



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 28, 2026 – 04:17 PM UTC

PDB ID : 4U4Q / pdb\_00004u4q  
Title : Crystal structure of Homoharringtonine bound to the yeast 80S ribosome  
Authors : Garreau de Loubresse, N.; Prokhorova, I.; Yusupova, G.; Yusupov, M.  
Deposited on : 2014-07-24  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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 : **FAILED**  
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

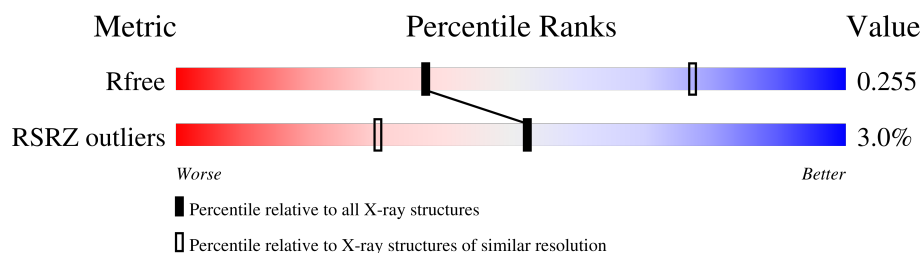
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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                      | 2672 (3.00-3.00)                                      |
| RSRZ outliers | 180081                      | 2671 (3.00-3.00)                                      |

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  | MG   | 1     | 3406 | -         | -        | -       | X                |
| 85  | MG   | 1     | 3494 | -         | -        | -       | X                |
| 85  | MG   | 1     | 3586 | -         | -        | -       | X                |
| 85  | MG   | 1     | 3594 | -         | -        | -       | X                |
| 85  | MG   | 1     | 3610 | -         | -        | -       | X                |
| 85  | MG   | 1     | 3654 | -         | -        | -       | X                |
| 85  | MG   | 1     | 3724 | -         | -        | -       | X                |
| 85  | MG   | 1     | 3809 | -         | -        | -       | X                |
| 85  | MG   | 1     | 3840 | -         | -        | -       | X                |
| 85  | MG   | 2     | 1901 | -         | -        | -       | X                |
| 85  | MG   | 2     | 1910 | -         | -        | -       | X                |
| 85  | MG   | 2     | 1914 | -         | -        | -       | X                |
| 85  | MG   | 2     | 1915 | -         | -        | -       | X                |
| 85  | MG   | 2     | 1917 | -         | -        | -       | X                |
| 85  | MG   | 2     | 1924 | -         | -        | -       | X                |
| 85  | MG   | 2     | 1926 | -         | -        | -       | X                |
| 85  | MG   | 2     | 1928 | -         | -        | -       | X                |
| 85  | MG   | 2     | 1931 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 85  | MG   | 2     | 1932 | -         | -        | -       | X                |
| 85  | MG   | 2     | 1938 | -         | -        | -       | X                |
| 85  | MG   | 2     | 1950 | -         | -        | -       | X                |
| 85  | MG   | 2     | 1951 | -         | -        | -       | X                |
| 85  | MG   | 2     | 1958 | -         | -        | -       | X                |
| 85  | MG   | 2     | 1959 | -         | -        | -       | X                |
| 85  | MG   | 2     | 1962 | -         | -        | -       | X                |
| 85  | MG   | 2     | 1968 | -         | -        | -       | X                |
| 85  | MG   | 2     | 1975 | -         | -        | -       | X                |
| 85  | MG   | 2     | 1978 | -         | -        | -       | X                |
| 85  | MG   | 2     | 1989 | -         | -        | -       | X                |
| 85  | MG   | 2     | 1990 | -         | -        | -       | X                |
| 85  | MG   | 2     | 1994 | -         | -        | -       | X                |
| 85  | MG   | 2     | 2008 | -         | -        | -       | X                |
| 85  | MG   | 2     | 2009 | -         | -        | -       | X                |
| 85  | MG   | 2     | 2016 | -         | -        | -       | X                |
| 85  | MG   | 2     | 2018 | -         | -        | -       | X                |
| 85  | MG   | 4     | 222  | -         | -        | -       | X                |
| 85  | MG   | 5     | 3588 | -         | -        | -       | X                |
| 85  | MG   | 5     | 3653 | -         | -        | -       | X                |
| 85  | MG   | 5     | 3884 | -         | -        | -       | X                |
| 85  | MG   | 5     | 3898 | -         | -        | -       | X                |
| 85  | MG   | 6     | 1922 | -         | -        | -       | X                |
| 85  | MG   | 6     | 1924 | -         | -        | -       | X                |
| 85  | MG   | 6     | 1930 | -         | -        | -       | X                |
| 85  | MG   | 6     | 1963 | -         | -        | -       | X                |
| 85  | MG   | 6     | 2016 | -         | -        | -       | X                |
| 85  | MG   | 6     | 2031 | -         | -        | -       | X                |
| 85  | MG   | 6     | 2037 | -         | -        | -       | X                |
| 85  | MG   | 6     | 2040 | -         | -        | -       | X                |
| 85  | MG   | 6     | 2041 | -         | -        | -       | X                |
| 85  | MG   | 6     | 2046 | -         | -        | -       | X                |
| 85  | MG   | n6    | 201  | -         | -        | -       | X                |
| 85  | MG   | o4    | 201  | -         | -        | -       | X                |

## 2 Entry composition [i](#)

There are 88 unique types of molecules in this entry. The entry contains 411245 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     | 1750     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 37283 | 16668 | 6591 | 12274 | 1750 |         |         |       |
| 1   | 6     | 1795     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 38238 | 17095 | 6758 | 12590 | 1795 |         |         |       |

- 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     |
|     |       |          | 1577  | 1014 | 278 | 283 | 2 |         |         |       |
| 2   | s0    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1583  | 1017 | 281 | 283 | 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     |
|     |       |          | 1799  | 1129 | 346 | 321 | 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   | S | 0       | 0       | 0     |
|     |       |          | 1481  | 951 | 265 | 265 |   |         |         |       |
| 9   | s7    | 186      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1491  | 957 | 267 | 267 |   |         |         |       |

- 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     |
|     |       |          | 773   | 500 | 126 | 145 | 2 |         |         |       |
| 12  | c0    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 762   | 491 | 125 | 144 | 2 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| C0    | 89      | ALA      | GLY    | conflict | UNP Q08745 |
| c0    | 89      | ALA      | GLY    | conflict | UNP Q08745 |

- Molecule 13 is a protein called 40S ribosomal protein S11-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | C1    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1214  | 775 | 230 | 206 | 3 |         |         |       |
| 13  | c1    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1168  | 747 | 221 | 197 | 3 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| C1    | 147     | ALA      | GLY    | conflict | UNP P0CX47 |
| c1    | 147     | ALA      | GLY    | conflict | UNP P0CX47 |

- 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 |         |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| C2    | 104     | ALA      | GLY    | conflict | UNP P48589 |
| C2    | 110     | ALA      | GLY    | conflict | UNP P48589 |
| c2    | 104     | ALA      | GLY    | conflict | UNP P48589 |
| c2    | 110     | ALA      | GLY    | conflict | UNP P48589 |

- 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 |  |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 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     |
|     |       |          | 926   | 577 | 177 | 170 | 2 |         |         |       |
| 19  | c7    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 906   | 563 | 174 | 167 | 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 |         |         |       |
| 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-B.

| 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     |
|     |       |          | 442   | 274 | 92 | 72 | 4 |         |         |       |
| 31  | d9    | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 442   | 274 | 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 |         |         |       |

- Molecule 33 is a protein called Ubiquitin-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  | 1544 | 419 | 470 | 8 |         |         |       |
| 34  | sR    | 318      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2442  | 1544 | 418 | 472 | 8 |         |         |       |

- Molecule 35 is a protein called 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     |
|     |       |          | 67376 | 30095 | 12145 | 21987 | 3149 |         |         |       |

- 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     |
|     |       |          | 1914  | 1191 | 388 | 334 | 1 |         |         |       |
| 39  | l2    | 252      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1912  | 1190 | 388 | 333 | 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     |
|     |       |          | 3075  | 1950 | 584 | 533 | 8 |         |         |       |
| 40  | l3    | 386      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3075  | 1950 | 584 | 533 | 8 |         |         |       |

- 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     |
|     |       |          | 2748  | 1729 | 522 | 494 | 3 |         |         |       |
| 41  | l4    | 361      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2748  | 1729 | 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  | l5    | 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  | l6    | 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  | l7    | 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     |
|     |       |          | 1804  | 1151 | 323 | 327 | 3 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 45  | l8    | 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  | l9    | 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     |
|     |       |          | 1705  | 1083 | 322 | 294 | 6 |         |         |       |
| 47  | m0    | 213      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1722  | 1094 | 325 | 297 | 6 |         |         |       |

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

| 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   | 0       | 0       | 0     |
|     |       |          | 1053  | 675 | 199 | 177 |         |         |       |
| 50  | m4    | 137      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1059  | 678 | 200 | 179 |         |         |       |

- 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 |         |         |       |
| 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   | 0       | 0       | 0     |
|     |       |          | 1420  | 882 | 281 | 257 |         |         |       |
| 53  | m7    | 155      | Total | C   | N   | O   | 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   | 0       | 0       | 0     |
|     |       |          | 1521  | 935 | 326 | 260 |         |         |       |
| 55  | m9    | 188      | Total | C   | N   | O   | 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     |
|     |       |          | 699   | 443 | 137 | 118 | 1 |         |         |       |
| 60  | n4    | 135      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1038  | 651 | 206 | 180 | 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     |
|     |       |          | 964   | 620 | 169 | 173 | 2 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 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     |
|     |       |          | 876   | 556 | 167 | 152 | 1 |         |         |       |
| 67  | o1    | 109      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 883   | 559 | 167 | 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 |         |         |       |
| 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     |
|     |       |          | 880   | 545 | 179 | 152 | 4 |         |         |       |
| 70  | o4    | 112      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 880   | 545 | 179 | 152 | 4 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| O4    | 121     | LYS      | -      | expression tag | UNP P87262 |
| o4    | 121     | LYS      | -      | expression tag | UNP P87262 |

- 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 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 71  | o5    | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 965   | 612 | 185 | 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     |
|     |       |          | 770   | 481 | 156 | 131 | 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     |
|     |       |          | 608   | 388 | 114 | 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 S30-A.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 80  | e0    | 62       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 491   | 309 | 101 | 80 | 1 |         |         |       |

- Molecule 81 is a protein called Unknown protein chain m2.

| 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 Unknown protein chain p1.

| 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 Unknown protein chain p2.

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

- Molecule 85 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 85  | 2     | 121      | Total | Mg  | 0       | 0       |
|     |       |          | 121   | 121 |         |         |
| 85  | S2    | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 85  | S4    | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 85  | S6    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 85  | S8    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 85  | C8    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 85  | D3    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 85  | 1     | 466      | Total | Mg  | 0       | 0       |
|     |       |          | 466   | 466 |         |         |
| 85  | 3     | 13       | Total | Mg  | 0       | 0       |
|     |       |          | 13    | 13  |         |         |
| 85  | 4     | 23       | Total | Mg  | 0       | 0       |
|     |       |          | 23    | 23  |         |         |
| 85  | L2    | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 85  | L3    | 3        | Total | Mg  | 0       | 0       |
|     |       |          | 3     | 3   |         |         |
| 85  | L4    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 85  | L5    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 85  | L6    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 85  | L7    | 4        | Total | Mg  | 0       | 0       |
|     |       |          | 4     | 4   |         |         |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 85  | L8    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | M0    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 85  | M1    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 85  | M3    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 85  | M5    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 85  | M6    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | M7    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 85  | M9    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 85  | N0    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | N3    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 85  | N5    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | N8    | 6        | Total<br>6   | Mg<br>6   | 0       | 0       |
| 85  | O1    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | O2    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | O3    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | O4    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | O7    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 85  | 6     | 147      | Total<br>147 | Mg<br>147 | 0       | 0       |
| 85  | s1    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | s4    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | s6    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

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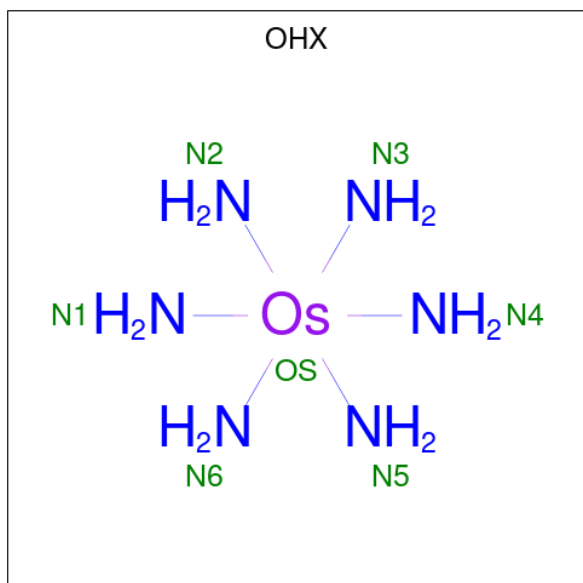
| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 85  | s8    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 85  | s9    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | c1    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | c7    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | c9    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 85  | d3    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 85  | d6    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | sM    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 85  | 5     | 500      | Total<br>500 | Mg<br>500 | 0       | 0       |
| 85  | 7     | 16       | Total<br>16  | Mg<br>16  | 0       | 0       |
| 85  | 8     | 15       | Total<br>15  | Mg<br>15  | 0       | 0       |
| 85  | l2    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 85  | l3    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 85  | l4    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | l5    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | l7    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 85  | l9    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | m0    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 85  | m1    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 85  | m6    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 85  | m7    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 85  | n0    | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 85  | n3    | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 85  | n6    | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 85  | n8    | 5        | Total<br>5 | Mg<br>5 | 0       | 0       |
| 85  | o1    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 85  | o3    | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 85  | o4    | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 85  | o7    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 85  | q0    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 85  | q1    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |

- Molecule 86 is osmium (III) hexammine (CCD ID: OHX) (formula:  $\text{H}_{12}\text{N}_6\text{Os}$ ).



| Mol | Chain | Residues | Atoms      |        |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|---------|
| 86  | 2     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 2     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | S8    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | C3    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | C5    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | C8    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | D9    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | SR    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
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| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
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| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
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| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
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| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
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| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
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| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
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| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 3     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms      |        |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|---------|
| 86  | 4     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 4     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 4     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 4     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 4     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 4     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 4     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 4     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 4     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 4     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 4     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 4     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 4     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 4     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 4     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | 4     | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | L3    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | L3    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | L4    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | M0    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | M5    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |
| 86  | M7    | 1        | Total<br>7 | N<br>6 | Os<br>1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | M7    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | M8    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | M9    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | N1    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | N9    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | O2    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | O3    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | O7    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | O7    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | O9    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | Q2    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 6     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | s1    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | s4    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | s8    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | s9    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | c3    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | c5    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | c8    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | d4    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | d9    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | sR    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
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| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 7     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 8     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 13    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 13    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 13    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 14    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 14    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | 15    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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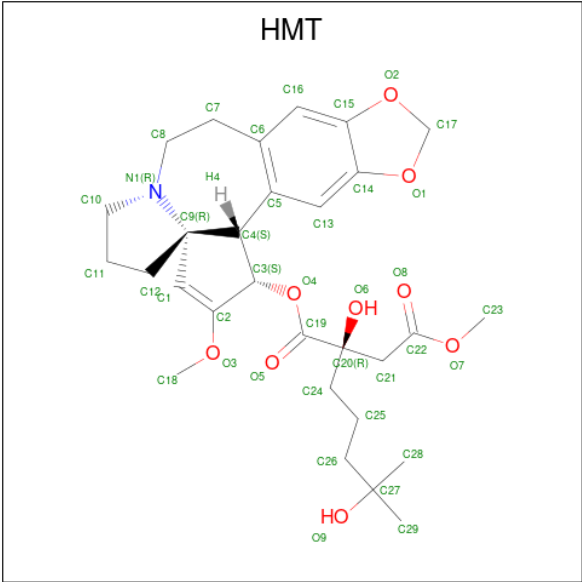
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| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 86  | l5    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | l5    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | l9    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | m0    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | m0    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | m1    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | m4    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | m5    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | m6    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | m7    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | m8    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | n3    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | n3    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | n9    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | o2    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | o3    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | o7    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | o9    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 86  | q2    | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

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

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

- Molecule 88 is (3beta)-O 3 -[(2R)-2,6-dihydroxy-2-(2-methoxy-2-oxoethyl)-6-methylheptano  
yl]cephalotaxine (CCD ID: HMT) (formula: C<sub>29</sub>H<sub>39</sub>NO<sub>9</sub>).



| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 88  | 1     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 39    | 29 | 1 | 9 |         |         |
| 88  | 5     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 39    | 29 | 1 | 9 |         |         |

