,97                 | 0     |
| 85  | OHX  | 1     | 3455 | 7/7   | 0.97 | 0.12 | 91,91,91,91                 | 0     |
| 85  | OHX  | 5     | 3528 | 7/7   | 0.97 | 0.10 | 117,117,117,117             | 0     |
| 85  | OHX  | 5     | 3529 | 7/7   | 0.97 | 0.12 | 102,102,102,102             | 0     |
| 85  | OHX  | 1     | 3552 | 7/7   | 0.97 | 0.17 | 104,104,104,104             | 0     |
| 85  | OHX  | 1     | 3507 | 7/7   | 0.97 | 0.10 | 106,106,106,106             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | MG   | 8     | 225  | 1/1   | 0.97 | 0.18 | 66,66,66,66                 | 0     |
| 85  | OHX  | 1     | 3508 | 7/7   | 0.97 | 0.15 | 111,111,111,111             | 0     |
| 86  | MG   | 4     | 227  | 1/1   | 0.97 | 0.05 | 47,47,47,47                 | 0     |
| 85  | OHX  | 1     | 3509 | 7/7   | 0.97 | 0.20 | 94,94,94,94                 | 0     |
| 85  | OHX  | 2     | 1987 | 7/7   | 0.97 | 0.09 | 147,147,147,147             | 0     |
| 85  | OHX  | 3     | 204  | 7/7   | 0.97 | 0.10 | 99,99,99,99                 | 0     |
| 85  | OHX  | 5     | 3537 | 7/7   | 0.97 | 0.18 | 92,92,92,92                 | 0     |
| 86  | MG   | 13    | 407  | 1/1   | 0.97 | 0.08 | 31,31,31,31                 | 0     |
| 85  | OHX  | 3     | 205  | 7/7   | 0.97 | 0.15 | 90,90,90,90                 | 0     |
| 86  | MG   | 5     | 3809 | 1/1   | 0.97 | 0.27 | 38,38,38,38                 | 0     |
| 85  | OHX  | 1     | 3694 | 7/7   | 0.97 | 0.18 | 98,98,98,98                 | 0     |
| 86  | MG   | 5     | 3938 | 1/1   | 0.97 | 0.20 | 33,33,33,33                 | 0     |
| 85  | OHX  | 7     | 203  | 7/7   | 0.97 | 0.15 | 95,95,95,95                 | 0     |
| 85  | OHX  | 1     | 3459 | 7/7   | 0.97 | 0.12 | 79,79,79,79                 | 0     |
| 85  | OHX  | 7     | 205  | 7/7   | 0.97 | 0.18 | 93,93,93,93                 | 0     |
| 86  | MG   | 5     | 3942 | 1/1   | 0.97 | 0.12 | 31,31,31,31                 | 0     |
| 85  | OHX  | 7     | 206  | 7/7   | 0.97 | 0.11 | 100,100,100,100             | 0     |
| 86  | MG   | L7    | 301  | 1/1   | 0.97 | 0.13 | 39,39,39,39                 | 0     |
| 85  | OHX  | 7     | 207  | 7/7   | 0.97 | 0.12 | 101,101,101,101             | 0     |
| 85  | OHX  | 1     | 3512 | 7/7   | 0.97 | 0.14 | 100,100,100,100             | 0     |
| 86  | MG   | 5     | 3947 | 1/1   | 0.97 | 0.13 | 38,38,38,38                 | 0     |
| 85  | OHX  | 5     | 3543 | 7/7   | 0.97 | 0.23 | 80,80,80,80                 | 0     |
| 85  | OHX  | 6     | 1962 | 7/7   | 0.97 | 0.18 | 97,97,97,97                 | 0     |
| 85  | OHX  | 1     | 3460 | 7/7   | 0.97 | 0.10 | 88,88,88,88                 | 0     |
| 85  | OHX  | 1     | 3561 | 7/7   | 0.97 | 0.20 | 97,97,97,97                 | 0     |
| 85  | OHX  | 8     | 203  | 7/7   | 0.97 | 0.11 | 114,114,114,114             | 0     |
| 85  | OHX  | 8     | 205  | 7/7   | 0.97 | 0.17 | 101,101,101,101             | 0     |
| 85  | OHX  | 8     | 206  | 7/7   | 0.97 | 0.11 | 115,115,115,115             | 0     |
| 85  | OHX  | 2     | 1977 | 7/7   | 0.97 | 0.12 | 113,113,113,113             | 0     |
| 85  | OHX  | 5     | 3548 | 7/7   | 0.97 | 0.21 | 86,86,86,86                 | 0     |
| 85  | OHX  | 2     | 1937 | 7/7   | 0.97 | 0.11 | 123,123,123,123             | 0     |
| 85  | OHX  | 8     | 210  | 7/7   | 0.97 | 0.08 | 139,139,139,139             | 0     |
| 85  | OHX  | 4     | 204  | 7/7   | 0.97 | 0.10 | 108,108,108,108             | 0     |