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, $\alpha$ , $\beta$ , $\gamma$                | 436.25Å 286.92Å 303.84Å<br>90.00° 98.90° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 49.69 – 3.00<br>49.69 – 3.00                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.8 (49.69-3.00)<br>98.8 (49.69-3.00)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.34                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.24 (at 3.01Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (phenix.refine: dev_1702)                            | Depositor        |
| R, $R_{free}$                                                           | 0.208 , 0.255<br>0.210 , 0.255                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 29029 reflections (1.98%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 74.0                                                        | Xtriage          |
| Anisotropy                                                              | 0.180                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 66.8                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.93                                                        | EDS              |
| Total number of atoms                                                   | 411245                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 71.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% 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 2562 ligands modelled in this entry, 1427 are monoatomic - leaving 1135 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 | $\# Z  > 2$ |
| 86  | OHX  | 6     | 2110 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 1     | 4107 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 2     | 2173 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 1     | 3961 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 1     | 4138 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 6     | 2093 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 5     | 4239 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 6     | 2179 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 1     | 3975 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 1     | 3967 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 1     | 3951 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 1     | 3998 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 6     | 2149 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 1     | 4098 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 5     | 4072 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 5     | 4150 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 2     | 2145 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 1     | 3920 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 6     | 2095 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 2     | 2121 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 5     | 3917 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 1     | 3939 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 6     | 2068 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 2     | 2035 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 6     | 2071 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 1     | 3904 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 2     | 2101 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 1     | 4192 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 1     | 3968 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 1     | 3966 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 6     | 2133 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 5     | 4207 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 5     | 4020 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 5     | 4253 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 2     | 2139 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 1     | 4072 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 5     | 3954 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 5     | 3919 | -    | 0,6,6        | -    | -           | -           |      |             |
| 86  | OHX  | 2     | 2136 | -    | 0,6,6        | -    | -           | -           |      |             |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 6     | 2206 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 8     | 224  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | Q2    | 502  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | C3    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4112 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2163 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4216 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | C8    | 202  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3888 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4166 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2056 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2102 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2092 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4028 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4188 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3964 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | S8    | 302  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4109 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4060 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3918 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2061 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4118 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4049 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3989 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4126 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3980 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3982 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2081 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4105 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4233 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4212 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3896 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3913 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4125 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2152 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2167 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3889 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4137 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2045 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2123 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4068 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4241 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4214 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 6     | 2076 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | N9    | 101  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4073 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 8     | 217  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2158 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2068 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3878 | -    | 0,6,6        | -    | -        | -           |      |          |
| 88  | HMT  | 1     | 4217 | -    | 41,43,43     | 0.59 | 0        | 43,66,66    | 0.92 | 3 (6%)   |
| 86  | OHX  | o2    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4054 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4244 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4150 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2153 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4195 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3959 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4191 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3912 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3908 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4030 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2178 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2117 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4226 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 8     | 222  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 4     | 237  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2053 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2055 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4210 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2183 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3947 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4175 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4008 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4085 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4193 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2111 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2170 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2144 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3977 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4193 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4251 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2062 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4179 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4007 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4219 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 6     | 2147 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3951 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2061 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2149 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3925 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4044 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4018 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4023 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2082 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4227 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2187 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4119 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4188 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2095 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4190 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | m6    | 203  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2067 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4045 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4160 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4211 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3922 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4140 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 3     | 216  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4249 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2138 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2107 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4080 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4174 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4088 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3921 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3982 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2169 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 7     | 217  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4066 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4059 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3992 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4164 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4198 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3958 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2059 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4224 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4177 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2118 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 5     | 3956 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4137 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4029 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3906 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4003 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2056 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4122 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3940 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2153 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4053 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4074 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2092 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3953 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2109 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4099 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4010 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4202 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 4     | 224  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2066 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4206 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 8     | 218  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3997 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2074 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2159 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4130 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3926 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2115 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2164 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3973 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4069 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4126 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4218 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3952 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4171 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4200 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2165 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2111 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4157 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4230 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3969 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4026 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2152 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3919 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 1     | 3941 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2027 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4136 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3909 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2069 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4083 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | O7    | 104  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4175 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4232 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | m7    | 206  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3885 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2042 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4209 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3996 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4180 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4158 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2076 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2089 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4027 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4112 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4179 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3915 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2193 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2139 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 7     | 221  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2040 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2125 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2069 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2052 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2125 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2057 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2096 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2124 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4209 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3946 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4021 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3976 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | L3    | 405  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2022 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4061 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3879 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4203 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3963 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 5     | 4178 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 7     | 225  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4025 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2075 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2097 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | sR    | 401  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4187 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2053 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4146 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4118 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3971 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3980 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3960 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3911 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2094 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 7     | 218  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4037 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4079 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3917 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2162 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 8     | 227  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4003 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2130 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2147 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2159 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 4     | 227  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3943 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4205 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | n3    | 204  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 3     | 221  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2116 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4068 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2073 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2146 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 8     | 229  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3887 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4207 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 4     | 226  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2180 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4032 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3883 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3926 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 3     | 219  | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 5     | 4160 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3929 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4127 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4220 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2043 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2024 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2155 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4023 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2106 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3992 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4139 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3870 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4104 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2089 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2141 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4028 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4030 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4100 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2046 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4043 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4073 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4213 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4165 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | O7    | 105  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4212 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4086 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4096 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4064 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2044 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4055 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3929 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4158 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4204 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3989 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4027 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4153 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4236 | 86   | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2079 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2066 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3984 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2140 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2177 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4095 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 5     | 4181 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2048 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | o7    | 503  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4208 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4106 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4012 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2072 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4178 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4168 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2174 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4082 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4006 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4016 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3941 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4022 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4071 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3954 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4004 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2105 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2071 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2168 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2176 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4047 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2064 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3942 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3948 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4201 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4097 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2156 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2026 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4159 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4170 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4138 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | o3    | 203  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4116 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4215 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2096 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2161 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | C5    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4183 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2083 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4021 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2172 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 7     | 228  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2155 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4037 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4247 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2120 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4185 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2143 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4146 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | N1    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4182 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4031 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4108 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 3     | 224  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4186 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4047 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2054 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3998 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4214 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2146 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2087 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4002 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4086 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4076 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4011 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3920 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4061 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 7     | 220  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | m0    | 302  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4088 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2086 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | L3    | 404  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | s8    | 303  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4057 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2142 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | n9    | 101  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4008 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4139 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4035 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2058 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 14    | 403  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4142 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3984 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2098 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 5     | 4001 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4164 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4091 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3877 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2129 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4042 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3956 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3971 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4092 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3934 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4167 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4113 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3912 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4168 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4205 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4203 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2196 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3963 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4053 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3910 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3985 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2141 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2131 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4005 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4211 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 13    | 405  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3987 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 4     | 233  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4026 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4242 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2195 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3955 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2150 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2135 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3911 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2065 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4069 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4004 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4196 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2177 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 8     | 216  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2079 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | M9    | 203  | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 1     | 4020 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4093 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4250 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3978 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2175 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4154 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | s1    | 302  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3943 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4152 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3968 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4162 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | n3    | 203  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3952 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2130 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4032 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4077 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2063 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3983 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4128 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4084 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4121 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4062 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2085 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3905 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4189 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2078 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3892 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4051 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2116 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3964 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4131 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4006 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2023 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4128 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4173 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3997 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3985 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2188 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4108 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2200 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2105 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3981 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | M7    | 206  | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 2     | 2034 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2077 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2086 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4114 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2185 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2029 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4189 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4197 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4206 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 3     | 218  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3946 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3950 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3976 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4161 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2088 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4009 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 4     | 234  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2154 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | m5    | 301  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4038 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2103 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4019 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | s4    | 302  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2090 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3874 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3928 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4194 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4049 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2136 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4077 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4058 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2166 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2060 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3907 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4107 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | O9    | 101  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2070 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2203 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2119 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | l5    | 304  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4167 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2102 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3918 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 5     | 4098 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4221 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 8     | 230  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | m8    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3983 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2127 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4169 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2110 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 8     | 221  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2054 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4109 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2122 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2113 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2186 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2087 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2198 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | c5    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2050 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | q2    | 502  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4063 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4187 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4071 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4235 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4014 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4045 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4223 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4064 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2108 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3962 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2031 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3868 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3895 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3902 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3987 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2078 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4144 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4066 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4170 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2091 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3931 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2123 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4017 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2160 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 6     | 2197 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2064 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4177 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4217 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4156 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2182 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2156 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4106 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2093 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2167 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3873 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2179 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3960 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2161 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4094 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3921 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4036 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 4     | 228  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3955 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4145 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2135 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4114 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 3     | 220  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | c8    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | m1    | 203  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | c3    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3986 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2163 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3973 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3988 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4012 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4018 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3977 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4234 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4123 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2070 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2133 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2174 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4238 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | O2    | 202  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4094 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4124 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2074 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 5     | 4199 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 8     | 228  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4155 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2170 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4148 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3932 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2114 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3937 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3910 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3944 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2117 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 13    | 404  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3949 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2081 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4101 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3933 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3970 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3958 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4147 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4199 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4015 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4194 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4210 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4025 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4243 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2067 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4195 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4172 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4041 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4110 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4043 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | m0    | 303  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4117 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4135 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4186 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4082 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2107 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4038 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2103 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4070 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 3     | 223  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3999 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2175 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 1     | 4135 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3884 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4031 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4110 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2178 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4154 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 8     | 225  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4052 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4067 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4095 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4132 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2037 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2121 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4033 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2204 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4173 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4017 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4091 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4134 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2169 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 4     | 231  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4124 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4191 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2127 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2060 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4144 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2059 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4202 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2148 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2194 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2118 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3894 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4121 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2055 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2115 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2164 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 15    | 302  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 4     | 230  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3901 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4039 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3966 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | M5    | 303  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | M8    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 5     | 3940 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4136 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4147 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4182 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | d4    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4065 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4105 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4159 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4087 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3995 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4141 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | O3    | 202  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 7     | 227  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 3     | 214  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4103 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2049 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4013 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4245 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2134 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4198 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4192 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4055 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3893 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2072 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4093 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4149 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4036 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2144 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2165 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4092 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4248 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2091 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4196 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4120 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2126 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4081 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2039 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3897 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2057 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 7     | 226  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3979 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3965 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4131 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 15    | 303  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4046 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4129 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4024 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3914 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 3     | 217  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4029 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 4     | 238  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3902 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 4     | 225  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2157 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4111 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4084 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4090 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3915 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3957 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2128 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4040 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2181 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4119 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4190 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3975 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3950 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4089 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4010 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2124 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3900 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2109 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4081 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3969 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4042 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4102 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4143 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3981 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4087 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2097 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4078 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2082 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2112 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4050 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2080 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3927 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3991 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 5     | 4005 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 3     | 215  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | o9    | 101  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4019 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4185 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 7     | 223  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4172 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3959 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4041 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | l3    | 406  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3930 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4046 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4122 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2199 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4016 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3891 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4153 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4148 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2160 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2062 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | d9    | 102  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3945 | 86   | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2038 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3974 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4085 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2051 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2098 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4141 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4204 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2158 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4034 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3923 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4103 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2033 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2052 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2132 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4171 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4134 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4184 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3974 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4079 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3906 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3939 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 5     | 4116 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4215 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 14    | 402  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4000 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3905 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2129 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | s9    | 202  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2106 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2171 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2075 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4149 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2148 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 7     | 224  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3947 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4133 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4208 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4213 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 7     | 222  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4165 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3913 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4022 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3979 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3916 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4200 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2094 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3970 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4222 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4157 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4083 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2114 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 4     | 235  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2171 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4048 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3942 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2162 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 8     | 223  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4040 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4097 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2049 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3978 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2180 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4132 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4101 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 5     | 4111 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3924 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | L4    | 402  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3938 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4129 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4166 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3881 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4078 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3936 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3962 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4052 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2126 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4155 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3949 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2138 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4231 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2025 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2131 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2073 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3944 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2168 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4123 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4048 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3953 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4145 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | SR    | 401  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3957 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4216 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2128 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3899 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2028 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3876 | -    | 0,6,6        | -    | -        | -           |      |          |
| 88  | HMT  | 5     | 4255 | -    | 41,43,43     | 0.58 | 0        | 43,66,66    | 0.79 | 2 (4%)   |
| 86  | OHX  | 5     | 4015 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3937 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3990 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2143 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4075 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4143 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2151 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2202 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3909 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2205 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 5     | 4039 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4125 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 8     | 220  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2083 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3933 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3972 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3869 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4065 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2032 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4104 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2104 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3961 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4181 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3890 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2140 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3867 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4035 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3903 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3898 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4228 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4229 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2099 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4000 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2134 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3988 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4070 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2154 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4033 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4054 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2030 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | M0    | 304  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4051 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 8     | 219  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2047 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2176 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4067 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3935 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4056 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3904 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3880 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3907 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4162 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 3     | 222  | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | M7    | 207  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3965 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4050 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2058 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3901 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4225 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3886 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2100 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4197 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4117 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 8     | 226  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3995 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2132 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4240 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2145 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4156 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2201 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2172 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3994 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4007 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4113 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4174 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 4     | 236  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2137 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4254 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4044 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2120 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2157 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3922 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4062 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4127 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2190 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4176 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3916 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3999 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2063 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4013 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4115 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3996 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4163 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4180 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3936 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3990 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 6     | 2080 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2108 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3994 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3948 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3934 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 7     | 219  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2036 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2112 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4183 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4161 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 19    | 202  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4252 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2099 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4090 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2173 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3927 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3924 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4060 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2085 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3945 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2088 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | m4    | 201  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4024 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4201 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3914 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4074 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4099 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4059 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4151 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4169 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4176 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2142 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4089 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2051 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3908 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4075 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4002 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4076 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4115 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4096 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4130 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 4     | 232  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4102 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 6     | 2101 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2100 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4151 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3930 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3967 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4009 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3993 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4014 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 4     | 229  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4133 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2090 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3871 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3932 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4011 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2065 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4001 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4246 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3872 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2166 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3991 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3972 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4063 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2137 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4058 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4163 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4080 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2041 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2113 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2151 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2104 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4142 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4152 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3925 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2050 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2191 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2119 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3875 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3935 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4100 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3903 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4057 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2084 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2192 | -    | 0,6,6        | -    | -        | -           |      |          |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | OHX  | 2     | 2150 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3931 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2048 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4056 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2084 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3993 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4184 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3882 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4237 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 4120 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3923 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2189 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2184 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3928 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 5     | 3986 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 3938 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4034 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 2     | 2122 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 1     | 4140 | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | D9    | 102  | -    | 0,6,6        | -    | -        | -           |      |          |
| 86  | OHX  | 6     | 2077 | -    | 0,6,6        | -    | -        | -           |      |          |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 88  | HMT  | 5     | 4255 | -    | -       | 4/27/74/74 | 0/5/5/5 |
| 88  | HMT  | 1     | 4217 | -    | -       | 7/27/74/74 | 0/5/5/5 |

There are no bond length outliers.

All (5) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 88  | 1     | 4217 | HMT  | C9-C4-C5    | 3.59  | 121.79      | 115.96   |
| 88  | 5     | 4255 | HMT  | C25-C26-C27 | -2.81 | 106.74      | 116.07   |
| 88  | 1     | 4217 | HMT  | C20-C21-C22 | 2.32  | 121.06      | 114.09   |
| 88  | 5     | 4255 | HMT  | C18-O3-C2   | -2.28 | 112.77      | 116.53   |
| 88  | 1     | 4217 | HMT  | C8-C7-C6    | -2.08 | 109.13      | 114.37   |

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

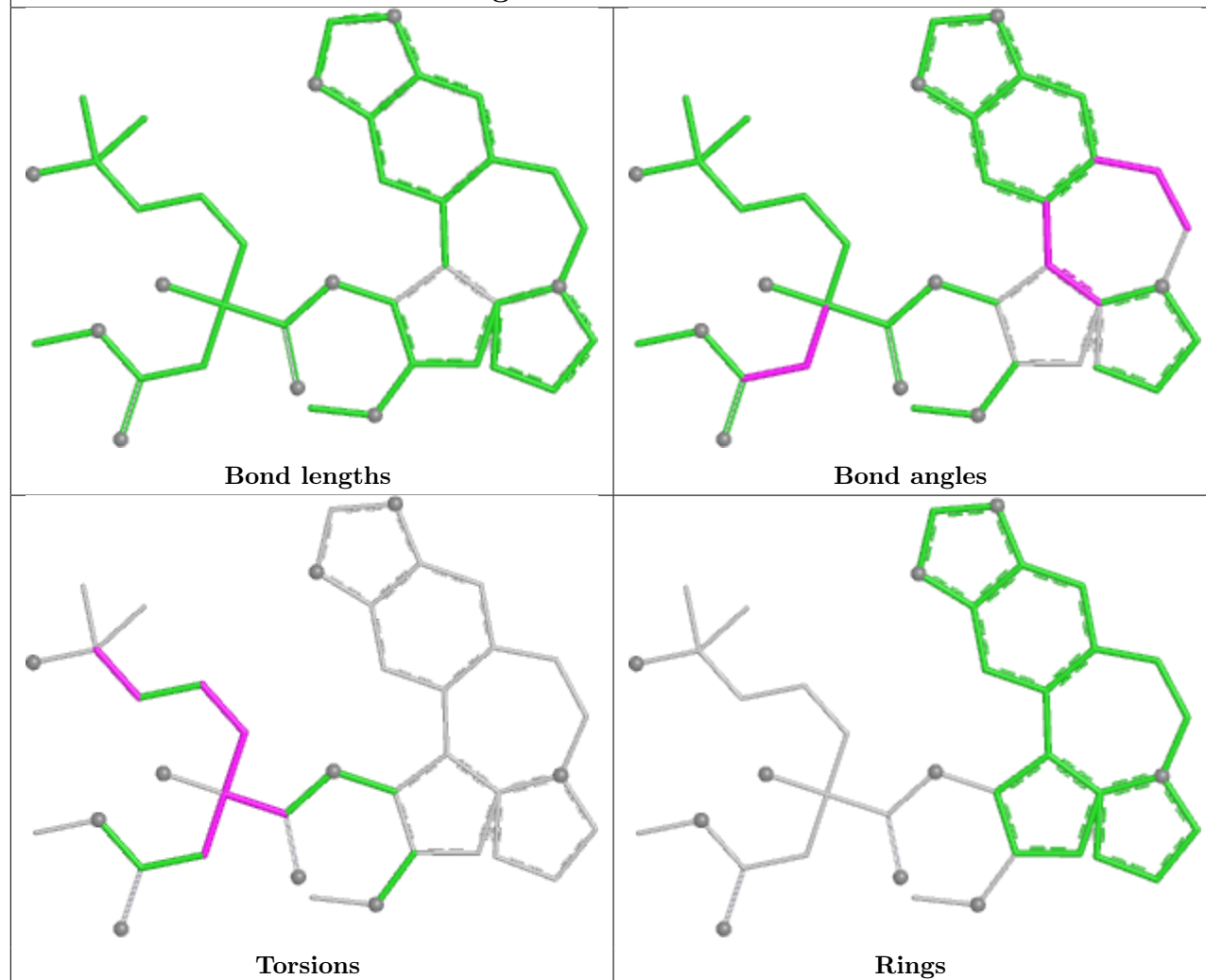
| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 88  | 1     | 4217 | HMT  | C19-C20-C24-C25 |
| 88  | 1     | 4217 | HMT  | C21-C20-C24-C25 |
| 88  | 1     | 4217 | HMT  | O6-C20-C24-C25  |
| 88  | 5     | 4255 | HMT  | C25-C26-C27-O9  |
| 88  | 1     | 4217 | HMT  | C20-C24-C25-C26 |

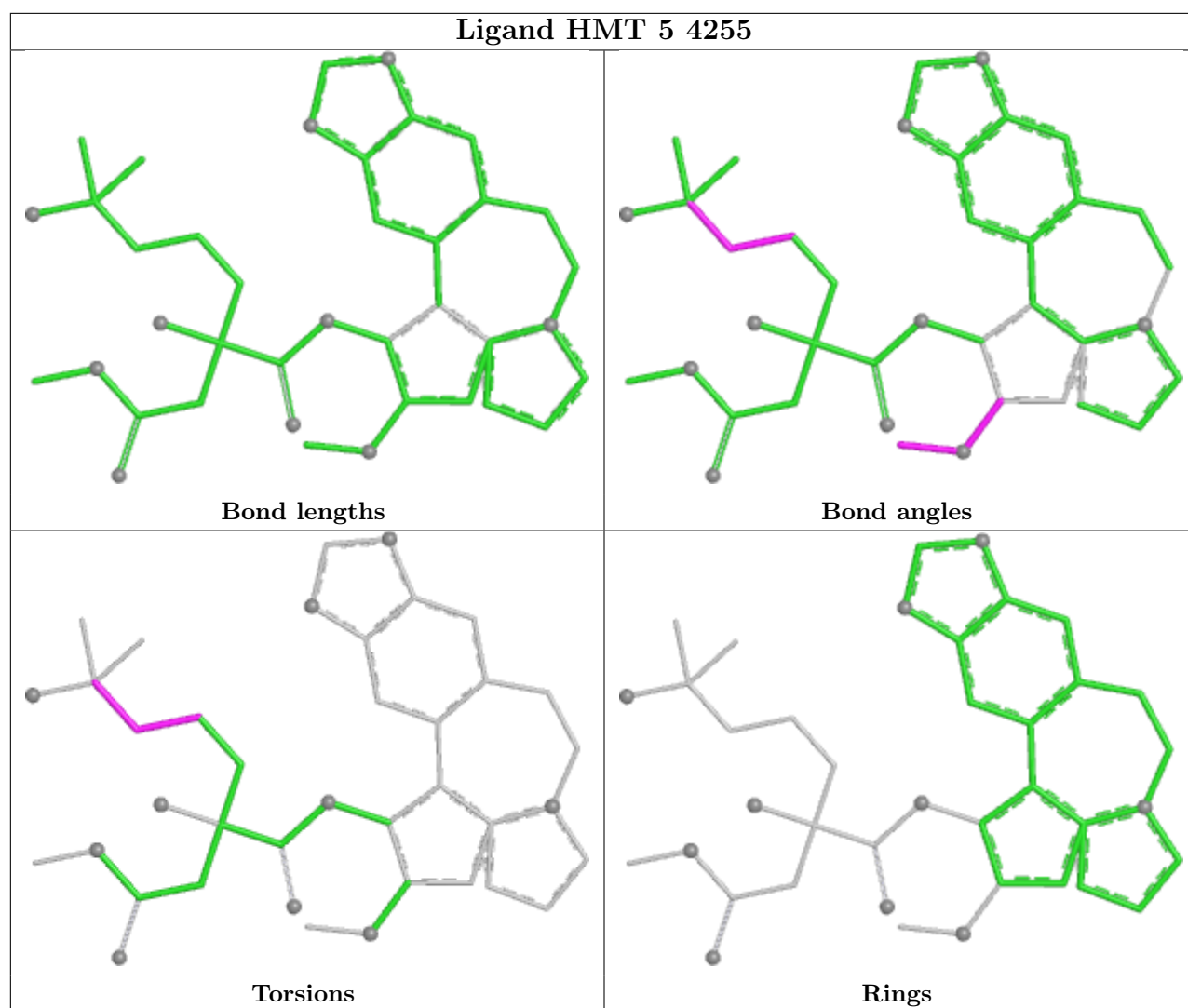
There are no ring outliers.

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.