| 85  | OHX  | 6     | 1968 | 7/7   | 0.97 | 0.11 | 123,123,123,123             | 0     |
| 85  | OHX  | 4     | 205  | 7/7   | 0.97 | 0.19 | 121,121,121,121             | 0     |
| 85  | OHX  | 1     | 3468 | 7/7   | 0.97 | 0.13 | 100,100,100,100             | 0     |
| 85  | OHX  | 2     | 1939 | 7/7   | 0.97 | 0.09 | 123,123,123,123             | 0     |
| 85  | OHX  | 6     | 1972 | 7/7   | 0.97 | 0.17 | 101,101,101,101             | 0     |
| 85  | OHX  | 2     | 1962 | 7/7   | 0.97 | 0.18 | 114,114,114,114             | 0     |
| 85  | OHX  | 1     | 3521 | 7/7   | 0.97 | 0.19 | 86,86,86,86                 | 0     |
| 85  | OHX  | 13    | 401  | 7/7   | 0.97 | 0.15 | 95,95,95,95                 | 0     |
| 85  | OHX  | 1     | 3475 | 7/7   | 0.97 | 0.10 | 119,119,119,119             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | OHX  | 1     | 3476 | 7/7   | 0.97 | 0.09 | 98,98,98,98                 | 0     |
| 85  | OHX  | 1     | 3478 | 7/7   | 0.97 | 0.15 | 96,96,96,96                 | 0     |
| 86  | MG   | 1     | 3951 | 1/1   | 0.97 | 0.12 | 40,40,40,40                 | 0     |
| 85  | OHX  | 6     | 1978 | 7/7   | 0.97 | 0.18 | 98,98,98,98                 | 0     |
| 85  | OHX  | 1     | 3573 | 7/7   | 0.97 | 0.17 | 110,110,110,110             | 0     |
| 86  | MG   | 5     | 3844 | 1/1   | 0.97 | 0.32 | 38,38,38,38                 | 0     |
| 86  | MG   | 6     | 2168 | 1/1   | 0.97 | 0.21 | 44,44,44,44                 | 0     |
| 85  | OHX  | 1     | 3480 | 7/7   | 0.97 | 0.11 | 105,105,105,105             | 0     |
| 85  | OHX  | 1     | 3467 | 7/7   | 0.98 | 0.09 | 87,87,87,87                 | 0     |
| 85  | OHX  | 5     | 3503 | 7/7   | 0.98 | 0.09 | 102,102,102,102             | 0     |
| 85  | OHX  | 6     | 1924 | 7/7   | 0.98 | 0.16 | 91,91,91,91                 | 0     |
| 85  | OHX  | 8     | 204  | 7/7   | 0.98 | 0.13 | 97,97,97,97                 | 0     |
| 85  | OHX  | 2     | 1906 | 7/7   | 0.98 | 0.10 | 103,103,103,103             | 0     |
| 85  | OHX  | 6     | 1926 | 7/7   | 0.98 | 0.21 | 87,87,87,87                 | 0     |
| 85  | OHX  | 5     | 3507 | 7/7   | 0.98 | 0.13 | 87,87,87,87                 | 0     |
| 85  | OHX  | 5     | 3508 | 7/7   | 0.98 | 0.17 | 93,93,93,93                 | 0     |
| 85  | OHX  | 1     | 3469 | 7/7   | 0.98 | 0.08 | 100,100,100,100             | 0     |
| 85  | OHX  | 5     | 3510 | 7/7   | 0.98 | 0.08 | 122,122,122,122             | 0     |
| 85  | OHX  | 6     | 1928 | 7/7   | 0.98 | 0.07 | 136,136,136,136             | 0     |
| 86  | MG   | 1     | 4002 | 1/1   | 0.98 | 0.08 | 43,43,43,43                 | 0     |
| 85  | OHX  | 5     | 3513 | 7/7   | 0.98 | 0.10 | 101,101,101,101             | 0     |
| 85  | OHX  | 2     | 1912 | 7/7   | 0.98 | 0.09 | 110,110,110,110             | 0     |
| 85  | OHX  | 1     | 3472 | 7/7   | 0.98 | 0.09 | 92,92,92,92                 | 0     |
| 85  | OHX  | 6     | 1932 | 7/7   | 0.98 | 0.11 | 90,90,90,90                 | 0     |
| 85  | OHX  | 2     | 1913 | 7/7   | 0.98 | 0.08 | 106,106,106,106             | 0     |
| 85  | OHX  | 6     | 1934 | 7/7   | 0.98 | 0.12 | 101,101,101,101             | 0     |
| 85  | OHX  | 1     | 3474 | 7/7   | 0.98 | 0.10 | 87,87,87,87                 | 0     |
| 85  | OHX  | 2     | 1948 | 7/7   | 0.98 | 0.09 | 124,124,124,124             | 0     |
| 85  | OHX  | 2     | 1914 | 7/7   | 0.98 | 0.10 | 97,97,97,97                 | 0     |
| 86  | MG   | 1     | 4013 | 1/1   | 0.98 | 0.12 | 34,34,34,34                 | 0     |