## Ligand HMT 1 4217





#### 4.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 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(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------|----|----|-----------------------|-------|
| 1   | 2     | 1750/1800 (97%) | 0.26   | 56 (3%)  | 50 | 29 | 52, 89, 160, 248      | 0     |
| 1   | 6     | 1795/1800 (99%) | 0.12   | 62 (3%)  | 47 | 27 | 38, 74, 169, 247      | 0     |
| 2   | S0    | 206/251 (82%)   | 0.70   | 14 (6%)  | 23 | 12 | 92, 106, 118, 143     | 0     |
| 2   | s0    | 206/251 (82%)   | 0.26   | 5 (2%)   | 59 | 36 | 71, 90, 103, 116      | 0     |
| 3   | S1    | 214/254 (84%)   | 1.05   | 31 (14%) | 6  | 3  | 99, 126, 152, 160     | 0     |
| 3   | s1    | 216/254 (85%)   | 0.25   | 5 (2%)   | 61 | 38 | 68, 82, 101, 110      | 0     |
| 4   | S2    | 217/253 (85%)   | 0.24   | 3 (1%)   | 73 | 51 | 71, 86, 102, 120      | 0     |
| 4   | s2    | 217/253 (85%)   | 0.18   | 6 (2%)   | 55 | 32 | 54, 70, 86, 97        | 0     |
| 5   | S3    | 223/239 (93%)   | 0.39   | 9 (4%)   | 42 | 23 | 76, 91, 120, 132      | 0     |
| 5   | s3    | 223/239 (93%)   | 0.45   | 6 (2%)   | 56 | 33 | 73, 104, 126, 134     | 0     |
| 6   | S4    | 260/260 (100%)  | 0.32   | 5 (1%)   | 66 | 43 | 63, 89, 101, 126      | 0     |
| 6   | s4    | 260/260 (100%)  | 0.04   | 3 (1%)   | 76 | 55 | 49, 73, 86, 113       | 0     |
| 7   | S5    | 206/224 (91%)   | 0.68   | 10 (4%)  | 35 | 18 | 99, 117, 129, 138     | 0     |
| 7   | s5    | 206/224 (91%)   | 0.44   | 5 (2%)   | 59 | 36 | 69, 91, 111, 124      | 0     |
| 8   | S6    | 226/236 (95%)   | 0.56   | 14 (6%)  | 26 | 14 | 64, 99, 119, 140      | 0     |
| 8   | s6    | 218/236 (92%)   | 0.14   | 1 (0%)   | 87 | 72 | 49, 78, 100, 121      | 0     |
| 9   | S7    | 184/189 (97%)   | 0.45   | 4 (2%)   | 62 | 39 | 86, 113, 137, 144     | 0     |
| 9   | s7    | 186/189 (98%)   | 0.49   | 8 (4%)   | 40 | 21 | 68, 100, 132, 138     | 0     |
| 10  | S8    | 188/200 (94%)   | 0.36   | 5 (2%)   | 56 | 33 | 56, 71, 111, 124      | 0     |
| 10  | s8    | 188/200 (94%)   | 0.20   | 5 (2%)   | 56 | 33 | 43, 64, 111, 126      | 0     |
| 11  | S9    | 185/196 (94%)   | 0.61   | 11 (5%)  | 28 | 14 | 83, 97, 132, 163      | 0     |
| 11  | s9    | 185/196 (94%)   | 0.33   | 10 (5%)  | 31 | 16 | 64, 77, 109, 140      | 0     |
| 12  | C0    | 96/105 (91%)    | 0.79   | 10 (10%) | 11 | 6  | 83, 104, 139, 152     | 0     |
| 12  | c0    | 96/105 (91%)    | 1.26   | 16 (16%) | 4  | 3  | 99, 134, 150, 170     | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 13  | C1    | 155/155 (100%) | 0.41   | 11 (7%) 22 11 | 60, 70, 114, 119      | 0     |
| 13  | c1    | 146/155 (94%)  | 0.27   | 8 (5%) 30 15  | 47, 62, 94, 115       | 0     |
| 14  | C2    | 124/142 (87%)  | 0.83   | 10 (8%) 18 9  | 129, 139, 155, 163    | 0     |
| 14  | c2    | 124/142 (87%)  | 1.39   | 24 (19%) 3 2  | 178, 189, 204, 208    | 0     |
| 15  | C3    | 150/150 (100%) | 0.46   | 8 (5%) 32 16  | 67, 87, 100, 107      | 0     |
| 15  | c3    | 150/150 (100%) | 0.10   | 1 (0%) 84 66  | 54, 69, 86, 97        | 0     |
| 16  | C4    | 127/136 (93%)  | 0.94   | 11 (8%) 16 8  | 69, 122, 136, 138     | 0     |
| 16  | c4    | 128/136 (94%)  | 0.31   | 4 (3%) 51 30  | 48, 82, 90, 97        | 0     |
| 17  | C5    | 124/141 (87%)  | 0.54   | 4 (3%) 50 29  | 80, 96, 129, 145      | 0     |
| 17  | c5    | 135/141 (95%)  | 0.75   | 13 (9%) 13 7  | 77, 99, 117, 129      | 0     |
| 18  | C6    | 141/142 (99%)  | 0.74   | 9 (6%) 25 13  | 82, 111, 116, 119     | 0     |
| 18  | c6    | 142/142 (100%) | 0.62   | 9 (6%) 26 13  | 64, 85, 102, 124      | 0     |
| 19  | C7    | 120/136 (88%)  | 1.07   | 17 (14%) 6 4  | 94, 109, 130, 132     | 0     |
| 19  | c7    | 117/136 (86%)  | 0.79   | 14 (11%) 9 5  | 78, 92, 112, 116      | 0     |
| 20  | C8    | 145/145 (100%) | 0.61   | 10 (6%) 23 12 | 78, 108, 129, 137     | 0     |
| 20  | c8    | 145/145 (100%) | 0.31   | 3 (2%) 63 40  | 68, 88, 110, 122      | 0     |
| 21  | C9    | 143/143 (100%) | 0.78   | 14 (9%) 13 7  | 92, 107, 122, 133     | 0     |
| 21  | c9    | 143/143 (100%) | 0.20   | 1 (0%) 84 66  | 64, 77, 94, 114       | 0     |
| 22  | D0    | 107/120 (89%)  | 0.88   | 11 (10%) 12 6 | 74, 108, 136, 139     | 0     |
| 22  | d0    | 110/120 (91%)  | 0.85   | 9 (8%) 17 9   | 69, 105, 138, 148     | 0     |
| 23  | D1    | 87/87 (100%)   | 0.24   | 2 (2%) 61 38  | 89, 95, 111, 121      | 0     |
| 23  | d1    | 87/87 (100%)   | -0.06  | 2 (2%) 61 38  | 68, 76, 97, 107       | 0     |
| 24  | D2    | 129/129 (100%) | 0.21   | 2 (1%) 70 47  | 70, 81, 90, 101       | 0     |
| 24  | d2    | 129/129 (100%) | 0.02   | 1 (0%) 82 64  | 52, 63, 70, 81        | 0     |
| 25  | D3    | 144/144 (100%) | 0.24   | 5 (3%) 47 27  | 58, 63, 74, 86        | 0     |
| 25  | d3    | 144/144 (100%) | -0.12  | 3 (2%) 63 40  | 43, 48, 60, 73        | 0     |
| 26  | D4    | 134/134 (100%) | 0.47   | 7 (5%) 33 17  | 75, 102, 116, 122     | 0     |
| 26  | d4    | 134/134 (100%) | 0.26   | 5 (3%) 45 25  | 57, 81, 95, 115       | 0     |
| 27  | D5    | 70/107 (65%)   | 0.69   | 5 (7%) 22 11  | 115, 129, 136, 137    | 0     |
| 27  | d5    | 69/107 (64%)   | 0.47   | 3 (4%) 40 21  | 83, 106, 118, 121     | 0     |
| 28  | D6    | 97/97 (100%)   | 0.66   | 5 (5%) 33 17  | 75, 90, 138, 143      | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 28  | d6    | 97/97 (100%)    | 0.30   | 2 (2%) 63 40  | 53, 66, 93, 101       | 0     |
| 29  | D7    | 81/81 (100%)    | 0.65   | 4 (4%) 35 18  | 84, 98, 125, 130      | 0     |
| 29  | d7    | 81/81 (100%)    | 0.17   | 0 100 100     | 64, 82, 120, 124      | 0     |
| 30  | D8    | 63/66 (95%)     | 0.74   | 2 (3%) 50 29  | 111, 125, 136, 141    | 0     |
| 30  | d8    | 63/66 (95%)     | 0.54   | 1 (1%) 70 47  | 88, 103, 116, 125     | 0     |
| 31  | D9    | 53/55 (96%)     | 0.65   | 6 (11%) 10 6  | 77, 82, 102, 109      | 0     |
| 31  | d9    | 53/55 (96%)     | 0.99   | 8 (15%) 5 3   | 70, 82, 124, 134      | 0     |
| 32  | E0    | 60/60 (100%)    | 0.45   | 3 (5%) 34 18  | 62, 95, 131, 137      | 0     |
| 33  | E1    | 71/76 (93%)     | 1.16   | 12 (16%) 4 3  | 99, 126, 138, 141     | 0     |
| 33  | e1    | 76/76 (100%)    | 1.75   | 24 (31%) 1 1  | 146, 165, 178, 179    | 0     |
| 34  | SR    | 318/318 (100%)  | 0.42   | 6 (1%) 66 43  | 66, 115, 133, 150     | 0     |
| 34  | sR    | 318/318 (100%)  | 0.57   | 22 (6%) 23 12 | 97, 115, 131, 147     | 0     |
| 35  | SM    | 159/273 (58%)   | 0.87   | 22 (13%) 6 4  | 62, 88, 139, 144      | 0     |
| 35  | sM    | 104/273 (38%)   | 0.84   | 11 (10%) 11 6 | 63, 100, 182, 188     | 0     |
| 36  | 1     | 3149/3396 (92%) | -0.28  | 74 (2%) 61 38 | 25, 49, 127, 239      | 0     |
| 36  | 5     | 3150/3396 (92%) | -0.34  | 67 (2%) 63 40 | 24, 47, 115, 209      | 0     |
| 37  | 3     | 121/121 (100%)  | -0.24  | 1 (0%) 82 64  | 38, 68, 85, 89        | 0     |
| 37  | 7     | 121/121 (100%)  | -0.54  | 1 (0%) 82 64  | 31, 50, 63, 72        | 0     |
| 38  | 4     | 158/158 (100%)  | -0.40  | 2 (1%) 75 53  | 32, 51, 91, 126       | 0     |
| 38  | 8     | 158/158 (100%)  | -0.28  | 5 (3%) 50 29  | 35, 57, 96, 117       | 0     |
| 39  | L2    | 252/253 (99%)   | -0.15  | 3 (1%) 76 55  | 32, 47, 64, 74        | 0     |
| 39  | l2    | 252/253 (99%)   | 0.06   | 8 (3%) 50 29  | 32, 50, 67, 78        | 0     |
| 40  | L3    | 386/386 (100%)  | -0.14  | 1 (0%) 90 79  | 30, 54, 68, 104       | 0     |
| 40  | l3    | 386/386 (100%)  | -0.43  | 2 (0%) 87 72  | 24, 39, 52, 83        | 0     |
| 41  | L4    | 361/361 (100%)  | -0.29  | 2 (0%) 85 69  | 27, 42, 60, 69        | 0     |
| 41  | l4    | 361/361 (100%)  | -0.26  | 1 (0%) 90 79  | 28, 47, 66, 79        | 0     |
| 42  | L5    | 296/296 (100%)  | 0.15   | 3 (1%) 79 59  | 49, 74, 93, 118       | 0     |
| 42  | l5    | 294/296 (99%)   | -0.09  | 2 (0%) 84 66  | 38, 54, 81, 121       | 0     |
| 43  | L6    | 156/175 (89%)   | -0.24  | 0 100 100     | 38, 45, 66, 87        | 0     |
| 43  | l6    | 157/175 (89%)   | -0.15  | 1 (0%) 85 69  | 39, 46, 67, 78        | 0     |
| 44  | L7    | 222/243 (91%)   | -0.34  | 0 100 100     | 31, 39, 68, 103       | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 44  | l7    | 223/243 (91%)  | -0.38  | 0 100 100     | 29, 36, 72, 113       | 0     |
| 45  | L8    | 233/255 (91%)  | 0.17   | 2 (0%) 81 61  | 55, 69, 102, 116      | 0     |
| 45  | l8    | 231/255 (90%)  | 0.37   | 14 (6%) 27 14 | 66, 79, 105, 117      | 0     |
| 46  | L9    | 191/191 (100%) | -0.05  | 0 100 100     | 49, 61, 77, 93        | 0     |
| 46  | l9    | 191/191 (100%) | -0.26  | 1 (0%) 87 72  | 33, 43, 61, 74        | 0     |
| 47  | M0    | 211/220 (95%)  | -0.11  | 3 (1%) 73 51  | 37, 50, 87, 99        | 0     |
| 47  | m0    | 213/220 (96%)  | -0.08  | 6 (2%) 55 32  | 33, 54, 79, 97        | 0     |
| 48  | M1    | 169/173 (97%)  | 0.30   | 4 (2%) 59 36  | 60, 79, 92, 98        | 0     |
| 48  | m1    | 169/173 (97%)  | -0.14  | 1 (0%) 85 69  | 41, 60, 72, 83        | 0     |
| 49  | M3    | 193/198 (97%)  | -0.10  | 2 (1%) 79 59  | 30, 51, 91, 119       | 0     |
| 49  | m3    | 194/198 (97%)  | -0.05  | 1 (0%) 87 72  | 38, 59, 97, 120       | 0     |
| 50  | M4    | 136/137 (99%)  | -0.25  | 1 (0%) 84 66  | 41, 49, 62, 73        | 0     |
| 50  | m4    | 137/137 (100%) | -0.32  | 2 (1%) 72 49  | 36, 41, 60, 71        | 0     |
| 51  | M5    | 203/203 (100%) | -0.05  | 0 100 100     | 30, 45, 55, 61        | 0     |
| 51  | m5    | 203/203 (100%) | 0.15   | 4 (1%) 65 41  | 37, 53, 64, 69        | 0     |
| 52  | M6    | 197/198 (99%)  | -0.13  | 2 (1%) 79 59  | 30, 40, 57, 62        | 0     |
| 52  | m6    | 197/198 (99%)  | -0.41  | 0 100 100     | 25, 30, 57, 63        | 0     |
| 53  | M7    | 183/183 (100%) | 0.15   | 13 (7%) 22 11 | 34, 42, 96, 127       | 0     |
| 53  | m7    | 155/183 (84%)  | -0.33  | 0 100 100     | 29, 36, 49, 79        | 0     |
| 54  | M8    | 185/185 (100%) | -0.11  | 2 (1%) 78 57  | 33, 42, 57, 72        | 0     |
| 54  | m8    | 185/185 (100%) | -0.22  | 0 100 100     | 36, 47, 55, 61        | 0     |
| 55  | M9    | 188/188 (100%) | 0.31   | 7 (3%) 45 25  | 50, 66, 148, 158      | 0     |
| 55  | m9    | 188/188 (100%) | 0.13   | 1 (0%) 87 72  | 44, 57, 127, 137      | 0     |
| 56  | N0    | 172/172 (100%) | -0.17  | 2 (1%) 76 55  | 40, 47, 63, 70        | 0     |
| 56  | n0    | 172/172 (100%) | -0.28  | 4 (2%) 61 38  | 30, 38, 49, 60        | 0     |
| 57  | N1    | 159/159 (100%) | -0.09  | 2 (1%) 75 53  | 35, 47, 89, 97        | 0     |
| 57  | n1    | 159/159 (100%) | -0.20  | 0 100 100     | 32, 39, 77, 84        | 0     |
| 58  | N2    | 100/120 (83%)  | 0.35   | 2 (2%) 65 41  | 83, 96, 110, 122      | 0     |
| 58  | n2    | 98/120 (81%)   | 0.37   | 2 (2%) 65 41  | 70, 83, 93, 100       | 0     |
| 59  | N3    | 136/136 (100%) | -0.21  | 1 (0%) 84 66  | 37, 48, 60, 69        | 0     |
| 59  | n3    | 136/136 (100%) | -0.36  | 2 (1%) 72 49  | 26, 37, 52, 56        | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2  |         | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|----------|---------|-----------------------|-------|
| 60  | N4    | 98/155 (63%)   | 0.62   | 11 (11%) | 10 6    | 48, 63, 145, 148      | 0     |
| 60  | n4    | 135/155 (87%)  | 0.33   | 10 (7%)  | 20 10   | 38, 85, 117, 135      | 0     |
| 61  | N5    | 121/141 (85%)  | 0.04   | 2 (1%)   | 69 45   | 43, 58, 73, 103       | 0     |
| 61  | n5    | 120/141 (85%)  | 0.02   | 2 (1%)   | 69 45   | 45, 61, 79, 88        | 0     |
| 62  | N6    | 126/126 (100%) | -0.11  | 1 (0%)   | 82 64   | 39, 51, 63, 73        | 0     |
| 62  | n6    | 126/126 (100%) | 0.10   | 2 (1%)   | 70 47   | 44, 56, 72, 80        | 0     |
| 63  | N7    | 135/135 (100%) | 0.15   | 0        | 100 100 | 68, 80, 96, 105       | 0     |
| 63  | n7    | 135/135 (100%) | 0.37   | 3 (2%)   | 62 39   | 72, 86, 107, 114      | 0     |
| 64  | N8    | 148/148 (100%) | -0.21  | 0        | 100 100 | 26, 44, 65, 76        | 0     |
| 64  | n8    | 148/148 (100%) | -0.24  | 0        | 100 100 | 28, 49, 68, 73        | 0     |
| 65  | N9    | 58/58 (100%)   | 0.10   | 4 (6%)   | 23 12   | 35, 52, 98, 114       | 0     |
| 65  | n9    | 58/58 (100%)   | 0.10   | 3 (5%)   | 33 17   | 31, 48, 73, 84        | 0     |
| 66  | O0    | 97/104 (93%)   | 0.09   | 3 (3%)   | 51 30   | 67, 75, 94, 100       | 0     |
| 66  | o0    | 100/104 (96%)  | 0.10   | 2 (2%)   | 65 41   | 65, 77, 99, 106       | 0     |
| 67  | O1    | 109/112 (97%)  | 0.10   | 1 (0%)   | 81 61   | 48, 61, 92, 105       | 0     |
| 67  | o1    | 109/112 (97%)  | -0.01  | 1 (0%)   | 81 61   | 38, 48, 82, 102       | 0     |
| 68  | O2    | 127/129 (98%)  | -0.23  | 2 (1%)   | 70 47   | 25, 39, 50, 65        | 0     |
| 68  | o2    | 127/129 (98%)  | -0.18  | 3 (2%)   | 59 36   | 26, 44, 57, 73        | 0     |
| 69  | O3    | 106/106 (100%) | -0.25  | 0        | 100 100 | 31, 37, 59, 68        | 0     |
| 69  | o3    | 106/106 (100%) | -0.37  | 0        | 100 100 | 29, 35, 59, 72        | 0     |
| 70  | O4    | 112/120 (93%)  | 0.35   | 2 (1%)   | 67 44   | 45, 64, 100, 112      | 0     |
| 70  | o4    | 112/120 (93%)  | 0.31   | 2 (1%)   | 67 44   | 45, 65, 110, 119      | 0     |
| 71  | O5    | 119/119 (100%) | 0.01   | 3 (2%)   | 58 35   | 43, 60, 68, 71        | 0     |
| 71  | o5    | 119/119 (100%) | 0.06   | 3 (2%)   | 58 35   | 50, 64, 76, 83        | 0     |
| 72  | O6    | 99/99 (100%)   | 0.01   | 2 (2%)   | 65 41   | 49, 59, 89, 103       | 0     |
| 72  | o6    | 99/99 (100%)   | 0.17   | 2 (2%)   | 65 41   | 53, 68, 91, 110       | 0     |
| 73  | O7    | 87/87 (100%)   | -0.14  | 2 (2%)   | 61 38   | 32, 37, 60, 85        | 0     |
| 73  | o7    | 87/87 (100%)   | 0.02   | 2 (2%)   | 61 38   | 33, 41, 70, 107       | 0     |
| 74  | O8    | 77/77 (100%)   | 0.29   | 2 (2%)   | 57 34   | 72, 82, 104, 109      | 0     |
| 74  | o8    | 77/77 (100%)   | 0.23   | 1 (1%)   | 75 53   | 73, 85, 103, 106      | 0     |
| 75  | O9    | 50/50 (100%)   | 0.02   | 2 (4%)   | 42 23   | 41, 44, 53, 57        | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2         | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 75  | o9    | 50/50 (100%)      | -0.11  | 0 100 100       | 43, 46, 58, 64        | 0     |
| 76  | Q0    | 52/52 (100%)      | 0.06   | 0 100 100       | 43, 50, 62, 73        | 0     |
| 76  | q0    | 52/52 (100%)      | -0.16  | 0 100 100       | 30, 34, 46, 51        | 0     |
| 77  | Q1    | 25/25 (100%)      | 0.23   | 0 100 100       | 54, 56, 59, 61        | 0     |
| 77  | q1    | 25/25 (100%)      | 0.16   | 0 100 100       | 41, 43, 55, 63        | 0     |
| 78  | Q2    | 105/105 (100%)    | 0.03   | 4 (3%) 44 24    | 35, 52, 72, 100       | 0     |
| 78  | q2    | 105/105 (100%)    | -0.07  | 2 (1%) 66 43    | 38, 50, 69, 93        | 0     |
| 79  | Q3    | 91/91 (100%)      | -0.22  | 0 100 100       | 40, 50, 68, 81        | 0     |
| 79  | q3    | 91/91 (100%)      | -0.16  | 1 (1%) 78 57    | 36, 50, 65, 75        | 0     |
| 80  | e0    | 62/62 (100%)      | 0.24   | 2 (3%) 50 29    | 52, 78, 106, 115      | 0     |
| 81  | m2    | 0/160             | -      | -               | -                     | -     |
| 82  | p0    | 143/311 (45%)     | 0.87   | 9 (6%) 26 13    | 84, 102, 180, 188     | 0     |
| 83  | p1    | 0/47              | -      | -               | -                     | -     |
| 84  | p2    | 0/46              | -      | -               | -                     | -     |
| All | All   | 33063/35346 (93%) | 0.08   | 1003 (3%) 52 30 | 24, 65, 129, 248      | 0     |