| 85  | OHX  | 1     | 3534 | 7/7   | 0.98 | 0.07 | 146,146,146,146             | 0     |
| 85  | OHX  | 1     | 3477 | 7/7   | 0.98 | 0.10 | 95,95,95,95                 | 0     |
| 85  | OHX  | 2     | 1907 | 7/7   | 0.98 | 0.08 | 101,101,101,101             | 0     |
| 85  | OHX  | 1     | 3479 | 7/7   | 0.98 | 0.16 | 85,85,85,85                 | 0     |
| 85  | OHX  | 2     | 1970 | 7/7   | 0.98 | 0.12 | 107,107,107,107             | 0     |
| 85  | OHX  | 2     | 1916 | 7/7   | 0.98 | 0.08 | 107,107,107,107             | 0     |
| 85  | OHX  | 1     | 3407 | 7/7   | 0.98 | 0.10 | 64,64,64,64                 | 0     |
| 85  | OHX  | m0    | 301  | 7/7   | 0.98 | 0.08 | 118,118,118,118             | 0     |
| 85  | OHX  | 1     | 3416 | 7/7   | 0.98 | 0.10 | 71,71,71,71                 | 0     |
| 85  | OHX  | 1     | 3418 | 7/7   | 0.98 | 0.10 | 72,72,72,72                 | 0     |
| 85  | OHX  | 1     | 3485 | 7/7   | 0.98 | 0.14 | 99,99,99,99                 | 0     |
| 85  | OHX  | 5     | 3532 | 7/7   | 0.98 | 0.14 | 79,79,79,79                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | OHX  | 1     | 3423 | 7/7   | 0.98 | 0.11 | 71,71,71,71                 | 0     |
| 85  | OHX  | 1     | 3426 | 7/7   | 0.98 | 0.11 | 82,82,82,82                 | 0     |
| 85  | OHX  | o2    | 201  | 7/7   | 0.98 | 0.16 | 86,86,86,86                 | 0     |
| 85  | OHX  | 1     | 3488 | 7/7   | 0.98 | 0.10 | 98,98,98,98                 | 0     |
| 85  | OHX  | 1     | 3427 | 7/7   | 0.98 | 0.09 | 70,70,70,70                 | 0     |
| 85  | OHX  | 1     | 3432 | 7/7   | 0.98 | 0.10 | 77,77,77,77                 | 0     |
| 85  | OHX  | q2    | 502  | 7/7   | 0.98 | 0.11 | 73,73,73,73                 | 0     |
| 85  | OHX  | 5     | 3538 | 7/7   | 0.98 | 0.09 | 108,108,108,108             | 0     |
| 85  | OHX  | 1     | 3433 | 7/7   | 0.98 | 0.09 | 77,77,77,77                 | 0     |
| 85  | OHX  | 1     | 3434 | 7/7   | 0.98 | 0.07 | 82,82,82,82                 | 0     |
| 85  | OHX  | 1     | 3493 | 7/7   | 0.98 | 0.10 | 102,102,102,102             | 0     |
| 85  | OHX  | 3     | 202  | 7/7   | 0.98 | 0.08 | 90,90,90,90                 | 0     |
| 85  | OHX  | 1     | 3435 | 7/7   | 0.98 | 0.09 | 85,85,85,85                 | 0     |
| 85  | OHX  | 2     | 1917 | 7/7   | 0.98 | 0.10 | 95,95,95,95                 | 0     |
| 86  | MG   | 5     | 3863 | 1/1   | 0.98 | 0.32 | 26,26,26,26                 | 0     |
| 85  | OHX  | 1     | 3496 | 7/7   | 0.98 | 0.10 | 108,108,108,108             | 0     |
| 85  | OHX  | 1     | 3443 | 7/7   | 0.98 | 0.11 | 81,81,81,81                 | 0     |
| 85  | OHX  | 1     | 3556 | 7/7   | 0.98 | 0.16 | 105,105,105,105             | 0     |
| 85  | OHX  | 1     | 3498 | 7/7   | 0.98 | 0.13 | 94,94,94,94                 | 0     |
| 85  | OHX  | 1     | 3444 | 7/7   | 0.98 | 0.07 | 92,92,92,92                 | 0     |
| 85  | OHX  | 2     | 1908 | 7/7   | 0.98 | 0.10 | 108,108,108,108             | 0     |
| 85  | OHX  | 1     | 3501 | 7/7   | 0.98 | 0.13 | 70,70,70,70                 | 0     |
| 85  | OHX  | 5     | 3677 | 7/7   | 0.98 | 0.17 | 74,74,74,74                 | 0     |
| 85  | OHX  | 4     | 202  | 7/7   | 0.98 | 0.11 | 77,77,77,77                 | 0     |
| 85  | OHX  | 2     | 1919 | 7/7   | 0.98 | 0.08 | 94,94,94,94                 | 0     |
| 85  | OHX  | s1    | 301  | 7/7   | 0.98 | 0.10 | 81,81,81,81                 | 0     |
| 86  | MG   | O1    | 201  | 1/1   | 0.98 | 0.08 | 75,75,75,75                 | 0     |
| 85  | OHX  | 1     | 3447 | 7/7   | 0.98 | 0.09 | 87,87,87,87                 | 0     |
| 85  | OHX  | 1     | 3563 | 7/7   | 0.98 | 0.11 | 119,119,119,119             | 0     |
| 85  | OHX  | 5     | 3557 | 7/7   | 0.98 | 0.15 | 91,91,91,91                 | 0     |
| 85  | OHX  | 1     | 3448 | 7/7   | 0.98 | 0.09 | 86,86,86,86                 | 0     |
| 85  | OHX  | 1     | 3449 | 7/7   | 0.98 | 0.08 | 82,82,82,82                 | 0     |
| 86  | MG   | 1     | 4056 | 1/1   | 0.98 | 0.11 | 38,38,38,38                 | 0     |
| 85  | OHX  | 2     | 1920 | 7/7   | 0.98 | 0.08 | 101,101,101,101             | 0     |
| 85  | OHX  | 2     | 1904 | 7/7   | 0.98 | 0.08 | 89,89,89,89                 | 0     |
| 85  | OHX  | 1     | 3453 | 7/7   | 0.98 | 0.08 | 94,94,94,94                 | 0     |
| 85  | OHX  | 2     | 1938 | 7/7   | 0.98 | 0.14 | 104,104,104,104             | 0     |
| 85  | OHX  | 2     | 1922 | 7/7   | 0.98 | 0.09 | 99,99,99,99                 | 0     |
| 85  | OHX  | 2     | 1923 | 7/7   | 0.98 | 0.10 | 101,101,101,101             | 0     |
| 85  | OHX  | 1     | 3572 | 7/7   | 0.98 | 0.17 | 85,85,85,85                 | 0     |
| 85  | OHX  | 5     | 3413 | 7/7   | 0.98 | 0.08 | 57,57,57,57                 | 0     |
| 86  | MG   | 5     | 4174 | 1/1   | 0.98 | 0.10 | 48,48,48,48                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | OHX  | 5     | 3419 | 7/7   | 0.98 | 0.09 | 61,61,61,61                 | 0     |
| 85  | OHX  | 5     | 3429 | 7/7   | 0.98 | 0.11 | 70,70,70,70                 | 0     |
| 85  | OHX  | 5     | 3434 | 7/7   | 0.98 | 0.09 | 68,68,68,68                 | 0     |
| 85  | OHX  | 5     | 3435 | 7/7   | 0.98 | 0.10 | 90,90,90,90                 | 0     |
| 85  | OHX  | 5     | 3439 | 7/7   | 0.98 | 0.09 | 69,69,69,69                 | 0     |
| 85  | OHX  | 5     | 3441 | 7/7   | 0.98 | 0.08 | 87,87,87,87                 | 0     |
| 85  | OHX  | 1     | 3457 | 7/7   | 0.98 | 0.12 | 91,91,91,91                 | 0     |
| 86  | MG   | 5     | 3897 | 1/1   | 0.98 | 0.28 | 25,25,25,25                 | 0     |
| 85  | OHX  | 5     | 3443 | 7/7   | 0.98 | 0.09 | 81,81,81,81                 | 0     |
| 85  | OHX  | 1     | 3513 | 7/7   | 0.98 | 0.15 | 101,101,101,101             | 0     |
| 85  | OHX  | 5     | 3703 | 7/7   | 0.98 | 0.17 | 83,83,83,83                 | 0     |
| 85  | OHX  | 5     | 3445 | 7/7   | 0.98 | 0.08 | 79,79,79,79                 | 0     |
| 85  | OHX  | 5     | 3446 | 7/7   | 0.98 | 0.07 | 85,85,85,85                 | 0     |
| 85  | OHX  | 5     | 3449 | 7/7   | 0.98 | 0.09 | 88,88,88,88                 | 0     |
| 85  | OHX  | 5     | 3451 | 7/7   | 0.98 | 0.08 | 96,96,96,96                 | 0     |
| 85  | OHX  | 5     | 3452 | 7/7   | 0.98 | 0.09 | 84,84,84,84                 | 0     |
| 85  | OHX  | 5     | 3582 | 7/7   | 0.98 | 0.16 | 85,85,85,85                 | 0     |
| 85  | OHX  | 1     | 3458 | 7/7   | 0.98 | 0.07 | 96,96,96,96                 | 0     |
| 85  | OHX  | 5     | 3454 | 7/7   | 0.98 | 0.08 | 98,98,98,98                 | 0     |
| 85  | OHX  | 5     | 3456 | 7/7   | 0.98 | 0.08 | 91,91,91,91                 | 0     |
| 85  | OHX  | 2     | 1924 | 7/7   | 0.98 | 0.09 | 117,117,117,117             | 0     |
| 86  | MG   | 13    | 403  | 1/1   | 0.98 | 0.35 | 27,27,27,27                 | 0     |
| 86  | MG   | 5     | 3770 | 1/1   | 0.98 | 0.16 | 37,37,37,37                 | 0     |