The worst 5 of 1003 RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 36  | 1     | 1349 | G    | 7.3  |
| 7   | S5    | 37   | GLN  | 7.0  |
| 3   | S1    | 156  | ALA  | 6.4  |
| 5   | S3    | 88   | ALA  | 6.4  |
| 47  | m0    | 111  | LEU  | 6.2  |

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

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

## 5.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.4 Ligands ⓘ

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

| Mol | Type | Chain | Res  | Atoms | RSCC  | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|----------------------------|-------|
| 85  | MG   | 1     | 3809 | 1/1   | -0.74 | 0.44 | 193,193,193,193            | 0     |
| 85  | MG   | 6     | 2041 | 1/1   | -0.34 | 0.51 | 110,110,110,110            | 0     |
| 85  | MG   | 1     | 3406 | 1/1   | -0.04 | 0.42 | 116,116,116,116            | 0     |
| 85  | MG   | 2     | 1968 | 1/1   | -0.03 | 0.46 | 123,123,123,123            | 0     |
| 85  | MG   | 1     | 3819 | 1/1   | 0.07  | 0.40 | 119,119,119,119            | 0     |
| 85  | MG   | 2     | 1975 | 1/1   | 0.22  | 0.59 | 87,87,87,87                | 0     |
| 85  | MG   | 6     | 1924 | 1/1   | 0.28  | 0.53 | 97,97,97,97                | 0     |
| 85  | MG   | 5     | 3773 | 1/1   | 0.31  | 0.33 | 102,102,102,102            | 0     |
| 85  | MG   | 2     | 2001 | 1/1   | 0.35  | 0.40 | 119,119,119,119            | 0     |
| 85  | MG   | 6     | 2016 | 1/1   | 0.36  | 0.40 | 133,133,133,133            | 0     |
| 85  | MG   | 2     | 2016 | 1/1   | 0.41  | 0.44 | 78,78,78,78                | 0     |
| 85  | MG   | 1     | 3654 | 1/1   | 0.44  | 0.44 | 92,92,92,92                | 0     |
| 85  | MG   | 6     | 1909 | 1/1   | 0.44  | 0.36 | 111,111,111,111            | 0     |
| 85  | MG   | 2     | 1915 | 1/1   | 0.44  | 0.53 | 73,73,73,73                | 0     |
| 85  | MG   | 2     | 1959 | 1/1   | 0.47  | 0.50 | 101,101,101,101            | 0     |
| 85  | MG   | 5     | 3467 | 1/1   | 0.48  | 0.36 | 93,93,93,93                | 0     |
| 85  | MG   | 2     | 1993 | 1/1   | 0.48  | 0.34 | 100,100,100,100            | 0     |
| 85  | MG   | 5     | 3898 | 1/1   | 0.48  | 0.41 | 94,94,94,94                | 0     |
| 85  | MG   | 5     | 3884 | 1/1   | 0.49  | 0.41 | 90,90,90,90                | 0     |
| 85  | MG   | 2     | 1978 | 1/1   | 0.50  | 0.44 | 99,99,99,99                | 0     |
| 85  | MG   | 2     | 1966 | 1/1   | 0.50  | 0.32 | 89,89,89,89                | 0     |
| 85  | MG   | 6     | 1904 | 1/1   | 0.52  | 0.40 | 70,70,70,70                | 0     |
| 85  | MG   | 2     | 1983 | 1/1   | 0.53  | 0.23 | 78,78,78,78                | 0     |
| 85  | MG   | 2     | 2000 | 1/1   | 0.54  | 0.36 | 87,87,87,87                | 0     |
| 85  | MG   | 2     | 1990 | 1/1   | 0.55  | 0.41 | 111,111,111,111            | 0     |
| 85  | MG   | 2     | 1963 | 1/1   | 0.55  | 0.18 | 143,143,143,143            | 0     |
| 85  | MG   | 5     | 3805 | 1/1   | 0.57  | 0.17 | 152,152,152,152            | 0     |
| 85  | MG   | 2     | 1986 | 1/1   | 0.58  | 0.36 | 104,104,104,104            | 0     |
| 85  | MG   | 4     | 222  | 1/1   | 0.58  | 0.46 | 90,90,90,90                | 0     |
| 85  | MG   | 6     | 2000 | 1/1   | 0.59  | 0.37 | 114,114,114,114            | 0     |
| 85  | MG   | O7    | 102  | 1/1   | 0.59  | 0.24 | 60,60,60,60                | 0     |
| 85  | MG   | 2     | 1946 | 1/1   | 0.59  | 0.29 | 94,94,94,94                | 0     |
| 85  | MG   | 6     | 1969 | 1/1   | 0.59  | 0.36 | 73,73,73,73                | 0     |
| 85  | MG   | 6     | 1907 | 1/1   | 0.60  | 0.37 | 70,70,70,70                | 0     |
| 85  | MG   | 2     | 1934 | 1/1   | 0.60  | 0.33 | 81,81,81,81                | 0     |
| 85  | MG   | 2     | 1926 | 1/1   | 0.60  | 0.52 | 96,96,96,96                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 6     | 1968 | 1/1   | 0.60 | 0.36 | 82,82,82,82                 | 0     |
| 85  | MG   | 6     | 2046 | 1/1   | 0.60 | 0.47 | 86,86,86,86                 | 0     |
| 85  | MG   | 1     | 3638 | 1/1   | 0.61 | 0.36 | 72,72,72,72                 | 0     |
| 85  | MG   | 1     | 3653 | 1/1   | 0.62 | 0.21 | 72,72,72,72                 | 0     |
| 85  | MG   | 1     | 3679 | 1/1   | 0.63 | 0.38 | 72,72,72,72                 | 0     |
| 85  | MG   | 2     | 1958 | 1/1   | 0.63 | 0.51 | 85,85,85,85                 | 0     |
| 85  | MG   | M3    | 202  | 1/1   | 0.63 | 0.38 | 93,93,93,93                 | 0     |
| 85  | MG   | 5     | 3682 | 1/1   | 0.63 | 0.36 | 83,83,83,83                 | 0     |
| 85  | MG   | o1    | 201  | 1/1   | 0.63 | 0.32 | 62,62,62,62                 | 0     |
| 85  | MG   | 5     | 3770 | 1/1   | 0.64 | 0.32 | 71,71,71,71                 | 0     |
| 85  | MG   | 5     | 3708 | 1/1   | 0.64 | 0.34 | 91,91,91,91                 | 0     |
| 85  | MG   | 6     | 1963 | 1/1   | 0.65 | 0.47 | 83,83,83,83                 | 0     |
| 85  | MG   | 5     | 3780 | 1/1   | 0.65 | 0.35 | 81,81,81,81                 | 0     |
| 86  | OHX  | 1     | 4193 | 7/7   | 0.65 | 0.29 | 131,131,131,131             | 0     |
| 85  | MG   | 5     | 3420 | 1/1   | 0.66 | 0.27 | 72,72,72,72                 | 0     |
| 85  | MG   | 6     | 1967 | 1/1   | 0.66 | 0.35 | 85,85,85,85                 | 0     |
| 85  | MG   | 6     | 1973 | 1/1   | 0.66 | 0.38 | 73,73,73,73                 | 0     |
| 85  | MG   | 2     | 1948 | 1/1   | 0.66 | 0.26 | 91,91,91,91                 | 0     |
| 85  | MG   | 2     | 1945 | 1/1   | 0.67 | 0.34 | 70,70,70,70                 | 0     |
| 85  | MG   | 2     | 1931 | 1/1   | 0.67 | 0.45 | 79,79,79,79                 | 0     |
| 86  | OHX  | 5     | 4240 | 7/7   | 0.67 | 0.22 | 147,147,147,147             | 0     |
| 85  | MG   | 6     | 2004 | 1/1   | 0.68 | 0.30 | 79,79,79,79                 | 0     |
| 85  | MG   | 1     | 3627 | 1/1   | 0.68 | 0.32 | 77,77,77,77                 | 0     |
| 85  | MG   | 4     | 204  | 1/1   | 0.68 | 0.39 | 70,70,70,70                 | 0     |
| 85  | MG   | 5     | 3792 | 1/1   | 0.68 | 0.29 | 90,90,90,90                 | 0     |
| 86  | OHX  | 5     | 4231 | 7/7   | 0.68 | 0.28 | 125,125,125,125             | 0     |
| 85  | MG   | 1     | 3420 | 1/1   | 0.68 | 0.34 | 90,90,90,90                 | 0     |
| 85  | MG   | 2     | 1982 | 1/1   | 0.69 | 0.35 | 90,90,90,90                 | 0     |
| 85  | MG   | 5     | 3685 | 1/1   | 0.69 | 0.37 | 64,64,64,64                 | 0     |
| 85  | MG   | 6     | 2040 | 1/1   | 0.69 | 0.47 | 87,87,87,87                 | 0     |
| 85  | MG   | 5     | 3769 | 1/1   | 0.69 | 0.19 | 98,98,98,98                 | 0     |
| 85  | MG   | 6     | 1964 | 1/1   | 0.69 | 0.26 | 99,99,99,99                 | 0     |
| 85  | MG   | 2     | 1976 | 1/1   | 0.70 | 0.33 | 58,58,58,58                 | 0     |
| 85  | MG   | 6     | 1966 | 1/1   | 0.70 | 0.26 | 67,67,67,67                 | 0     |
| 86  | OHX  | 2     | 2180 | 7/7   | 0.70 | 0.20 | 164,164,164,164             | 0     |
| 85  | MG   | 2     | 1964 | 1/1   | 0.70 | 0.33 | 100,100,100,100             | 0     |
| 85  | MG   | 5     | 3861 | 1/1   | 0.70 | 0.30 | 79,79,79,79                 | 0     |
| 85  | MG   | 2     | 2017 | 1/1   | 0.70 | 0.35 | 79,79,79,79                 | 0     |
| 85  | MG   | 2     | 1950 | 1/1   | 0.71 | 0.51 | 88,88,88,88                 | 0     |
| 85  | MG   | 6     | 1985 | 1/1   | 0.71 | 0.22 | 79,79,79,79                 | 0     |
| 85  | MG   | 6     | 1991 | 1/1   | 0.71 | 0.31 | 72,72,72,72                 | 0     |
| 85  | MG   | 1     | 3840 | 1/1   | 0.71 | 0.44 | 63,63,63,63                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 2     | 2163 | 7/7   | 0.71 | 0.18 | 168,168,168,168             | 0     |
| 86  | OHX  | 2     | 2178 | 7/7   | 0.71 | 0.19 | 168,168,168,168             | 0     |
| 85  | MG   | 5     | 3421 | 1/1   | 0.71 | 0.31 | 97,97,97,97                 | 0     |
| 85  | MG   | 1     | 3774 | 1/1   | 0.71 | 0.17 | 52,52,52,52                 | 0     |
| 86  | OHX  | O9    | 101  | 7/7   | 0.71 | 0.25 | 118,118,118,118             | 0     |
| 85  | MG   | 5     | 3588 | 1/1   | 0.71 | 0.41 | 56,56,56,56                 | 0     |
| 85  | MG   | 1     | 3641 | 1/1   | 0.71 | 0.26 | 55,55,55,55                 | 0     |
| 86  | OHX  | 14    | 403  | 7/7   | 0.71 | 0.22 | 143,143,143,143             | 0     |
| 85  | MG   | 6     | 1935 | 1/1   | 0.72 | 0.40 | 59,59,59,59                 | 0     |
| 85  | MG   | 5     | 3745 | 1/1   | 0.72 | 0.27 | 62,62,62,62                 | 0     |
| 85  | MG   | 6     | 1982 | 1/1   | 0.72 | 0.31 | 78,78,78,78                 | 0     |
| 85  | MG   | 2     | 1951 | 1/1   | 0.72 | 0.43 | 102,102,102,102             | 0     |
| 85  | MG   | 2     | 2005 | 1/1   | 0.72 | 0.35 | 81,81,81,81                 | 0     |
| 86  | OHX  | 1     | 4190 | 7/7   | 0.72 | 0.18 | 181,181,181,181             | 0     |
| 85  | MG   | 2     | 1952 | 1/1   | 0.72 | 0.24 | 102,102,102,102             | 0     |
| 86  | OHX  | L4    | 402  | 7/7   | 0.72 | 0.20 | 138,138,138,138             | 0     |
| 85  | MG   | 5     | 3570 | 1/1   | 0.72 | 0.38 | 28,28,28,28                 | 0     |
| 85  | MG   | 6     | 1914 | 1/1   | 0.72 | 0.36 | 73,73,73,73                 | 0     |
| 85  | MG   | 2     | 1989 | 1/1   | 0.72 | 0.47 | 61,61,61,61                 | 0     |
| 85  | MG   | 6     | 1934 | 1/1   | 0.72 | 0.34 | 80,80,80,80                 | 0     |
| 85  | MG   | 2     | 1988 | 1/1   | 0.73 | 0.27 | 83,83,83,83                 | 0     |
| 85  | MG   | 2     | 1961 | 1/1   | 0.73 | 0.36 | 59,59,59,59                 | 0     |
| 85  | MG   | 1     | 3666 | 1/1   | 0.73 | 0.14 | 60,60,60,60                 | 0     |
| 85  | MG   | 2     | 1908 | 1/1   | 0.73 | 0.32 | 78,78,78,78                 | 0     |
| 85  | MG   | 1     | 3730 | 1/1   | 0.73 | 0.26 | 61,61,61,61                 | 0     |
| 85  | MG   | 1     | 3758 | 1/1   | 0.73 | 0.33 | 99,99,99,99                 | 0     |
| 86  | OHX  | 1     | 4198 | 7/7   | 0.73 | 0.22 | 129,129,129,129             | 0     |
| 85  | MG   | 2     | 1954 | 1/1   | 0.73 | 0.21 | 105,105,105,105             | 0     |
| 85  | MG   | 2     | 1928 | 1/1   | 0.73 | 0.41 | 86,86,86,86                 | 0     |
| 86  | OHX  | 6     | 2186 | 7/7   | 0.73 | 0.24 | 132,132,132,132             | 0     |
| 85  | MG   | 2     | 1917 | 1/1   | 0.73 | 0.45 | 64,64,64,64                 | 0     |
| 86  | OHX  | 5     | 4238 | 7/7   | 0.73 | 0.22 | 139,139,139,139             | 0     |
| 85  | MG   | 1     | 3640 | 1/1   | 0.73 | 0.15 | 51,51,51,51                 | 0     |
| 85  | MG   | 2     | 1972 | 1/1   | 0.73 | 0.32 | 89,89,89,89                 | 0     |
| 85  | MG   | 6     | 1952 | 1/1   | 0.74 | 0.29 | 63,63,63,63                 | 0     |
| 85  | MG   | 2     | 1992 | 1/1   | 0.74 | 0.26 | 70,70,70,70                 | 0     |
| 85  | MG   | 6     | 1992 | 1/1   | 0.74 | 0.34 | 80,80,80,80                 | 0     |
| 85  | MG   | 5     | 3653 | 1/1   | 0.74 | 0.43 | 35,35,35,35                 | 0     |
| 85  | MG   | 5     | 3661 | 1/1   | 0.74 | 0.29 | 31,31,31,31                 | 0     |
| 85  | MG   | 2     | 1901 | 1/1   | 0.74 | 0.45 | 83,83,83,83                 | 0     |
| 85  | MG   | 6     | 2001 | 1/1   | 0.74 | 0.17 | 55,55,55,55                 | 0     |
| 86  | OHX  | 1     | 4179 | 7/7   | 0.74 | 0.19 | 143,143,143,143             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 1     | 3421 | 1/1   | 0.74 | 0.38 | 74,74,74,74                 | 0     |
| 85  | MG   | 5     | 3726 | 1/1   | 0.74 | 0.24 | 96,96,96,96                 | 0     |
| 85  | MG   | 1     | 3530 | 1/1   | 0.74 | 0.35 | 47,47,47,47                 | 0     |
| 85  | MG   | 6     | 2022 | 1/1   | 0.74 | 0.26 | 112,112,112,112             | 0     |
| 85  | MG   | 3     | 211  | 1/1   | 0.74 | 0.20 | 74,74,74,74                 | 0     |
| 86  | OHX  | 6     | 2172 | 7/7   | 0.74 | 0.19 | 147,147,147,147             | 0     |
| 85  | MG   | 2     | 1994 | 1/1   | 0.74 | 0.45 | 72,72,72,72                 | 0     |
| 86  | OHX  | 6     | 2193 | 7/7   | 0.74 | 0.21 | 153,153,153,153             | 0     |
| 85  | MG   | 2     | 1914 | 1/1   | 0.74 | 0.42 | 71,71,71,71                 | 0     |
| 85  | MG   | 6     | 1981 | 1/1   | 0.74 | 0.27 | 67,67,67,67                 | 0     |
| 85  | MG   | S4    | 302  | 1/1   | 0.74 | 0.39 | 74,74,74,74                 | 0     |
| 85  | MG   | 5     | 3810 | 1/1   | 0.74 | 0.25 | 74,74,74,74                 | 0     |
| 86  | OHX  | m4    | 201  | 7/7   | 0.74 | 0.14 | 197,197,197,197             | 0     |
| 85  | MG   | 2     | 2015 | 1/1   | 0.75 | 0.32 | 70,70,70,70                 | 0     |
| 85  | MG   | 1     | 3769 | 1/1   | 0.75 | 0.30 | 56,56,56,56                 | 0     |
| 85  | MG   | 3     | 208  | 1/1   | 0.75 | 0.28 | 78,78,78,78                 | 0     |
| 86  | OHX  | 6     | 2158 | 7/7   | 0.75 | 0.17 | 169,169,169,169             | 0     |
| 86  | OHX  | 2     | 2099 | 7/7   | 0.75 | 0.19 | 154,154,154,154             | 0     |
| 85  | MG   | 6     | 1929 | 1/1   | 0.75 | 0.34 | 57,57,57,57                 | 0     |
| 86  | OHX  | 6     | 2192 | 7/7   | 0.75 | 0.20 | 142,142,142,142             | 0     |
| 85  | MG   | 5     | 3703 | 1/1   | 0.75 | 0.26 | 69,69,69,69                 | 0     |
| 86  | OHX  | s1    | 302  | 7/7   | 0.75 | 0.21 | 158,158,158,158             | 0     |
| 86  | OHX  | 5     | 4191 | 7/7   | 0.75 | 0.18 | 153,153,153,153             | 0     |
| 85  | MG   | 2     | 1962 | 1/1   | 0.75 | 0.40 | 76,76,76,76                 | 0     |
| 86  | OHX  | 5     | 4237 | 7/7   | 0.75 | 0.22 | 148,148,148,148             | 0     |
| 86  | OHX  | 1     | 4169 | 7/7   | 0.75 | 0.14 | 201,201,201,201             | 0     |
| 85  | MG   | 6     | 1988 | 1/1   | 0.75 | 0.29 | 69,69,69,69                 | 0     |
| 86  | OHX  | 14    | 402  | 7/7   | 0.75 | 0.17 | 153,153,153,153             | 0     |
| 85  | MG   | 1     | 3594 | 1/1   | 0.75 | 0.40 | 58,58,58,58                 | 0     |
| 85  | MG   | 5     | 3878 | 1/1   | 0.75 | 0.25 | 38,38,38,38                 | 0     |
| 85  | MG   | 2     | 1977 | 1/1   | 0.76 | 0.35 | 88,88,88,88                 | 0     |
| 85  | MG   | 1     | 3842 | 1/1   | 0.76 | 0.31 | 62,62,62,62                 | 0     |