| 85  | OHX  | 5     | 3458 | 7/7   | 0.98 | 0.09 | 92,92,92,92                 | 0     |
| 85  | OHX  | 1     | 3639 | 7/7   | 0.98 | 0.16 | 107,107,107,107             | 0     |
| 85  | OHX  | 2     | 1925 | 7/7   | 0.98 | 0.11 | 133,133,133,133             | 0     |
| 85  | OHX  | 1     | 3461 | 7/7   | 0.98 | 0.12 | 80,80,80,80                 | 0     |
| 85  | OHX  | 5     | 3462 | 7/7   | 0.98 | 0.08 | 73,73,73,73                 | 0     |
| 85  | OHX  | 5     | 3463 | 7/7   | 0.98 | 0.11 | 90,90,90,90                 | 0     |
| 85  | OHX  | 1     | 3518 | 7/7   | 0.98 | 0.14 | 76,76,76,76                 | 0     |
| 85  | OHX  | 2     | 1943 | 7/7   | 0.98 | 0.16 | 104,104,104,104             | 0     |
| 85  | OHX  | 5     | 3467 | 7/7   | 0.98 | 0.10 | 92,92,92,92                 | 0     |
| 85  | OHX  | N9    | 102  | 7/7   | 0.98 | 0.09 | 63,63,63,63                 | 0     |
| 85  | OHX  | 1     | 3463 | 7/7   | 0.98 | 0.12 | 84,84,84,84                 | 0     |
| 85  | OHX  | 5     | 3470 | 7/7   | 0.98 | 0.08 | 87,87,87,87                 | 0     |
| 85  | OHX  | 5     | 3471 | 7/7   | 0.98 | 0.10 | 91,91,91,91                 | 0     |
| 85  | OHX  | 5     | 3472 | 7/7   | 0.98 | 0.09 | 99,99,99,99                 | 0     |
| 85  | OHX  | 5     | 3473 | 7/7   | 0.98 | 0.17 | 85,85,85,85                 | 0     |
| 85  | OHX  | 2     | 1910 | 7/7   | 0.98 | 0.09 | 100,100,100,100             | 0     |
| 85  | OHX  | 5     | 3475 | 7/7   | 0.98 | 0.11 | 80,80,80,80                 | 0     |
| 85  | OHX  | O7    | 102  | 7/7   | 0.98 | 0.10 | 94,94,94,94                 | 0     |
| 85  | OHX  | 5     | 3477 | 7/7   | 0.98 | 0.08 | 90,90,90,90                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | OHX  | 5     | 3478 | 7/7   | 0.98 | 0.10 | 96,96,96,96                 | 0     |
| 85  | OHX  | 5     | 3479 | 7/7   | 0.98 | 0.11 | 83,83,83,83                 | 0     |
| 85  | OHX  | O7    | 103  | 7/7   | 0.98 | 0.13 | 92,92,92,92                 | 0     |
| 85  | OHX  | Q2    | 502  | 7/7   | 0.98 | 0.14 | 71,71,71,71                 | 0     |
| 85  | OHX  | 6     | 1902 | 7/7   | 0.98 | 0.14 | 79,79,79,79                 | 0     |
| 85  | OHX  | 1     | 3465 | 7/7   | 0.98 | 0.10 | 98,98,98,98                 | 0     |
| 85  | OHX  | 6     | 1907 | 7/7   | 0.98 | 0.10 | 82,82,82,82                 | 0     |
| 85  | OHX  | 6     | 1908 | 7/7   | 0.98 | 0.10 | 80,80,80,80                 | 0     |
| 85  | OHX  | 5     | 3614 | 7/7   | 0.98 | 0.17 | 81,81,81,81                 | 0     |
| 85  | OHX  | 6     | 1909 | 7/7   | 0.98 | 0.09 | 96,96,96,96                 | 0     |
| 85  | OHX  | 5     | 3488 | 7/7   | 0.98 | 0.12 | 83,83,83,83                 | 0     |
| 85  | OHX  | 5     | 3489 | 7/7   | 0.98 | 0.17 | 86,86,86,86                 | 0     |
| 85  | OHX  | 6     | 1912 | 7/7   | 0.98 | 0.09 | 87,87,87,87                 | 0     |
| 85  | OHX  | 5     | 3491 | 7/7   | 0.98 | 0.08 | 118,118,118,118             | 0     |
| 85  | OHX  | 7     | 201  | 7/7   | 0.98 | 0.09 | 80,80,80,80                 | 0     |
| 86  | MG   | 5     | 4088 | 1/1   | 0.98 | 0.12 | 35,35,35,35                 | 0     |
| 85  | OHX  | 7     | 202  | 7/7   | 0.98 | 0.12 | 88,88,88,88                 | 0     |
| 86  | MG   | 1     | 3982 | 1/1   | 0.98 | 0.30 | 32,32,32,32                 | 0     |
| 85  | OHX  | 6     | 1913 | 7/7   | 0.98 | 0.08 | 94,94,94,94                 | 0     |