| 86  | OHX  | 2     | 2160 | 7/7   | 0.76 | 0.26 | 129,129,129,129             | 0     |
| 85  | MG   | 1     | 3494 | 1/1   | 0.76 | 0.41 | 83,83,83,83                 | 0     |
| 86  | OHX  | 6     | 2190 | 7/7   | 0.76 | 0.22 | 142,142,142,142             | 0     |
| 86  | OHX  | 2     | 2164 | 7/7   | 0.76 | 0.23 | 133,133,133,133             | 0     |
| 86  | OHX  | 2     | 2172 | 7/7   | 0.76 | 0.21 | 143,143,143,143             | 0     |
| 85  | MG   | 1     | 3795 | 1/1   | 0.76 | 0.22 | 66,66,66,66                 | 0     |
| 85  | MG   | 1     | 3642 | 1/1   | 0.76 | 0.32 | 60,60,60,60                 | 0     |
| 86  | OHX  | 5     | 4224 | 7/7   | 0.76 | 0.19 | 165,165,165,165             | 0     |
| 85  | MG   | 5     | 3823 | 1/1   | 0.76 | 0.22 | 90,90,90,90                 | 0     |
| 86  | OHX  | 5     | 4233 | 7/7   | 0.76 | 0.20 | 149,149,149,149             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 1     | 4175 | 7/7   | 0.76 | 0.25 | 133,133,133,133             | 0     |
| 85  | MG   | 6     | 1911 | 1/1   | 0.76 | 0.37 | 83,83,83,83                 | 0     |
| 85  | MG   | 1     | 3762 | 1/1   | 0.76 | 0.14 | 54,54,54,54                 | 0     |
| 85  | MG   | 6     | 1922 | 1/1   | 0.76 | 0.41 | 57,57,57,57                 | 0     |
| 85  | MG   | 5     | 3887 | 1/1   | 0.76 | 0.32 | 71,71,71,71                 | 0     |
| 86  | OHX  | 15    | 304  | 7/7   | 0.76 | 0.22 | 140,140,140,140             | 0     |
| 85  | MG   | 5     | 3656 | 1/1   | 0.76 | 0.10 | 42,42,42,42                 | 0     |
| 87  | ZN   | D7    | 101  | 1/1   | 0.76 | 0.18 | 144,144,144,144             | 0     |
| 86  | OHX  | 1     | 4208 | 7/7   | 0.77 | 0.23 | 128,128,128,128             | 0     |
| 85  | MG   | 5     | 3637 | 1/1   | 0.77 | 0.28 | 51,51,51,51                 | 0     |
| 85  | MG   | 3     | 201  | 1/1   | 0.77 | 0.31 | 74,74,74,74                 | 0     |
| 85  | MG   | 2     | 1924 | 1/1   | 0.77 | 0.51 | 85,85,85,85                 | 0     |
| 85  | MG   | 1     | 3710 | 1/1   | 0.77 | 0.14 | 55,55,55,55                 | 0     |
| 85  | MG   | 2     | 1938 | 1/1   | 0.77 | 0.44 | 62,62,62,62                 | 0     |
| 85  | MG   | 4     | 219  | 1/1   | 0.77 | 0.19 | 48,48,48,48                 | 0     |
| 85  | MG   | 6     | 2033 | 1/1   | 0.77 | 0.27 | 71,71,71,71                 | 0     |
| 86  | OHX  | 2     | 2145 | 7/7   | 0.77 | 0.19 | 143,143,143,143             | 0     |
| 85  | MG   | 6     | 2037 | 1/1   | 0.77 | 0.40 | 87,87,87,87                 | 0     |
| 86  | OHX  | 5     | 4167 | 7/7   | 0.77 | 0.18 | 166,166,166,166             | 0     |
| 85  | MG   | 1     | 3481 | 1/1   | 0.77 | 0.29 | 78,78,78,78                 | 0     |
| 85  | MG   | 6     | 1923 | 1/1   | 0.77 | 0.34 | 67,67,67,67                 | 0     |
| 86  | OHX  | 5     | 4226 | 7/7   | 0.77 | 0.25 | 118,118,118,118             | 0     |
| 85  | MG   | L7    | 303  | 1/1   | 0.77 | 0.19 | 47,47,47,47                 | 0     |
| 85  | MG   | M1    | 201  | 1/1   | 0.77 | 0.21 | 79,79,79,79                 | 0     |
| 85  | MG   | 2     | 1910 | 1/1   | 0.77 | 0.43 | 56,56,56,56                 | 0     |
| 86  | OHX  | 1     | 4131 | 7/7   | 0.77 | 0.18 | 146,146,146,146             | 0     |
| 85  | MG   | 5     | 3450 | 1/1   | 0.77 | 0.26 | 62,62,62,62                 | 0     |
| 85  | MG   | 5     | 3781 | 1/1   | 0.77 | 0.25 | 76,76,76,76                 | 0     |
| 85  | MG   | N0    | 201  | 1/1   | 0.77 | 0.32 | 45,45,45,45                 | 0     |
| 85  | MG   | 5     | 3480 | 1/1   | 0.77 | 0.34 | 62,62,62,62                 | 0     |
| 85  | MG   | 1     | 3500 | 1/1   | 0.77 | 0.37 | 68,68,68,68                 | 0     |
| 85  | MG   | 6     | 1961 | 1/1   | 0.77 | 0.39 | 86,86,86,86                 | 0     |
| 85  | MG   | 6     | 2031 | 1/1   | 0.78 | 0.50 | 89,89,89,89                 | 0     |
| 86  | OHX  | M9    | 203  | 7/7   | 0.78 | 0.16 | 154,154,154,154             | 0     |
| 85  | MG   | 1     | 3586 | 1/1   | 0.78 | 0.41 | 52,52,52,52                 | 0     |
| 85  | MG   | 6     | 1930 | 1/1   | 0.78 | 0.44 | 61,61,61,61                 | 0     |
| 86  | OHX  | 1     | 4066 | 7/7   | 0.78 | 0.23 | 125,125,125,125             | 0     |
| 86  | OHX  | 6     | 2182 | 7/7   | 0.78 | 0.23 | 133,133,133,133             | 0     |
| 86  | OHX  | 6     | 2185 | 7/7   | 0.78 | 0.20 | 141,141,141,141             | 0     |
| 85  | MG   | 2     | 2009 | 1/1   | 0.78 | 0.45 | 75,75,75,75                 | 0     |
| 86  | OHX  | 6     | 2187 | 7/7   | 0.78 | 0.16 | 161,161,161,161             | 0     |
| 86  | OHX  | 1     | 4142 | 7/7   | 0.78 | 0.21 | 133,133,133,133             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 1     | 4145 | 7/7   | 0.78 | 0.24 | 129,129,129,129             | 0     |
| 85  | MG   | 15    | 301  | 1/1   | 0.78 | 0.18 | 61,61,61,61                 | 0     |
| 86  | OHX  | 6     | 2202 | 7/7   | 0.78 | 0.20 | 148,148,148,148             | 0     |
| 86  | OHX  | 6     | 2206 | 7/7   | 0.78 | 0.21 | 145,145,145,145             | 0     |
| 86  | OHX  | 1     | 4173 | 7/7   | 0.78 | 0.18 | 153,153,153,153             | 0     |
| 86  | OHX  | 1     | 4174 | 7/7   | 0.78 | 0.19 | 157,157,157,157             | 0     |
| 85  | MG   | 1     | 3655 | 1/1   | 0.78 | 0.40 | 70,70,70,70                 | 0     |
| 86  | OHX  | 5     | 4199 | 7/7   | 0.78 | 0.18 | 142,142,142,142             | 0     |
| 86  | OHX  | 5     | 4210 | 7/7   | 0.78 | 0.21 | 136,136,136,136             | 0     |
| 85  | MG   | 1     | 3610 | 1/1   | 0.78 | 0.44 | 63,63,63,63                 | 0     |
| 86  | OHX  | 1     | 4181 | 7/7   | 0.78 | 0.20 | 142,142,142,142             | 0     |
| 86  | OHX  | 5     | 4227 | 7/7   | 0.78 | 0.20 | 146,146,146,146             | 0     |
| 85  | MG   | 2     | 1971 | 1/1   | 0.78 | 0.32 | 69,69,69,69                 | 0     |
| 86  | OHX  | 1     | 4191 | 7/7   | 0.78 | 0.20 | 135,135,135,135             | 0     |
| 85  | MG   | 5     | 3715 | 1/1   | 0.78 | 0.21 | 48,48,48,48                 | 0     |
| 86  | OHX  | 1     | 4195 | 7/7   | 0.78 | 0.16 | 143,143,143,143             | 0     |
| 86  | OHX  | 1     | 4197 | 7/7   | 0.78 | 0.20 | 131,131,131,131             | 0     |
| 85  | MG   | 5     | 3638 | 1/1   | 0.78 | 0.25 | 56,56,56,56                 | 0     |
| 85  | MG   | 5     | 3650 | 1/1   | 0.78 | 0.18 | 89,89,89,89                 | 0     |
| 86  | OHX  | 1     | 4215 | 7/7   | 0.78 | 0.23 | 130,130,130,130             | 0     |
| 86  | OHX  | 4     | 235  | 7/7   | 0.78 | 0.19 | 143,143,143,143             | 0     |
| 86  | OHX  | 4     | 238  | 7/7   | 0.78 | 0.27 | 139,139,139,139             | 0     |
| 86  | OHX  | 1     | 4192 | 7/7   | 0.79 | 0.23 | 122,122,122,122             | 0     |
| 85  | MG   | 5     | 3815 | 1/1   | 0.79 | 0.12 | 59,59,59,59                 | 0     |
| 85  | MG   | 6     | 2021 | 1/1   | 0.79 | 0.10 | 49,49,49,49                 | 0     |
| 85  | MG   | 5     | 3848 | 1/1   | 0.79 | 0.11 | 56,56,56,56                 | 0     |
| 85  | MG   | 5     | 3731 | 1/1   | 0.79 | 0.27 | 61,61,61,61                 | 0     |
| 86  | OHX  | 5     | 4156 | 7/7   | 0.79 | 0.27 | 111,111,111,111             | 0     |
| 86  | OHX  | 1     | 4199 | 7/7   | 0.79 | 0.17 | 155,155,155,155             | 0     |
| 86  | OHX  | 1     | 4203 | 7/7   | 0.79 | 0.20 | 143,143,143,143             | 0     |
| 85  | MG   | 2     | 2008 | 1/1   | 0.79 | 0.42 | 77,77,77,77                 | 0     |
| 85  | MG   | 1     | 3724 | 1/1   | 0.79 | 0.43 | 37,37,37,37                 | 0     |
| 85  | MG   | 2     | 1932 | 1/1   | 0.79 | 0.43 | 61,61,61,61                 | 0     |
| 85  | MG   | 5     | 3470 | 1/1   | 0.79 | 0.19 | 107,107,107,107             | 0     |
| 85  | MG   | 2     | 2018 | 1/1   | 0.79 | 0.52 | 79,79,79,79                 | 0     |
| 85  | MG   | n6    | 201  | 1/1   | 0.79 | 0.42 | 55,55,55,55                 | 0     |
| 85  | MG   | 2     | 2020 | 1/1   | 0.79 | 0.35 | 92,92,92,92                 | 0     |
| 86  | OHX  | 6     | 2150 | 7/7   | 0.79 | 0.20 | 127,127,127,127             | 0     |
| 85  | MG   | o4    | 201  | 1/1   | 0.79 | 0.40 | 52,52,52,52                 | 0     |
| 85  | MG   | 5     | 3580 | 1/1   | 0.79 | 0.25 | 33,33,33,33                 | 0     |
| 86  | OHX  | 5     | 4250 | 7/7   | 0.79 | 0.19 | 137,137,137,137             | 0     |
| 86  | OHX  | 2     | 2134 | 7/7   | 0.79 | 0.20 | 138,138,138,138             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 6     | 2006 | 1/1   | 0.79 | 0.28 | 95,95,95,95                 | 0     |
| 86  | OHX  | 1     | 4189 | 7/7   | 0.79 | 0.20 | 138,138,138,138             | 0     |
| 86  | OHX  | 2     | 2159 | 7/7   | 0.79 | 0.19 | 148,148,148,148             | 0     |
| 85  | MG   | 2     | 1969 | 1/1   | 0.79 | 0.32 | 84,84,84,84                 | 0     |
| 85  | MG   | 1     | 3515 | 1/1   | 0.80 | 0.31 | 26,26,26,26                 | 0     |
| 85  | MG   | S8    | 301  | 1/1   | 0.80 | 0.22 | 62,62,62,62                 | 0     |
| 85  | MG   | 1     | 3854 | 1/1   | 0.80 | 0.25 | 60,60,60,60                 | 0     |
| 86  | OHX  | 1     | 4186 | 7/7   | 0.80 | 0.20 | 136,136,136,136             | 0     |
| 85  | MG   | 6     | 2014 | 1/1   | 0.80 | 0.21 | 48,48,48,48                 | 0     |
| 86  | OHX  | 6     | 2195 | 7/7   | 0.80 | 0.16 | 168,168,168,168             | 0     |
| 85  | MG   | o4    | 202  | 1/1   | 0.80 | 0.32 | 69,69,69,69                 | 0     |
| 85  | MG   | 2     | 1904 | 1/1   | 0.80 | 0.37 | 74,74,74,74                 | 0     |
| 85  | MG   | M9    | 202  | 1/1   | 0.80 | 0.32 | 72,72,72,72                 | 0     |
| 85  | MG   | 5     | 3778 | 1/1   | 0.80 | 0.17 | 71,71,71,71                 | 0     |
| 85  | MG   | 1     | 3801 | 1/1   | 0.80 | 0.13 | 49,49,49,49                 | 0     |
| 85  | MG   | N5    | 201  | 1/1   | 0.80 | 0.18 | 68,68,68,68                 | 0     |
| 85  | MG   | 1     | 3419 | 1/1   | 0.80 | 0.26 | 56,56,56,56                 | 0     |
| 85  | MG   | 6     | 1902 | 1/1   | 0.80 | 0.24 | 54,54,54,54                 | 0     |
| 85  | MG   | 5     | 3807 | 1/1   | 0.80 | 0.23 | 96,96,96,96                 | 0     |
| 86  | OHX  | 2     | 2175 | 7/7   | 0.80 | 0.21 | 161,161,161,161             | 0     |
| 85  | MG   | 6     | 2038 | 1/1   | 0.80 | 0.34 | 78,78,78,78                 | 0     |
| 85  | MG   | 6     | 1987 | 1/1   | 0.80 | 0.22 | 55,55,55,55                 | 0     |
| 85  | MG   | 6     | 1950 | 1/1   | 0.80 | 0.30 | 45,45,45,45                 | 0     |
| 86  | OHX  | 1     | 4115 | 7/7   | 0.80 | 0.20 | 138,138,138,138             | 0     |
| 85  | MG   | 3     | 212  | 1/1   | 0.80 | 0.30 | 58,58,58,58                 | 0     |
| 86  | OHX  | 1     | 4133 | 7/7   | 0.80 | 0.16 | 155,155,155,155             | 0     |
| 86  | OHX  | 5     | 4242 | 7/7   | 0.80 | 0.19 | 139,139,139,139             | 0     |
| 86  | OHX  | 5     | 4243 | 7/7   | 0.80 | 0.16 | 171,171,171,171             | 0     |
| 86  | OHX  | 5     | 4244 | 7/7   | 0.80 | 0.14 | 207,207,207,207             | 0     |
| 86  | OHX  | 5     | 4248 | 7/7   | 0.80 | 0.20 | 145,145,145,145             | 0     |
| 86  | OHX  | 6     | 2109 | 7/7   | 0.80 | 0.20 | 134,134,134,134             | 0     |
| 86  | OHX  | 5     | 4252 | 7/7   | 0.80 | 0.20 | 154,154,154,154             | 0     |
| 86  | OHX  | 7     | 226  | 7/7   | 0.80 | 0.20 | 150,150,150,150             | 0     |
| 85  | MG   | c9    | 201  | 1/1   | 0.80 | 0.25 | 72,72,72,72                 | 0     |
| 85  | MG   | 1     | 3815 | 1/1   | 0.80 | 0.18 | 54,54,54,54                 | 0     |
| 85  | MG   | S6    | 301  | 1/1   | 0.80 | 0.27 | 90,90,90,90                 | 0     |
| 86  | OHX  | m1    | 203  | 7/7   | 0.80 | 0.17 | 142,142,142,142             | 0     |
| 85  | MG   | 5     | 3431 | 1/1   | 0.80 | 0.23 | 74,74,74,74                 | 0     |
| 85  | MG   | 5     | 3721 | 1/1   | 0.80 | 0.20 | 54,54,54,54                 | 0     |
| 85  | MG   | 1     | 3556 | 1/1   | 0.81 | 0.27 | 32,32,32,32                 | 0     |
| 85  | MG   | 5     | 3615 | 1/1   | 0.81 | 0.22 | 46,46,46,46                 | 0     |
| 86  | OHX  | 1     | 4099 | 7/7   | 0.81 | 0.17 | 139,139,139,139             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 1     | 4104 | 7/7   | 0.81 | 0.17 | 151,151,151,151             | 0     |
| 85  | MG   | 5     | 3636 | 1/1   | 0.81 | 0.16 | 49,49,49,49                 | 0     |
| 85  | MG   | 6     | 1958 | 1/1   | 0.81 | 0.44 | 53,53,53,53                 | 0     |
| 85  | MG   | 2     | 2007 | 1/1   | 0.81 | 0.34 | 58,58,58,58                 | 0     |
| 86  | OHX  | 6     | 2188 | 7/7   | 0.81 | 0.19 | 141,141,141,141             | 0     |
| 85  | MG   | 2     | 1929 | 1/1   | 0.81 | 0.46 | 72,72,72,72                 | 0     |
| 85  | MG   | 5     | 3651 | 1/1   | 0.81 | 0.26 | 71,71,71,71                 | 0     |
| 86  | OHX  | 1     | 4163 | 7/7   | 0.81 | 0.17 | 145,145,145,145             | 0     |
| 86  | OHX  | 1     | 4164 | 7/7   | 0.81 | 0.17 | 148,148,148,148             | 0     |
| 85  | MG   | 1     | 3699 | 1/1   | 0.81 | 0.14 | 46,46,46,46                 | 0     |
| 85  | MG   | 1     | 3701 | 1/1   | 0.81 | 0.35 | 68,68,68,68                 | 0     |
| 85  | MG   | 1     | 3607 | 1/1   | 0.81 | 0.13 | 56,56,56,56                 | 0     |
| 85  | MG   | 5     | 3678 | 1/1   | 0.81 | 0.17 | 91,91,91,91                 | 0     |
| 85  | MG   | S2    | 301  | 1/1   | 0.81 | 0.38 | 57,57,57,57                 | 0     |
| 85  | MG   | 8     | 206  | 1/1   | 0.81 | 0.19 | 69,69,69,69                 | 0     |
| 86  | OHX  | 1     | 4183 | 7/7   | 0.81 | 0.22 | 131,131,131,131             | 0     |
| 86  | OHX  | 5     | 4207 | 7/7   | 0.81 | 0.20 | 137,137,137,137             | 0     |
| 85  | MG   | 1     | 3444 | 1/1   | 0.81 | 0.20 | 83,83,83,83                 | 0     |
| 86  | OHX  | 5     | 4223 | 7/7   | 0.81 | 0.19 | 137,137,137,137             | 0     |
| 85  | MG   | 1     | 3735 | 1/1   | 0.81 | 0.22 | 81,81,81,81                 | 0     |
| 85  | MG   | 6     | 1920 | 1/1   | 0.81 | 0.41 | 61,61,61,61                 | 0     |
| 85  | MG   | 1     | 3632 | 1/1   | 0.81 | 0.27 | 41,41,41,41                 | 0     |
| 85  | MG   | 5     | 3718 | 1/1   | 0.81 | 0.33 | 59,59,59,59                 | 0     |
| 85  | MG   | 4     | 218  | 1/1   | 0.81 | 0.19 | 61,61,61,61                 | 0     |