| 85  | OHX  | 6     | 1915 | 7/7   | 0.98 | 0.09 | 84,84,84,84                 | 0     |
| 87  | ZN   | D6    | 500  | 1/1   | 0.98 | 0.05 | 93,93,93,93                 | 0     |
| 85  | OHX  | 6     | 1917 | 7/7   | 0.98 | 0.09 | 86,86,86,86                 | 0     |
| 87  | ZN   | D9    | 101  | 1/1   | 0.98 | 0.04 | 89,89,89,89                 | 0     |
| 85  | OHX  | 1     | 3466 | 7/7   | 0.98 | 0.15 | 95,95,95,95                 | 0     |
| 85  | OHX  | 6     | 1919 | 7/7   | 0.98 | 0.08 | 108,108,108,108             | 0     |
| 85  | OHX  | 1     | 3524 | 7/7   | 0.98 | 0.15 | 109,109,109,109             | 0     |
| 87  | ZN   | d9    | 101  | 1/1   | 0.98 | 0.04 | 97,97,97,97                 | 0     |
| 85  | OHX  | 6     | 1922 | 7/7   | 0.98 | 0.16 | 90,90,90,90                 | 0     |
| 85  | OHX  | 5     | 3501 | 7/7   | 0.98 | 0.11 | 106,106,106,106             | 0     |
| 85  | OHX  | 1     | 3430 | 7/7   | 0.99 | 0.08 | 75,75,75,75                 | 0     |
| 85  | OHX  | 5     | 3414 | 7/7   | 0.99 | 0.08 | 61,61,61,61                 | 0     |
| 85  | OHX  | 5     | 3415 | 7/7   | 0.99 | 0.07 | 65,65,65,65                 | 0     |
| 85  | OHX  | 5     | 3416 | 7/7   | 0.99 | 0.07 | 65,65,65,65                 | 0     |
| 85  | OHX  | 5     | 3417 | 7/7   | 0.99 | 0.07 | 57,57,57,57                 | 0     |
| 85  | OHX  | 5     | 3418 | 7/7   | 0.99 | 0.07 | 69,69,69,69                 | 0     |
| 85  | OHX  | 1     | 3431 | 7/7   | 0.99 | 0.09 | 70,70,70,70                 | 0     |
| 85  | OHX  | 5     | 3420 | 7/7   | 0.99 | 0.07 | 62,62,62,62                 | 0     |
| 85  | OHX  | 5     | 3421 | 7/7   | 0.99 | 0.07 | 67,67,67,67                 | 0     |
| 85  | OHX  | 5     | 3511 | 7/7   | 0.99 | 0.10 | 63,63,63,63                 | 0     |
| 85  | OHX  | 5     | 3422 | 7/7   | 0.99 | 0.07 | 70,70,70,70                 | 0     |
| 85  | OHX  | 5     | 3423 | 7/7   | 0.99 | 0.06 | 67,67,67,67                 | 0     |
| 85  | OHX  | 5     | 3424 | 7/7   | 0.99 | 0.06 | 66,66,66,66                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | OHX  | 5     | 3425 | 7/7   | 0.99 | 0.07 | 71,71,71,71                 | 0     |
| 85  | OHX  | 5     | 3426 | 7/7   | 0.99 | 0.10 | 70,70,70,70                 | 0     |
| 85  | OHX  | 5     | 3427 | 7/7   | 0.99 | 0.07 | 69,69,69,69                 | 0     |
| 85  | OHX  | 5     | 3428 | 7/7   | 0.99 | 0.07 | 60,60,60,60                 | 0     |
| 86  | MG   | 5     | 4071 | 1/1   | 0.99 | 0.04 | 53,53,53,53                 | 0     |
| 85  | OHX  | 6     | 1921 | 7/7   | 0.99 | 0.11 | 86,86,86,86                 | 0     |
| 85  | OHX  | n3    | 201  | 7/7   | 0.99 | 0.10 | 85,85,85,85                 | 0     |
| 85  | OHX  | 5     | 3430 | 7/7   | 0.99 | 0.07 | 77,77,77,77                 | 0     |
| 85  | OHX  | n9    | 101  | 7/7   | 0.99 | 0.07 | 64,64,64,64                 | 0     |
| 85  | OHX  | 5     | 3431 | 7/7   | 0.99 | 0.07 | 73,73,73,73                 | 0     |
| 85  | OHX  | 5     | 3432 | 7/7   | 0.99 | 0.09 | 67,67,67,67                 | 0     |
| 85  | OHX  | 5     | 3433 | 7/7   | 0.99 | 0.08 | 64,64,64,64                 | 0     |
| 86  | MG   | 1     | 4004 | 1/1   | 0.99 | 0.04 | 42,42,42,42                 | 0     |
| 85  | OHX  | 1     | 3404 | 7/7   | 0.99 | 0.08 | 55,55,55,55                 | 0     |
| 85  | OHX  | 1     | 3405 | 7/7   | 0.99 | 0.10 | 58,58,58,58                 | 0     |
| 85  | OHX  | 5     | 3436 | 7/7   | 0.99 | 0.07 | 66,66,66,66                 | 0     |