| 86  | OHX  | 5     | 4234 | 7/7   | 0.81 | 0.24 | 128,128,128,128             | 0     |
| 85  | MG   | 2     | 1953 | 1/1   | 0.81 | 0.39 | 89,89,89,89                 | 0     |
| 85  | MG   | 2     | 1909 | 1/1   | 0.81 | 0.44 | 77,77,77,77                 | 0     |
| 86  | OHX  | 2     | 2158 | 7/7   | 0.81 | 0.10 | 281,281,281,281             | 0     |
| 85  | MG   | 2     | 1941 | 1/1   | 0.81 | 0.30 | 64,64,64,64                 | 0     |
| 86  | OHX  | 1     | 4200 | 7/7   | 0.81 | 0.23 | 123,123,123,123             | 0     |
| 85  | MG   | 5     | 3456 | 1/1   | 0.81 | 0.28 | 86,86,86,86                 | 0     |
| 86  | OHX  | 2     | 2161 | 7/7   | 0.81 | 0.18 | 144,144,144,144             | 0     |
| 86  | OHX  | 1     | 4209 | 7/7   | 0.81 | 0.23 | 121,121,121,121             | 0     |
| 85  | MG   | 2     | 1907 | 1/1   | 0.81 | 0.49 | 59,59,59,59                 | 0     |
| 85  | MG   | 1     | 3418 | 1/1   | 0.81 | 0.30 | 47,47,47,47                 | 0     |
| 85  | MG   | 6     | 1936 | 1/1   | 0.81 | 0.28 | 77,77,77,77                 | 0     |
| 85  | MG   | 6     | 1939 | 1/1   | 0.81 | 0.44 | 66,66,66,66                 | 0     |
| 86  | OHX  | 2     | 2177 | 7/7   | 0.81 | 0.15 | 168,168,168,168             | 0     |
| 85  | MG   | 1     | 3532 | 1/1   | 0.81 | 0.36 | 67,67,67,67                 | 0     |
| 86  | OHX  | 2     | 2179 | 7/7   | 0.81 | 0.23 | 145,145,145,145             | 0     |
| 86  | OHX  | o9    | 101  | 7/7   | 0.81 | 0.24 | 114,114,114,114             | 0     |
| 86  | OHX  | 6     | 2138 | 7/7   | 0.81 | 0.20 | 130,130,130,130             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 1     | 3565 | 1/1   | 0.82 | 0.31 | 49,49,49,49                 | 0     |
| 85  | MG   | 5     | 3845 | 1/1   | 0.82 | 0.15 | 49,49,49,49                 | 0     |
| 85  | MG   | 5     | 3424 | 1/1   | 0.82 | 0.24 | 60,60,60,60                 | 0     |
| 86  | OHX  | d9    | 102  | 7/7   | 0.82 | 0.18 | 161,161,161,161             | 0     |
| 86  | OHX  | 5     | 3932 | 7/7   | 0.82 | 0.25 | 109,109,109,109             | 0     |
| 85  | MG   | 5     | 3849 | 1/1   | 0.82 | 0.20 | 46,46,46,46                 | 0     |
| 85  | MG   | 1     | 3576 | 1/1   | 0.82 | 0.38 | 41,41,41,41                 | 0     |
| 85  | MG   | 1     | 3476 | 1/1   | 0.82 | 0.41 | 73,73,73,73                 | 0     |
| 86  | OHX  | 5     | 4195 | 7/7   | 0.82 | 0.23 | 115,115,115,115             | 0     |
| 85  | MG   | 1     | 3591 | 1/1   | 0.82 | 0.48 | 45,45,45,45                 | 0     |
| 86  | OHX  | 1     | 4205 | 7/7   | 0.82 | 0.22 | 135,135,135,135             | 0     |
| 86  | OHX  | 1     | 4207 | 7/7   | 0.82 | 0.20 | 125,125,125,125             | 0     |
| 86  | OHX  | 5     | 4222 | 7/7   | 0.82 | 0.14 | 166,166,166,166             | 0     |
| 85  | MG   | 2     | 1927 | 1/1   | 0.82 | 0.43 | 64,64,64,64                 | 0     |
| 85  | MG   | 2     | 2006 | 1/1   | 0.82 | 0.45 | 53,53,53,53                 | 0     |
| 85  | MG   | 7     | 202  | 1/1   | 0.82 | 0.28 | 40,40,40,40                 | 0     |
| 85  | MG   | 8     | 201  | 1/1   | 0.82 | 0.19 | 33,33,33,33                 | 0     |
| 86  | OHX  | 5     | 4228 | 7/7   | 0.82 | 0.17 | 138,138,138,138             | 0     |
| 85  | MG   | 1     | 3499 | 1/1   | 0.82 | 0.32 | 32,32,32,32                 | 0     |
| 85  | MG   | 5     | 3488 | 1/1   | 0.82 | 0.23 | 51,51,51,51                 | 0     |
| 86  | OHX  | 1     | 4143 | 7/7   | 0.82 | 0.27 | 109,109,109,109             | 0     |
| 85  | MG   | 1     | 3816 | 1/1   | 0.82 | 0.17 | 52,52,52,52                 | 0     |
| 85  | MG   | 1     | 3817 | 1/1   | 0.82 | 0.30 | 63,63,63,63                 | 0     |
| 85  | MG   | 6     | 2027 | 1/1   | 0.82 | 0.20 | 67,67,67,67                 | 0     |
| 85  | MG   | 6     | 1972 | 1/1   | 0.82 | 0.14 | 70,70,70,70                 | 0     |
| 85  | MG   | 1     | 3618 | 1/1   | 0.82 | 0.16 | 62,62,62,62                 | 0     |
| 86  | OHX  | 6     | 2169 | 7/7   | 0.82 | 0.14 | 171,171,171,171             | 0     |
| 85  | MG   | 6     | 1980 | 1/1   | 0.82 | 0.17 | 77,77,77,77                 | 0     |
| 85  | MG   | 2     | 1998 | 1/1   | 0.82 | 0.38 | 73,73,73,73                 | 0     |
| 86  | OHX  | 6     | 2184 | 7/7   | 0.82 | 0.19 | 131,131,131,131             | 0     |
| 86  | OHX  | 2     | 2149 | 7/7   | 0.82 | 0.14 | 161,161,161,161             | 0     |
| 86  | OHX  | 8     | 227  | 7/7   | 0.82 | 0.20 | 123,123,123,123             | 0     |
| 86  | OHX  | 2     | 2156 | 7/7   | 0.82 | 0.11 | 227,227,227,227             | 0     |
| 85  | MG   | 2     | 1943 | 1/1   | 0.82 | 0.25 | 70,70,70,70                 | 0     |
| 85  | MG   | 1     | 3433 | 1/1   | 0.82 | 0.42 | 48,48,48,48                 | 0     |
| 85  | MG   | 1     | 3443 | 1/1   | 0.82 | 0.28 | 25,25,25,25                 | 0     |
| 85  | MG   | 6     | 1940 | 1/1   | 0.82 | 0.44 | 89,89,89,89                 | 0     |
| 86  | OHX  | m7    | 206  | 7/7   | 0.82 | 0.21 | 115,115,115,115             | 0     |
| 85  | MG   | 2     | 1930 | 1/1   | 0.82 | 0.29 | 67,67,67,67                 | 0     |
| 85  | MG   | 5     | 3663 | 1/1   | 0.82 | 0.50 | 66,66,66,66                 | 0     |
| 85  | MG   | s6    | 301  | 1/1   | 0.83 | 0.30 | 75,75,75,75                 | 0     |
| 86  | OHX  | 5     | 4098 | 7/7   | 0.83 | 0.17 | 145,145,145,145             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 5     | 4144 | 7/7   | 0.83 | 0.19 | 123,123,123,123             | 0     |
| 85  | MG   | 2     | 1912 | 1/1   | 0.83 | 0.34 | 72,72,72,72                 | 0     |
| 85  | MG   | m1    | 202  | 1/1   | 0.83 | 0.24 | 57,57,57,57                 | 0     |
| 86  | OHX  | 5     | 4182 | 7/7   | 0.83 | 0.18 | 140,140,140,140             | 0     |
| 85  | MG   | 1     | 3465 | 1/1   | 0.83 | 0.11 | 44,44,44,44                 | 0     |
| 85  | MG   | 2     | 1940 | 1/1   | 0.83 | 0.31 | 68,68,68,68                 | 0     |
| 86  | OHX  | 1     | 4210 | 7/7   | 0.83 | 0.20 | 129,129,129,129             | 0     |
| 85  | MG   | 2     | 1974 | 1/1   | 0.83 | 0.30 | 70,70,70,70                 | 0     |
| 85  | MG   | 1     | 3739 | 1/1   | 0.83 | 0.15 | 36,36,36,36                 | 0     |
| 86  | OHX  | 5     | 4213 | 7/7   | 0.83 | 0.24 | 107,107,107,107             | 0     |
| 86  | OHX  | 5     | 4215 | 7/7   | 0.83 | 0.17 | 145,145,145,145             | 0     |
| 86  | OHX  | 1     | 4146 | 7/7   | 0.83 | 0.15 | 139,139,139,139             | 0     |
| 86  | OHX  | 1     | 4148 | 7/7   | 0.83 | 0.16 | 147,147,147,147             | 0     |
| 85  | MG   | 1     | 3583 | 1/1   | 0.83 | 0.30 | 38,38,38,38                 | 0     |
| 85  | MG   | 2     | 1997 | 1/1   | 0.83 | 0.12 | 103,103,103,103             | 0     |
| 86  | OHX  | 1     | 4168 | 7/7   | 0.83 | 0.21 | 119,119,119,119             | 0     |
| 85  | MG   | 1     | 3498 | 1/1   | 0.83 | 0.29 | 45,45,45,45                 | 0     |
| 86  | OHX  | 1     | 4172 | 7/7   | 0.83 | 0.22 | 109,109,109,109             | 0     |
| 85  | MG   | 2     | 2021 | 1/1   | 0.83 | 0.62 | 97,97,97,97                 | 0     |
| 86  | OHX  | 2     | 2153 | 7/7   | 0.83 | 0.15 | 167,167,167,167             | 0     |
| 85  | MG   | 5     | 3816 | 1/1   | 0.83 | 0.21 | 62,62,62,62                 | 0     |
| 85  | MG   | 6     | 1977 | 1/1   | 0.83 | 0.26 | 68,68,68,68                 | 0     |
| 86  | OHX  | 6     | 2183 | 7/7   | 0.83 | 0.21 | 135,135,135,135             | 0     |
| 85  | MG   | 6     | 1938 | 1/1   | 0.83 | 0.24 | 43,43,43,43                 | 0     |
| 85  | MG   | 5     | 3710 | 1/1   | 0.83 | 0.27 | 90,90,90,90                 | 0     |
| 85  | MG   | 5     | 3490 | 1/1   | 0.83 | 0.15 | 27,27,27,27                 | 0     |
| 86  | OHX  | 5     | 4247 | 7/7   | 0.83 | 0.21 | 136,136,136,136             | 0     |
| 85  | MG   | 5     | 3855 | 1/1   | 0.83 | 0.28 | 54,54,54,54                 | 0     |
| 85  | MG   | 2     | 1979 | 1/1   | 0.83 | 0.39 | 59,59,59,59                 | 0     |
| 86  | OHX  | 5     | 4251 | 7/7   | 0.83 | 0.20 | 121,121,121,121             | 0     |
| 85  | MG   | 1     | 3509 | 1/1   | 0.83 | 0.32 | 29,29,29,29                 | 0     |
| 86  | OHX  | 5     | 4254 | 7/7   | 0.83 | 0.17 | 153,153,153,153             | 0     |
| 85  | MG   | 5     | 3879 | 1/1   | 0.83 | 0.39 | 57,57,57,57                 | 0     |
| 85  | MG   | 4     | 205  | 1/1   | 0.83 | 0.29 | 46,46,46,46                 | 0     |
| 86  | OHX  | 6     | 2194 | 7/7   | 0.83 | 0.16 | 149,149,149,149             | 0     |
| 85  | MG   | 6     | 1951 | 1/1   | 0.83 | 0.44 | 75,75,75,75                 | 0     |
| 86  | OHX  | 6     | 2197 | 7/7   | 0.83 | 0.17 | 156,156,156,156             | 0     |
| 86  | OHX  | 19    | 202  | 7/7   | 0.83 | 0.19 | 121,121,121,121             | 0     |
| 85  | MG   | 2     | 1999 | 1/1   | 0.83 | 0.24 | 87,87,87,87                 | 0     |
| 85  | MG   | 5     | 3747 | 1/1   | 0.83 | 0.32 | 36,36,36,36                 | 0     |
| 85  | MG   | 7     | 204  | 1/1   | 0.83 | 0.34 | 53,53,53,53                 | 0     |
| 86  | OHX  | s9    | 202  | 7/7   | 0.83 | 0.24 | 121,121,121,121             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 2     | 1916 | 1/1   | 0.83 | 0.33 | 58,58,58,58                 | 0     |
| 85  | MG   | 5     | 3888 | 1/1   | 0.84 | 0.31 | 54,54,54,54                 | 0     |
| 85  | MG   | 5     | 3695 | 1/1   | 0.84 | 0.37 | 74,74,74,74                 | 0     |
| 85  | MG   | 1     | 3864 | 1/1   | 0.84 | 0.37 | 70,70,70,70                 | 0     |
| 85  | MG   | 2     | 1960 | 1/1   | 0.84 | 0.32 | 63,63,63,63                 | 0     |
| 85  | MG   | 7     | 205  | 1/1   | 0.84 | 0.27 | 71,71,71,71                 | 0     |
| 86  | OHX  | 1     | 4150 | 7/7   | 0.84 | 0.18 | 135,135,135,135             | 0     |
| 86  | OHX  | 1     | 4151 | 7/7   | 0.84 | 0.17 | 140,140,140,140             | 0     |
| 85  | MG   | 1     | 3668 | 1/1   | 0.84 | 0.26 | 53,53,53,53                 | 0     |
| 85  | MG   | 2     | 1949 | 1/1   | 0.84 | 0.25 | 59,59,59,59                 | 0     |
| 86  | OHX  | 6     | 2198 | 7/7   | 0.84 | 0.14 | 163,163,163,163             | 0     |
| 86  | OHX  | 6     | 2201 | 7/7   | 0.84 | 0.21 | 139,139,139,139             | 0     |
| 85  | MG   | 8     | 210  | 1/1   | 0.84 | 0.26 | 59,59,59,59                 | 0     |
| 85  | MG   | 2     | 2012 | 1/1   | 0.84 | 0.23 | 61,61,61,61                 | 0     |
| 86  | OHX  | 1     | 4171 | 7/7   | 0.84 | 0.19 | 113,113,113,113             | 0     |
| 86  | OHX  | s8    | 303  | 7/7   | 0.84 | 0.14 | 156,156,156,156             | 0     |
| 85  | MG   | m1    | 201  | 1/1   | 0.84 | 0.28 | 64,64,64,64                 | 0     |
| 86  | OHX  | c3    | 201  | 7/7   | 0.84 | 0.15 | 146,146,146,146             | 0     |
| 86  | OHX  | d4    | 201  | 7/7   | 0.84 | 0.15 | 145,145,145,145             | 0     |
| 85  | MG   | 5     | 3482 | 1/1   | 0.84 | 0.28 | 42,42,42,42                 | 0     |
| 85  | MG   | 5     | 3483 | 1/1   | 0.84 | 0.35 | 71,71,71,71                 | 0     |
| 85  | MG   | n8    | 201  | 1/1   | 0.84 | 0.23 | 37,37,37,37                 | 0     |
| 85  | MG   | 5     | 3485 | 1/1   | 0.84 | 0.18 | 68,68,68,68                 | 0     |
| 86  | OHX  | 5     | 4149 | 7/7   | 0.84 | 0.24 | 107,107,107,107             | 0     |
| 85  | MG   | 1     | 3784 | 1/1   | 0.84 | 0.15 | 51,51,51,51                 | 0     |
| 86  | OHX  | 5     | 4158 | 7/7   | 0.84 | 0.18 | 137,137,137,137             | 0     |
| 86  | OHX  | 5     | 4166 | 7/7   | 0.84 | 0.18 | 140,140,140,140             | 0     |
| 85  | MG   | 2     | 2003 | 1/1   | 0.84 | 0.25 | 66,66,66,66                 | 0     |
| 86  | OHX  | 5     | 4174 | 7/7   | 0.84 | 0.17 | 158,158,158,158             | 0     |
| 85  | MG   | 5     | 3493 | 1/1   | 0.84 | 0.43 | 59,59,59,59                 | 0     |
| 86  | OHX  | 5     | 4184 | 7/7   | 0.84 | 0.18 | 132,132,132,132             | 0     |
| 86  | OHX  | 5     | 4189 | 7/7   | 0.84 | 0.21 | 121,121,121,121             | 0     |
| 85  | MG   | 5     | 3503 | 1/1   | 0.84 | 0.33 | 40,40,40,40                 | 0     |
| 86  | OHX  | 2     | 2143 | 7/7   | 0.84 | 0.22 | 123,123,123,123             | 0     |
| 86  | OHX  | 2     | 2144 | 7/7   | 0.84 | 0.14 | 168,168,168,168             | 0     |
| 86  | OHX  | 5     | 4205 | 7/7   | 0.84 | 0.17 | 130,130,130,130             | 0     |
| 85  | MG   | 5     | 3549 | 1/1   | 0.84 | 0.43 | 43,43,43,43                 | 0     |
| 86  | OHX  | 5     | 4209 | 7/7   | 0.84 | 0.22 | 139,139,139,139             | 0     |
| 86  | OHX  | 2     | 2148 | 7/7   | 0.84 | 0.22 | 109,109,109,109             | 0     |
| 85  | MG   | 5     | 3554 | 1/1   | 0.84 | 0.30 | 32,32,32,32                 | 0     |
| 85  | MG   | 5     | 3559 | 1/1   | 0.84 | 0.35 | 31,31,31,31                 | 0     |
| 86  | OHX  | 5     | 4220 | 7/7   | 0.84 | 0.17 | 142,142,142,142             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 5     | 4221 | 7/7   | 0.84 | 0.22 | 124,124,124,124             | 0     |
| 85  | MG   | 2     | 1965 | 1/1   | 0.84 | 0.39 | 63,63,63,63                 | 0     |
| 85  | MG   | 1     | 3716 | 1/1   | 0.84 | 0.42 | 76,76,76,76                 | 0     |
| 85  | MG   | 5     | 3799 | 1/1   | 0.84 | 0.21 | 71,71,71,71                 | 0     |
| 85  | MG   | 6     | 1928 | 1/1   | 0.84 | 0.41 | 71,71,71,71                 | 0     |
| 85  | MG   | 1     | 3719 | 1/1   | 0.84 | 0.15 | 47,47,47,47                 | 0     |
| 85  | MG   | L5    | 301  | 1/1   | 0.84 | 0.34 | 68,68,68,68                 | 0     |
| 86  | OHX  | 5     | 4230 | 7/7   | 0.84 | 0.15 | 151,151,151,151             | 0     |
| 85  | MG   | 5     | 3814 | 1/1   | 0.84 | 0.11 | 81,81,81,81                 | 0     |
| 85  | MG   | 2     | 1947 | 1/1   | 0.84 | 0.19 | 63,63,63,63                 | 0     |
| 86  | OHX  | 2     | 2174 | 7/7   | 0.84 | 0.18 | 158,158,158,158             | 0     |
| 86  | OHX  | 1     | 4214 | 7/7   | 0.84 | 0.16 | 160,160,160,160             | 0     |
| 85  | MG   | 2     | 1985 | 1/1   | 0.84 | 0.18 | 65,65,65,65                 | 0     |
| 86  | OHX  | 2     | 2176 | 7/7   | 0.84 | 0.18 | 141,141,141,141             | 0     |
| 85  | MG   | 6     | 2042 | 1/1   | 0.84 | 0.33 | 71,71,71,71                 | 0     |