| 85  | OHX  | 5     | 3437 | 7/7   | 0.99 | 0.08 | 74,74,74,74                 | 0     |
| 85  | OHX  | 5     | 3438 | 7/7   | 0.99 | 0.08 | 76,76,76,76                 | 0     |
| 85  | OHX  | 1     | 3406 | 7/7   | 0.99 | 0.07 | 54,54,54,54                 | 0     |
| 85  | OHX  | 5     | 3440 | 7/7   | 0.99 | 0.08 | 83,83,83,83                 | 0     |
| 85  | OHX  | 2     | 1905 | 7/7   | 0.99 | 0.08 | 86,86,86,86                 | 0     |
| 85  | OHX  | 1     | 3470 | 7/7   | 0.99 | 0.09 | 77,77,77,77                 | 0     |
| 85  | OHX  | 1     | 3436 | 7/7   | 0.99 | 0.06 | 83,83,83,83                 | 0     |
| 85  | OHX  | 1     | 3437 | 7/7   | 0.99 | 0.06 | 67,67,67,67                 | 0     |
| 85  | OHX  | 6     | 1929 | 7/7   | 0.99 | 0.10 | 81,81,81,81                 | 0     |
| 85  | OHX  | 1     | 3438 | 7/7   | 0.99 | 0.06 | 76,76,76,76                 | 0     |
| 85  | OHX  | 5     | 3447 | 7/7   | 0.99 | 0.09 | 73,73,73,73                 | 0     |
| 85  | OHX  | 5     | 3448 | 7/7   | 0.99 | 0.07 | 69,69,69,69                 | 0     |
| 85  | OHX  | 1     | 3439 | 7/7   | 0.99 | 0.07 | 75,75,75,75                 | 0     |
| 85  | OHX  | 5     | 3450 | 7/7   | 0.99 | 0.07 | 91,91,91,91                 | 0     |
| 85  | OHX  | 1     | 3440 | 7/7   | 0.99 | 0.09 | 68,68,68,68                 | 0     |
| 85  | OHX  | 1     | 3581 | 7/7   | 0.99 | 0.11 | 101,101,101,101             | 0     |
| 85  | OHX  | 1     | 3409 | 7/7   | 0.99 | 0.08 | 64,64,64,64                 | 0     |
| 85  | OHX  | 1     | 3442 | 7/7   | 0.99 | 0.07 | 85,85,85,85                 | 0     |
| 85  | OHX  | 5     | 3455 | 7/7   | 0.99 | 0.08 | 65,65,65,65                 | 0     |
| 85  | OHX  | 1     | 3410 | 7/7   | 0.99 | 0.07 | 63,63,63,63                 | 0     |
| 85  | OHX  | 1     | 3411 | 7/7   | 0.99 | 0.08 | 59,59,59,59                 | 0     |
| 85  | OHX  | 1     | 3412 | 7/7   | 0.99 | 0.08 | 67,67,67,67                 | 0     |
| 85  | OHX  | 1     | 3413 | 7/7   | 0.99 | 0.05 | 66,66,66,66                 | 0     |
| 85  | OHX  | 1     | 3414 | 7/7   | 0.99 | 0.08 | 65,65,65,65                 | 0     |
| 85  | OHX  | 1     | 3415 | 7/7   | 0.99 | 0.06 | 68,68,68,68                 | 0     |
| 85  | OHX  | N1    | 201  | 7/7   | 0.99 | 0.07 | 68,68,68,68                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | OHX  | 2     | 1901 | 7/7   | 0.99 | 0.13 | 79,79,79,79                 | 0     |
| 85  | OHX  | 5     | 3464 | 7/7   | 0.99 | 0.07 | 87,87,87,87                 | 0     |
| 85  | OHX  | 1     | 3450 | 7/7   | 0.99 | 0.07 | 90,90,90,90                 | 0     |
| 85  | OHX  | 1     | 3417 | 7/7   | 0.99 | 0.07 | 65,65,65,65                 | 0     |
| 85  | OHX  | 2     | 1902 | 7/7   | 0.99 | 0.06 | 86,86,86,86                 | 0     |
| 85  | OHX  | 1     | 3419 | 7/7   | 0.99 | 0.09 | 70,70,70,70                 | 0     |
| 85  | OHX  | 1     | 3420 | 7/7   | 0.99 | 0.08 | 63,63,63,63                 | 0     |
| 85  | OHX  | 6     | 1901 | 7/7   | 0.99 | 0.11 | 61,61,61,61                 | 0     |
| 85  | OHX  | 1     | 3421 | 7/7   | 0.99 | 0.09 | 74,74,74,74                 | 0     |
| 85  | OHX  | 6     | 1903 | 7/7   | 0.99 | 0.08 | 70,70,70,70                 | 0     |
| 85  | OHX  | 6     | 1904 | 7/7   | 0.99 | 0.07 | 70,70,70,70                 | 0     |
| 85  | OHX  | 1     | 3422 | 7/7   | 0.99 | 0.08 | 73,73,73,73                 | 0     |