| 85  | MG   | 1     | 3818 | 1/1   | 0.84 | 0.20 | 53,53,53,53                 | 0     |
| 86  | OHX  | M7    | 207  | 7/7   | 0.84 | 0.19 | 133,133,133,133             | 0     |
| 86  | OHX  | 5     | 4246 | 7/7   | 0.84 | 0.16 | 158,158,158,158             | 0     |
| 85  | MG   | 1     | 3408 | 1/1   | 0.84 | 0.33 | 43,43,43,43                 | 0     |
| 85  | MG   | 1     | 3834 | 1/1   | 0.84 | 0.34 | 47,47,47,47                 | 0     |
| 86  | OHX  | 1     | 4031 | 7/7   | 0.84 | 0.21 | 109,109,109,109             | 0     |
| 85  | MG   | 1     | 3738 | 1/1   | 0.84 | 0.18 | 58,58,58,58                 | 0     |
| 86  | OHX  | 1     | 4067 | 7/7   | 0.84 | 0.21 | 122,122,122,122             | 0     |
| 86  | OHX  | 1     | 4074 | 7/7   | 0.84 | 0.17 | 134,134,134,134             | 0     |
| 86  | OHX  | 6     | 2166 | 7/7   | 0.84 | 0.14 | 179,179,179,179             | 0     |
| 86  | OHX  | 7     | 228  | 7/7   | 0.84 | 0.17 | 137,137,137,137             | 0     |
| 85  | MG   | 6     | 1946 | 1/1   | 0.84 | 0.44 | 66,66,66,66                 | 0     |
| 86  | OHX  | 6     | 2171 | 7/7   | 0.84 | 0.17 | 148,148,148,148             | 0     |
| 85  | MG   | 2     | 2019 | 1/1   | 0.84 | 0.48 | 84,84,84,84                 | 0     |
| 86  | OHX  | 6     | 2175 | 7/7   | 0.84 | 0.21 | 145,145,145,145             | 0     |
| 86  | OHX  | 6     | 2176 | 7/7   | 0.84 | 0.24 | 123,123,123,123             | 0     |
| 86  | OHX  | 6     | 2177 | 7/7   | 0.84 | 0.16 | 148,148,148,148             | 0     |
| 85  | MG   | 1     | 3754 | 1/1   | 0.84 | 0.28 | 61,61,61,61                 | 0     |
| 86  | OHX  | 1     | 4116 | 7/7   | 0.84 | 0.27 | 108,108,108,108             | 0     |
| 85  | MG   | 5     | 3449 | 1/1   | 0.84 | 0.20 | 52,52,52,52                 | 0     |
| 85  | MG   | 5     | 3686 | 1/1   | 0.84 | 0.30 | 73,73,73,73                 | 0     |
| 85  | MG   | 5     | 3843 | 1/1   | 0.85 | 0.15 | 50,50,50,50                 | 0     |
| 86  | OHX  | 1     | 4184 | 7/7   | 0.85 | 0.22 | 128,128,128,128             | 0     |
| 85  | MG   | 1     | 3673 | 1/1   | 0.85 | 0.20 | 80,80,80,80                 | 0     |
| 86  | OHX  | 1     | 4188 | 7/7   | 0.85 | 0.22 | 121,121,121,121             | 0     |
| 85  | MG   | 1     | 3503 | 1/1   | 0.85 | 0.42 | 49,49,49,49                 | 0     |
| 85  | MG   | 2     | 1942 | 1/1   | 0.85 | 0.30 | 71,71,71,71                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 2     | 2162 | 7/7   | 0.85 | 0.16 | 160,160,160,160             | 0     |
| 86  | OHX  | 5     | 4090 | 7/7   | 0.85 | 0.26 | 104,104,104,104             | 0     |
| 85  | MG   | 5     | 3481 | 1/1   | 0.85 | 0.31 | 68,68,68,68                 | 0     |
| 85  | MG   | 1     | 3484 | 1/1   | 0.85 | 0.24 | 52,52,52,52                 | 0     |
| 85  | MG   | 5     | 3876 | 1/1   | 0.85 | 0.33 | 48,48,48,48                 | 0     |
| 86  | OHX  | 5     | 4150 | 7/7   | 0.85 | 0.20 | 125,125,125,125             | 0     |
| 86  | OHX  | 5     | 4154 | 7/7   | 0.85 | 0.17 | 140,140,140,140             | 0     |
| 85  | MG   | 4     | 213  | 1/1   | 0.85 | 0.21 | 52,52,52,52                 | 0     |
| 85  | MG   | 1     | 3526 | 1/1   | 0.85 | 0.18 | 39,39,39,39                 | 0     |
| 86  | OHX  | 5     | 4163 | 7/7   | 0.85 | 0.20 | 114,114,114,114             | 0     |
| 85  | MG   | 6     | 1979 | 1/1   | 0.85 | 0.31 | 46,46,46,46                 | 0     |
| 85  | MG   | 2     | 1905 | 1/1   | 0.85 | 0.45 | 65,65,65,65                 | 0     |
| 85  | MG   | 1     | 3456 | 1/1   | 0.85 | 0.36 | 58,58,58,58                 | 0     |
| 86  | OHX  | 5     | 4179 | 7/7   | 0.85 | 0.18 | 134,134,134,134             | 0     |
| 86  | OHX  | 5     | 4181 | 7/7   | 0.85 | 0.24 | 107,107,107,107             | 0     |
| 85  | MG   | 5     | 3896 | 1/1   | 0.85 | 0.30 | 52,52,52,52                 | 0     |
| 85  | MG   | 6     | 1941 | 1/1   | 0.85 | 0.34 | 48,48,48,48                 | 0     |
| 86  | OHX  | 5     | 4186 | 7/7   | 0.85 | 0.18 | 132,132,132,132             | 0     |
| 85  | MG   | 5     | 3506 | 1/1   | 0.85 | 0.22 | 31,31,31,31                 | 0     |
| 85  | MG   | 5     | 3728 | 1/1   | 0.85 | 0.35 | 76,76,76,76                 | 0     |
| 85  | MG   | 5     | 3536 | 1/1   | 0.85 | 0.34 | 40,40,40,40                 | 0     |
| 86  | OHX  | 5     | 4198 | 7/7   | 0.85 | 0.21 | 125,125,125,125             | 0     |
| 86  | OHX  | 1     | 4073 | 7/7   | 0.85 | 0.22 | 112,112,112,112             | 0     |
| 86  | OHX  | 5     | 4200 | 7/7   | 0.85 | 0.21 | 114,114,114,114             | 0     |
| 85  | MG   | 5     | 3737 | 1/1   | 0.85 | 0.13 | 41,41,41,41                 | 0     |
| 86  | OHX  | 4     | 234  | 7/7   | 0.85 | 0.21 | 111,111,111,111             | 0     |
| 86  | OHX  | 1     | 4084 | 7/7   | 0.85 | 0.20 | 112,112,112,112             | 0     |
| 86  | OHX  | 1     | 4098 | 7/7   | 0.85 | 0.20 | 125,125,125,125             | 0     |
| 86  | OHX  | 5     | 4211 | 7/7   | 0.85 | 0.15 | 149,149,149,149             | 0     |
| 86  | OHX  | L3    | 405  | 7/7   | 0.85 | 0.15 | 153,153,153,153             | 0     |
| 85  | MG   | L3    | 402  | 1/1   | 0.85 | 0.32 | 35,35,35,35                 | 0     |
| 86  | OHX  | 5     | 4216 | 7/7   | 0.85 | 0.24 | 114,114,114,114             | 0     |
| 86  | OHX  | M7    | 206  | 7/7   | 0.85 | 0.46 | 103,103,103,103             | 0     |
| 85  | MG   | 6     | 1949 | 1/1   | 0.85 | 0.40 | 54,54,54,54                 | 0     |
| 86  | OHX  | 1     | 4113 | 7/7   | 0.85 | 0.17 | 131,131,131,131             | 0     |
| 85  | MG   | 5     | 3762 | 1/1   | 0.85 | 0.22 | 44,44,44,44                 | 0     |
| 85  | MG   | 6     | 1916 | 1/1   | 0.85 | 0.48 | 65,65,65,65                 | 0     |
| 86  | OHX  | 5     | 4225 | 7/7   | 0.85 | 0.16 | 137,137,137,137             | 0     |
| 86  | OHX  | 6     | 2135 | 7/7   | 0.85 | 0.17 | 155,155,155,155             | 0     |
| 86  | OHX  | 1     | 4119 | 7/7   | 0.85 | 0.19 | 119,119,119,119             | 0     |
| 86  | OHX  | 1     | 4129 | 7/7   | 0.85 | 0.26 | 112,112,112,112             | 0     |
| 85  | MG   | s9    | 201  | 1/1   | 0.85 | 0.44 | 70,70,70,70                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | c1    | 201  | 1/1   | 0.85 | 0.18 | 50,50,50,50                 | 0     |
| 86  | OHX  | 6     | 2167 | 7/7   | 0.85 | 0.17 | 143,143,143,143             | 0     |
| 85  | MG   | c7    | 201  | 1/1   | 0.85 | 0.27 | 74,74,74,74                 | 0     |
| 85  | MG   | 5     | 3607 | 1/1   | 0.85 | 0.25 | 48,48,48,48                 | 0     |
| 85  | MG   | 6     | 1990 | 1/1   | 0.85 | 0.18 | 88,88,88,88                 | 0     |
| 85  | MG   | sM    | 301  | 1/1   | 0.85 | 0.13 | 44,44,44,44                 | 0     |
| 86  | OHX  | 2     | 2090 | 7/7   | 0.85 | 0.17 | 138,138,138,138             | 0     |
| 86  | OHX  | 1     | 4149 | 7/7   | 0.85 | 0.19 | 141,141,141,141             | 0     |
| 85  | MG   | 6     | 1917 | 1/1   | 0.85 | 0.32 | 56,56,56,56                 | 0     |
| 86  | OHX  | 2     | 2119 | 7/7   | 0.85 | 0.20 | 131,131,131,131             | 0     |
| 86  | OHX  | 1     | 4153 | 7/7   | 0.85 | 0.15 | 145,145,145,145             | 0     |
| 86  | OHX  | 1     | 4162 | 7/7   | 0.85 | 0.20 | 125,125,125,125             | 0     |
| 86  | OHX  | 5     | 4249 | 7/7   | 0.85 | 0.20 | 133,133,133,133             | 0     |
| 86  | OHX  | 2     | 2123 | 7/7   | 0.85 | 0.20 | 148,148,148,148             | 0     |
| 85  | MG   | 1     | 3844 | 1/1   | 0.85 | 0.23 | 55,55,55,55                 | 0     |
| 86  | OHX  | 2     | 2136 | 7/7   | 0.85 | 0.20 | 128,128,128,128             | 0     |
| 86  | OHX  | 6     | 2189 | 7/7   | 0.85 | 0.15 | 154,154,154,154             | 0     |
| 85  | MG   | 2     | 1944 | 1/1   | 0.85 | 0.20 | 69,69,69,69                 | 0     |
| 85  | MG   | 1     | 3613 | 1/1   | 0.85 | 0.12 | 44,44,44,44                 | 0     |
| 85  | MG   | 1     | 3562 | 1/1   | 0.85 | 0.34 | 38,38,38,38                 | 0     |
| 85  | MG   | 6     | 1925 | 1/1   | 0.85 | 0.41 | 42,42,42,42                 | 0     |
| 85  | MG   | 2     | 1970 | 1/1   | 0.85 | 0.37 | 76,76,76,76                 | 0     |
| 86  | OHX  | 6     | 2196 | 7/7   | 0.85 | 0.14 | 174,174,174,174             | 0     |
| 86  | OHX  | 2     | 2151 | 7/7   | 0.85 | 0.14 | 177,177,177,177             | 0     |
| 86  | OHX  | m0    | 303  | 7/7   | 0.85 | 0.20 | 120,120,120,120             | 0     |
| 85  | MG   | 5     | 3460 | 1/1   | 0.85 | 0.23 | 31,31,31,31                 | 0     |
| 86  | OHX  | 1     | 4180 | 7/7   | 0.85 | 0.24 | 113,113,113,113             | 0     |
| 85  | MG   | 5     | 3835 | 1/1   | 0.85 | 0.17 | 36,36,36,36                 | 0     |
| 86  | OHX  | 6     | 2205 | 7/7   | 0.85 | 0.21 | 148,148,148,148             | 0     |
| 86  | OHX  | 1     | 4182 | 7/7   | 0.85 | 0.09 | 216,216,216,216             | 0     |
| 87  | ZN   | d7    | 101  | 1/1   | 0.85 | 0.23 | 139,139,139,139             | 0     |
| 85  | MG   | 5     | 3572 | 1/1   | 0.86 | 0.31 | 37,37,37,37                 | 0     |
| 86  | OHX  | 1     | 4211 | 7/7   | 0.86 | 0.23 | 117,117,117,117             | 0     |
| 86  | OHX  | 1     | 4212 | 7/7   | 0.86 | 0.22 | 126,126,126,126             | 0     |
| 85  | MG   | L2    | 302  | 1/1   | 0.86 | 0.10 | 40,40,40,40                 | 0     |
| 85  | MG   | 5     | 3776 | 1/1   | 0.86 | 0.26 | 82,82,82,82                 | 0     |
| 86  | OHX  | 5     | 4162 | 7/7   | 0.86 | 0.22 | 125,125,125,125             | 0     |
| 86  | OHX  | 3     | 222  | 7/7   | 0.86 | 0.15 | 150,150,150,150             | 0     |
| 85  | MG   | 1     | 3496 | 1/1   | 0.86 | 0.23 | 48,48,48,48                 | 0     |
| 85  | MG   | 5     | 3590 | 1/1   | 0.86 | 0.31 | 33,33,33,33                 | 0     |
| 86  | OHX  | 5     | 4173 | 7/7   | 0.86 | 0.11 | 180,180,180,180             | 0     |
| 85  | MG   | 5     | 3605 | 1/1   | 0.86 | 0.09 | 28,28,28,28                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | L3    | 403  | 1/1   | 0.86 | 0.27 | 52,52,52,52                 | 0     |
| 86  | OHX  | 2     | 2107 | 7/7   | 0.86 | 0.18 | 136,136,136,136             | 0     |
| 86  | OHX  | 2     | 2115 | 7/7   | 0.86 | 0.16 | 146,146,146,146             | 0     |
| 85  | MG   | 5     | 3405 | 1/1   | 0.86 | 0.21 | 30,30,30,30                 | 0     |
| 85  | MG   | 5     | 3621 | 1/1   | 0.86 | 0.22 | 48,48,48,48                 | 0     |
| 86  | OHX  | 5     | 4187 | 7/7   | 0.86 | 0.20 | 115,115,115,115             | 0     |
| 86  | OHX  | 5     | 4188 | 7/7   | 0.86 | 0.19 | 116,116,116,116             | 0     |
| 85  | MG   | 2     | 1955 | 1/1   | 0.86 | 0.30 | 64,64,64,64                 | 0     |
| 85  | MG   | 1     | 3826 | 1/1   | 0.86 | 0.17 | 47,47,47,47                 | 0     |
| 86  | OHX  | 6     | 2119 | 7/7   | 0.86 | 0.18 | 137,137,137,137             | 0     |
| 86  | OHX  | 2     | 2137 | 7/7   | 0.86 | 0.14 | 157,157,157,157             | 0     |
| 86  | OHX  | 2     | 2139 | 7/7   | 0.86 | 0.20 | 152,152,152,152             | 0     |
| 86  | OHX  | 6     | 2143 | 7/7   | 0.86 | 0.13 | 165,165,165,165             | 0     |
| 86  | OHX  | 6     | 2146 | 7/7   | 0.86 | 0.18 | 128,128,128,128             | 0     |
| 85  | MG   | 2     | 1981 | 1/1   | 0.86 | 0.38 | 61,61,61,61                 | 0     |
| 86  | OHX  | 5     | 4208 | 7/7   | 0.86 | 0.18 | 132,132,132,132             | 0     |
| 86  | OHX  | 6     | 2154 | 7/7   | 0.86 | 0.17 | 148,148,148,148             | 0     |
| 85  | MG   | 1     | 3837 | 1/1   | 0.86 | 0.30 | 49,49,49,49                 | 0     |
| 85  | MG   | 1     | 3839 | 1/1   | 0.86 | 0.32 | 49,49,49,49                 | 0     |
| 86  | OHX  | 1     | 4156 | 7/7   | 0.86 | 0.17 | 136,136,136,136             | 0     |
| 86  | OHX  | 1     | 4161 | 7/7   | 0.86 | 0.15 | 137,137,137,137             | 0     |
| 85  | MG   | 1     | 3469 | 1/1   | 0.86 | 0.23 | 43,43,43,43                 | 0     |
| 85  | MG   | 5     | 3825 | 1/1   | 0.86 | 0.17 | 42,42,42,42                 | 0     |
| 86  | OHX  | 6     | 2174 | 7/7   | 0.86 | 0.16 | 143,143,143,143             | 0     |
| 86  | OHX  | 2     | 2150 | 7/7   | 0.86 | 0.16 | 154,154,154,154             | 0     |
| 86  | OHX  | 1     | 4167 | 7/7   | 0.86 | 0.14 | 158,158,158,158             | 0     |
| 85  | MG   | N3    | 202  | 1/1   | 0.86 | 0.27 | 68,68,68,68                 | 0     |
| 86  | OHX  | 6     | 2180 | 7/7   | 0.86 | 0.17 | 135,135,135,135             | 0     |
| 86  | OHX  | 6     | 2181 | 7/7   | 0.86 | 0.15 | 143,143,143,143             | 0     |
| 85  | MG   | 2     | 1936 | 1/1   | 0.86 | 0.40 | 49,49,49,49                 | 0     |
| 86  | OHX  | 2     | 2154 | 7/7   | 0.86 | 0.15 | 149,149,149,149             | 0     |
| 85  | MG   | O1    | 201  | 1/1   | 0.86 | 0.21 | 70,70,70,70                 | 0     |
| 85  | MG   | 1     | 3759 | 1/1   | 0.86 | 0.16 | 50,50,50,50                 | 0     |
| 86  | OHX  | 5     | 4232 | 7/7   | 0.86 | 0.12 | 167,167,167,167             | 0     |
| 85  | MG   | 5     | 3473 | 1/1   | 0.86 | 0.09 | 33,33,33,33                 | 0     |
| 85  | MG   | 5     | 3476 | 1/1   | 0.86 | 0.27 | 73,73,73,73                 | 0     |
| 86  | OHX  | 5     | 4235 | 7/7   | 0.86 | 0.14 | 158,158,158,158             | 0     |
| 85  | MG   | 1     | 3682 | 1/1   | 0.86 | 0.13 | 41,41,41,41                 | 0     |
| 85  | MG   | 5     | 3870 | 1/1   | 0.86 | 0.19 | 23,23,23,23                 | 0     |
| 86  | OHX  | 5     | 4239 | 7/7   | 0.86 | 0.22 | 126,126,126,126             | 0     |
| 85  | MG   | 5     | 3689 | 1/1   | 0.86 | 0.22 | 48,48,48,48                 | 0     |
| 86  | OHX  | 5     | 4241 | 7/7   | 0.86 | 0.14 | 139,139,139,139             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 5     | 3693 | 1/1   | 0.86 | 0.22 | 50,50,50,50                 | 0     |
| 86  | OHX  | 2     | 2165 | 7/7   | 0.86 | 0.14 | 168,168,168,168             | 0     |
| 85  | MG   | 1     | 3764 | 1/1   | 0.86 | 0.13 | 43,43,43,43                 | 0     |
| 85  | MG   | 6     | 1959 | 1/1   | 0.86 | 0.44 | 60,60,60,60                 | 0     |
| 85  | MG   | 1     | 3865 | 1/1   | 0.86 | 0.27 | 65,65,65,65                 | 0     |
| 85  | MG   | 1     | 3689 | 1/1   | 0.86 | 0.20 | 82,82,82,82                 | 0     |