| 85  | OHX  | 6     | 1906 | 7/7   | 0.99 | 0.09 | 71,71,71,71                 | 0     |
| 85  | OHX  | 1     | 3401 | 7/7   | 0.99 | 0.10 | 44,44,44,44                 | 0     |
| 85  | OHX  | 1     | 3424 | 7/7   | 0.99 | 0.07 | 76,76,76,76                 | 0     |
| 85  | OHX  | 1     | 3425 | 7/7   | 0.99 | 0.08 | 77,77,77,77                 | 0     |
| 85  | OHX  | 6     | 1910 | 7/7   | 0.99 | 0.08 | 73,73,73,73                 | 0     |
| 85  | OHX  | 6     | 1911 | 7/7   | 0.99 | 0.06 | 78,78,78,78                 | 0     |
| 85  | OHX  | 1     | 3402 | 7/7   | 0.99 | 0.07 | 53,53,53,53                 | 0     |
| 85  | OHX  | 1     | 3403 | 7/7   | 0.99 | 0.07 | 45,45,45,45                 | 0     |
| 85  | OHX  | 6     | 1914 | 7/7   | 0.99 | 0.07 | 83,83,83,83                 | 0     |
| 85  | OHX  | 1     | 3428 | 7/7   | 0.99 | 0.07 | 68,68,68,68                 | 0     |
| 85  | OHX  | 5     | 3485 | 7/7   | 0.99 | 0.09 | 75,75,75,75                 | 0     |
| 85  | OHX  | 6     | 1916 | 7/7   | 0.99 | 0.07 | 88,88,88,88                 | 0     |
| 85  | OHX  | 4     | 201  | 7/7   | 0.99 | 0.08 | 57,57,57,57                 | 0     |
| 85  | OHX  | 1     | 3429 | 7/7   | 0.99 | 0.06 | 72,72,72,72                 | 0     |
| 85  | OHX  | 8     | 201  | 7/7   | 0.99 | 0.08 | 57,57,57,57                 | 0     |
| 85  | OHX  | 8     | 202  | 7/7   | 0.99 | 0.09 | 74,74,74,74                 | 0     |
| 85  | OHX  | 5     | 3401 | 7/7   | 0.99 | 0.12 | 48,48,48,48                 | 0     |
| 85  | OHX  | 5     | 3402 | 7/7   | 0.99 | 0.11 | 43,43,43,43                 | 0     |
| 85  | OHX  | 5     | 3403 | 7/7   | 0.99 | 0.07 | 42,42,42,42                 | 0     |
| 85  | OHX  | 5     | 3492 | 7/7   | 0.99 | 0.06 | 73,73,73,73                 | 0     |
| 85  | OHX  | 5     | 3404 | 7/7   | 0.99 | 0.06 | 51,51,51,51                 | 0     |
| 85  | OHX  | 5     | 3494 | 7/7   | 0.99 | 0.12 | 86,86,86,86                 | 0     |
| 85  | OHX  | 5     | 3405 | 7/7   | 0.99 | 0.10 | 55,55,55,55                 | 0     |
| 85  | OHX  | 5     | 3407 | 7/7   | 0.99 | 0.06 | 59,59,59,59                 | 0     |
| 87  | ZN   | O7    | 101  | 1/1   | 0.99 | 0.06 | 45,45,45,45                 | 0     |
| 85  | OHX  | 5     | 3408 | 7/7   | 0.99 | 0.08 | 59,59,59,59                 | 0     |
| 87  | ZN   | Q3    | 501  | 1/1   | 0.99 | 0.04 | 68,68,68,68                 | 0     |
| 87  | ZN   | d6    | 500  | 1/1   | 0.99 | 0.04 | 71,71,71,71                 | 0     |
| 85  | OHX  | 5     | 3409 | 7/7   | 0.99 | 0.09 | 58,58,58,58                 | 0     |
| 85  | OHX  | 5     | 3410 | 7/7   | 0.99 | 0.09 | 59,59,59,59                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | OHX  | 5     | 3411 | 7/7   | 0.99 | 0.09 | 44,44,44,44                 | 0     |
| 87  | ZN   | o7    | 501  | 1/1   | 0.99 | 0.03 | 46,46,46,46                 | 0     |
| 87  | ZN   | q0    | 201  | 1/1   | 0.99 | 0.03 | 37,37,37,37                 | 0     |
| 85  | OHX  | 5     | 3412 | 7/7   | 0.99 | 0.12 | 68,68,68,68                 | 0     |
| 87  | ZN   | q3    | 501  | 1/1   | 0.99 | 0.03 | 65,65,65,65                 | 0     |
| 85  | OHX  | 5     | 3406 | 7/7   | 1.00 | 0.05 | 55,55,55,55                 | 0     |
| 87  | ZN   | Q0    | 201  | 1/1   | 1.00 | 0.02 | 49,49,49,49                 | 0     |
| 85  | OHX  | 1     | 3408 | 7/7   | 1.00 | 0.05 | 50,50,50,50                 | 0     |

## 5.5 Other polymers [i](#)

There are no such residues in this entry.