| 85  | MG   | 1     | 3690 | 1/1   | 0.86 | 0.16 | 47,47,47,47                 | 0     |
| 85  | MG   | 3     | 209  | 1/1   | 0.86 | 0.25 | 62,62,62,62                 | 0     |
| 85  | MG   | 1     | 3775 | 1/1   | 0.86 | 0.23 | 51,51,51,51                 | 0     |
| 86  | OHX  | 6     | 2203 | 7/7   | 0.86 | 0.18 | 142,142,142,142             | 0     |
| 85  | MG   | 1     | 3415 | 1/1   | 0.86 | 0.27 | 34,34,34,34                 | 0     |
| 86  | OHX  | D9    | 102  | 7/7   | 0.86 | 0.18 | 147,147,147,147             | 0     |
| 85  | MG   | 1     | 3416 | 1/1   | 0.86 | 0.10 | 49,49,49,49                 | 0     |
| 86  | OHX  | 8     | 226  | 7/7   | 0.86 | 0.19 | 135,135,135,135             | 0     |
| 86  | OHX  | 1     | 4039 | 7/7   | 0.86 | 0.20 | 124,124,124,124             | 0     |
| 85  | MG   | 5     | 3526 | 1/1   | 0.86 | 0.22 | 46,46,46,46                 | 0     |
| 85  | MG   | 1     | 3585 | 1/1   | 0.86 | 0.34 | 39,39,39,39                 | 0     |
| 86  | OHX  | 1     | 4071 | 7/7   | 0.86 | 0.20 | 125,125,125,125             | 0     |
| 86  | OHX  | 1     | 4204 | 7/7   | 0.86 | 0.20 | 130,130,130,130             | 0     |
| 85  | MG   | 1     | 3518 | 1/1   | 0.86 | 0.31 | 37,37,37,37                 | 0     |
| 85  | MG   | 1     | 3588 | 1/1   | 0.86 | 0.38 | 36,36,36,36                 | 0     |
| 85  | MG   | 1     | 3521 | 1/1   | 0.86 | 0.27 | 41,41,41,41                 | 0     |
| 86  | OHX  | 5     | 4101 | 7/7   | 0.86 | 0.22 | 115,115,115,115             | 0     |
| 86  | OHX  | 5     | 4102 | 7/7   | 0.86 | 0.18 | 126,126,126,126             | 0     |
| 86  | OHX  | 5     | 4130 | 7/7   | 0.86 | 0.18 | 127,127,127,127             | 0     |
| 85  | MG   | 2     | 2004 | 1/1   | 0.86 | 0.14 | 59,59,59,59                 | 0     |
| 85  | MG   | 1     | 3630 | 1/1   | 0.87 | 0.15 | 69,69,69,69                 | 0     |
| 85  | MG   | 5     | 3564 | 1/1   | 0.87 | 0.33 | 28,28,28,28                 | 0     |
| 86  | OHX  | 1     | 4177 | 7/7   | 0.87 | 0.13 | 165,165,165,165             | 0     |
| 86  | OHX  | 1     | 4178 | 7/7   | 0.87 | 0.16 | 141,141,141,141             | 0     |
| 85  | MG   | 1     | 3560 | 1/1   | 0.87 | 0.31 | 47,47,47,47                 | 0     |
| 86  | OHX  | 2     | 2142 | 7/7   | 0.87 | 0.17 | 136,136,136,136             | 0     |
| 85  | MG   | 5     | 3784 | 1/1   | 0.87 | 0.24 | 30,30,30,30                 | 0     |
| 86  | OHX  | 5     | 4099 | 7/7   | 0.87 | 0.18 | 121,121,121,121             | 0     |
| 85  | MG   | 1     | 3459 | 1/1   | 0.87 | 0.23 | 39,39,39,39                 | 0     |
| 85  | MG   | 5     | 3574 | 1/1   | 0.87 | 0.44 | 35,35,35,35                 | 0     |
| 86  | OHX  | 5     | 4111 | 7/7   | 0.87 | 0.21 | 105,105,105,105             | 0     |
| 86  | OHX  | 5     | 4122 | 7/7   | 0.87 | 0.19 | 117,117,117,117             | 0     |
| 86  | OHX  | 2     | 2147 | 7/7   | 0.87 | 0.13 | 166,166,166,166             | 0     |
| 86  | OHX  | 5     | 4134 | 7/7   | 0.87 | 0.13 | 177,177,177,177             | 0     |
| 86  | OHX  | 5     | 4140 | 7/7   | 0.87 | 0.16 | 116,116,116,116             | 0     |
| 86  | OHX  | 5     | 4141 | 7/7   | 0.87 | 0.22 | 122,122,122,122             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 5     | 4143 | 7/7   | 0.87 | 0.19 | 123,123,123,123             | 0     |
| 85  | MG   | 5     | 3800 | 1/1   | 0.87 | 0.06 | 36,36,36,36                 | 0     |
| 85  | MG   | 1     | 3639 | 1/1   | 0.87 | 0.33 | 71,71,71,71                 | 0     |
| 85  | MG   | 1     | 3405 | 1/1   | 0.87 | 0.27 | 56,56,56,56                 | 0     |
| 85  | MG   | 5     | 3809 | 1/1   | 0.87 | 0.24 | 36,36,36,36                 | 0     |
| 86  | OHX  | 5     | 4155 | 7/7   | 0.87 | 0.23 | 107,107,107,107             | 0     |
| 85  | MG   | 1     | 3566 | 1/1   | 0.87 | 0.27 | 38,38,38,38                 | 0     |
| 85  | MG   | 1     | 3857 | 1/1   | 0.87 | 0.28 | 41,41,41,41                 | 0     |
| 86  | OHX  | 5     | 4161 | 7/7   | 0.87 | 0.20 | 105,105,105,105             | 0     |
| 86  | OHX  | 2     | 2155 | 7/7   | 0.87 | 0.16 | 143,143,143,143             | 0     |
| 86  | OHX  | 1     | 4194 | 7/7   | 0.87 | 0.16 | 141,141,141,141             | 0     |
| 85  | MG   | 1     | 3747 | 1/1   | 0.87 | 0.22 | 59,59,59,59                 | 0     |
| 85  | MG   | 5     | 3611 | 1/1   | 0.87 | 0.18 | 35,35,35,35                 | 0     |
| 85  | MG   | 5     | 3822 | 1/1   | 0.87 | 0.14 | 40,40,40,40                 | 0     |
| 85  | MG   | 1     | 3752 | 1/1   | 0.87 | 0.13 | 47,47,47,47                 | 0     |
| 85  | MG   | 1     | 3753 | 1/1   | 0.87 | 0.21 | 53,53,53,53                 | 0     |
| 86  | OHX  | 1     | 4202 | 7/7   | 0.87 | 0.21 | 120,120,120,120             | 0     |
| 85  | MG   | 5     | 3634 | 1/1   | 0.87 | 0.09 | 35,35,35,35                 | 0     |
| 85  | MG   | 1     | 3573 | 1/1   | 0.87 | 0.39 | 44,44,44,44                 | 0     |
| 86  | OHX  | 5     | 4185 | 7/7   | 0.87 | 0.15 | 139,139,139,139             | 0     |
| 85  | MG   | 5     | 3418 | 1/1   | 0.87 | 0.28 | 24,24,24,24                 | 0     |
| 85  | MG   | 1     | 3647 | 1/1   | 0.87 | 0.25 | 45,45,45,45                 | 0     |
| 86  | OHX  | 2     | 2169 | 7/7   | 0.87 | 0.17 | 149,149,149,149             | 0     |
| 85  | MG   | 1     | 3648 | 1/1   | 0.87 | 0.18 | 64,64,64,64                 | 0     |
| 86  | OHX  | 5     | 4190 | 7/7   | 0.87 | 0.24 | 108,108,108,108             | 0     |
| 85  | MG   | 2     | 1937 | 1/1   | 0.87 | 0.36 | 59,59,59,59                 | 0     |
| 85  | MG   | 3     | 213  | 1/1   | 0.87 | 0.27 | 61,61,61,61                 | 0     |
| 86  | OHX  | 5     | 4197 | 7/7   | 0.87 | 0.14 | 164,164,164,164             | 0     |
| 85  | MG   | 5     | 3868 | 1/1   | 0.87 | 0.08 | 49,49,49,49                 | 0     |
| 86  | OHX  | 1     | 4213 | 7/7   | 0.87 | 0.24 | 121,121,121,121             | 0     |
| 85  | MG   | 4     | 202  | 1/1   | 0.87 | 0.35 | 50,50,50,50                 | 0     |
| 85  | MG   | 5     | 3660 | 1/1   | 0.87 | 0.10 | 39,39,39,39                 | 0     |
| 86  | OHX  | 5     | 4206 | 7/7   | 0.87 | 0.21 | 126,126,126,126             | 0     |
| 85  | MG   | 1     | 3472 | 1/1   | 0.87 | 0.14 | 43,43,43,43                 | 0     |
| 85  | MG   | 1     | 3407 | 1/1   | 0.87 | 0.28 | 38,38,38,38                 | 0     |
| 86  | OHX  | S8    | 302  | 7/7   | 0.87 | 0.13 | 157,157,157,157             | 0     |
| 86  | OHX  | 4     | 237  | 7/7   | 0.87 | 0.18 | 135,135,135,135             | 0     |
| 85  | MG   | 1     | 3480 | 1/1   | 0.87 | 0.21 | 80,80,80,80                 | 0     |
| 85  | MG   | 5     | 3465 | 1/1   | 0.87 | 0.09 | 34,34,34,34                 | 0     |
| 85  | MG   | 2     | 1922 | 1/1   | 0.87 | 0.34 | 65,65,65,65                 | 0     |
| 85  | MG   | 5     | 3890 | 1/1   | 0.87 | 0.24 | 37,37,37,37                 | 0     |
| 86  | OHX  | 5     | 4218 | 7/7   | 0.87 | 0.20 | 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  | MG   | 1     | 3523 | 1/1   | 0.87 | 0.20 | 82,82,82,82                 | 0     |
| 85  | MG   | 6     | 1997 | 1/1   | 0.87 | 0.18 | 74,74,74,74                 | 0     |
| 85  | MG   | 1     | 3439 | 1/1   | 0.87 | 0.27 | 50,50,50,50                 | 0     |
| 85  | MG   | 4     | 223  | 1/1   | 0.87 | 0.19 | 46,46,46,46                 | 0     |
| 86  | OHX  | 1     | 4083 | 7/7   | 0.87 | 0.21 | 119,119,119,119             | 0     |
| 85  | MG   | 2     | 2011 | 1/1   | 0.87 | 0.36 | 78,78,78,78                 | 0     |
| 86  | OHX  | 1     | 4093 | 7/7   | 0.87 | 0.16 | 131,131,131,131             | 0     |
| 85  | MG   | 7     | 216  | 1/1   | 0.87 | 0.22 | 47,47,47,47                 | 0     |
| 85  | MG   | 2     | 1939 | 1/1   | 0.87 | 0.41 | 70,70,70,70                 | 0     |
| 86  | OHX  | 5     | 4229 | 7/7   | 0.87 | 0.18 | 127,127,127,127             | 0     |
| 85  | MG   | 1     | 3612 | 1/1   | 0.87 | 0.12 | 43,43,43,43                 | 0     |
| 86  | OHX  | 1     | 4108 | 7/7   | 0.87 | 0.20 | 120,120,120,120             | 0     |
| 86  | OHX  | 1     | 4111 | 7/7   | 0.87 | 0.17 | 128,128,128,128             | 0     |
| 86  | OHX  | 1     | 4112 | 7/7   | 0.87 | 0.18 | 121,121,121,121             | 0     |
| 85  | MG   | 8     | 209  | 1/1   | 0.87 | 0.13 | 43,43,43,43                 | 0     |
| 85  | MG   | 5     | 3713 | 1/1   | 0.87 | 0.12 | 43,43,43,43                 | 0     |
| 85  | MG   | 8     | 214  | 1/1   | 0.87 | 0.30 | 56,56,56,56                 | 0     |
| 85  | MG   | 13    | 403  | 1/1   | 0.87 | 0.19 | 31,31,31,31                 | 0     |
| 86  | OHX  | 1     | 4125 | 7/7   | 0.87 | 0.16 | 140,140,140,140             | 0     |
| 85  | MG   | 6     | 2015 | 1/1   | 0.87 | 0.21 | 70,70,70,70                 | 0     |
| 85  | MG   | 17    | 302  | 1/1   | 0.87 | 0.21 | 40,40,40,40                 | 0     |
| 85  | MG   | 1     | 3542 | 1/1   | 0.87 | 0.27 | 65,65,65,65                 | 0     |
| 86  | OHX  | 1     | 4134 | 7/7   | 0.87 | 0.18 | 143,143,143,143             | 0     |
| 86  | OHX  | 1     | 4135 | 7/7   | 0.87 | 0.15 | 154,154,154,154             | 0     |
| 86  | OHX  | 1     | 4136 | 7/7   | 0.87 | 0.18 | 111,111,111,111             | 0     |
| 85  | MG   | 1     | 3614 | 1/1   | 0.87 | 0.28 | 49,49,49,49                 | 0     |
| 85  | MG   | 5     | 3722 | 1/1   | 0.87 | 0.24 | 43,43,43,43                 | 0     |
| 86  | OHX  | 1     | 4144 | 7/7   | 0.87 | 0.17 | 127,127,127,127             | 0     |
| 85  | MG   | M0    | 303  | 1/1   | 0.87 | 0.28 | 34,34,34,34                 | 0     |
| 85  | MG   | 5     | 3502 | 1/1   | 0.87 | 0.22 | 46,46,46,46                 | 0     |
| 86  | OHX  | 1     | 4147 | 7/7   | 0.87 | 0.21 | 108,108,108,108             | 0     |
| 86  | OHX  | 5     | 4253 | 7/7   | 0.87 | 0.17 | 135,135,135,135             | 0     |
| 85  | MG   | 1     | 3707 | 1/1   | 0.87 | 0.39 | 63,63,63,63                 | 0     |
| 85  | MG   | 5     | 3505 | 1/1   | 0.87 | 0.29 | 52,52,52,52                 | 0     |
| 86  | OHX  | 7     | 227  | 7/7   | 0.87 | 0.21 | 112,112,112,112             | 0     |
| 85  | MG   | 1     | 3548 | 1/1   | 0.87 | 0.36 | 65,65,65,65                 | 0     |
| 86  | OHX  | 2     | 2092 | 7/7   | 0.87 | 0.15 | 147,147,147,147             | 0     |
| 85  | MG   | 1     | 3714 | 1/1   | 0.87 | 0.21 | 57,57,57,57                 | 0     |
| 86  | OHX  | 8     | 229  | 7/7   | 0.87 | 0.18 | 119,119,119,119             | 0     |
| 86  | OHX  | 8     | 230  | 7/7   | 0.87 | 0.19 | 132,132,132,132             | 0     |
| 86  | OHX  | 2     | 2102 | 7/7   | 0.87 | 0.16 | 142,142,142,142             | 0     |
| 85  | MG   | 5     | 3533 | 1/1   | 0.87 | 0.18 | 52,52,52,52                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 2     | 2111 | 7/7   | 0.87 | 0.14 | 153,153,153,153             | 0     |
| 85  | MG   | 6     | 2036 | 1/1   | 0.87 | 0.44 | 67,67,67,67                 | 0     |
| 85  | MG   | 5     | 3543 | 1/1   | 0.87 | 0.35 | 69,69,69,69                 | 0     |
| 86  | OHX  | 2     | 2122 | 7/7   | 0.87 | 0.16 | 137,137,137,137             | 0     |
| 85  | MG   | 6     | 1955 | 1/1   | 0.87 | 0.44 | 42,42,42,42                 | 0     |
| 86  | OHX  | 2     | 2129 | 7/7   | 0.87 | 0.13 | 188,188,188,188             | 0     |
| 86  | OHX  | m8    | 201  | 7/7   | 0.87 | 0.21 | 123,123,123,123             | 0     |
| 86  | OHX  | 2     | 2131 | 7/7   | 0.87 | 0.20 | 131,131,131,131             | 0     |
| 85  | MG   | 2     | 1933 | 1/1   | 0.87 | 0.33 | 71,71,71,71                 | 0     |
| 86  | OHX  | 2     | 2135 | 7/7   | 0.87 | 0.18 | 124,124,124,124             | 0     |
| 87  | ZN   | e1    | 501  | 1/1   | 0.87 | 0.09 | 172,172,172,172             | 0     |
| 86  | OHX  | 5     | 4108 | 7/7   | 0.88 | 0.18 | 111,111,111,111             | 0     |
| 85  | MG   | 5     | 3643 | 1/1   | 0.88 | 0.32 | 56,56,56,56                 | 0     |
| 86  | OHX  | 5     | 4113 | 7/7   | 0.88 | 0.17 | 131,131,131,131             | 0     |
| 86  | OHX  | 5     | 4120 | 7/7   | 0.88 | 0.19 | 117,117,117,117             | 0     |
| 85  | MG   | 5     | 3644 | 1/1   | 0.88 | 0.10 | 33,33,33,33                 | 0     |
| 86  | OHX  | 1     | 4187 | 7/7   | 0.88 | 0.15 | 145,145,145,145             | 0     |
| 85  | MG   | 6     | 2012 | 1/1   | 0.88 | 0.30 | 58,58,58,58                 | 0     |
| 85  | MG   | 5     | 3864 | 1/1   | 0.88 | 0.07 | 38,38,38,38                 | 0     |
| 85  | MG   | 6     | 2013 | 1/1   | 0.88 | 0.15 | 59,59,59,59                 | 0     |
| 86  | OHX  | 5     | 4142 | 7/7   | 0.88 | 0.15 | 134,134,134,134             | 0     |
| 85  | MG   | 1     | 3425 | 1/1   | 0.88 | 0.25 | 48,48,48,48                 | 0     |
| 85  | MG   | 6     | 1908 | 1/1   | 0.88 | 0.19 | 48,48,48,48                 | 0     |
| 85  | MG   | 4     | 207  | 1/1   | 0.88 | 0.30 | 34,34,34,34                 | 0     |
| 86  | OHX  | 2     | 2170 | 7/7   | 0.88 | 0.16 | 139,139,139,139             | 0     |
| 86  | OHX  | 5     | 4152 | 7/7   | 0.88 | 0.16 | 142,142,142,142             | 0     |
| 85  | MG   | 4     | 212  | 1/1   | 0.88 | 0.28 | 50,50,50,50                 | 0     |
| 86  | OHX  | 2     | 2173 | 7/7   | 0.88 | 0.17 | 144,144,144,144             | 0     |
| 85  | MG   | 1     | 3538 | 1/1   | 0.88 | 0.37 | 48,48,48,48                 | 0     |
| 85  | MG   | 5     | 3674 | 1/1   | 0.88 | 0.20 | 63,63,63,63                 | 0     |
| 86  | OHX  | 5     | 4160 | 7/7   | 0.88 | 0.17 | 132,132,132,132             | 0     |
| 85  | MG   | 1     | 3431 | 1/1   | 0.88 | 0.32 | 47,47,47,47                 | 0     |
| 85  | MG   | 1     | 3458 | 1/1   | 0.88 | 0.22 | 27,27,27,27                 | 0     |
| 85  | MG   | 6     | 2032 | 1/1   | 0.88 | 0.27 | 98,98,98,98                 | 0     |
| 86  | OHX  | 5     | 4164 | 7/7   | 0.88 | 0.22 | 109,109,109,109             | 0     |
| 85  | MG   | 5     | 3489 | 1/1   | 0.88 | 0.29 | 25,25,25,25                 | 0     |
| 85  | MG   | 6     | 1965 | 1/1   | 0.88 | 0.30 | 58,58,58,58                 | 0     |
| 86  | OHX  | 1     | 4206 | 7/7   | 0.88 | 0.17 | 125,125,125,125             | 0     |
| 85  | MG   | 5     | 3690 | 1/1   | 0.88 | 0.33 | 43,43,43,43                 | 0     |
| 85  | MG   | 6     | 1919 | 1/1   | 0.88 | 0.33 | 42,42,42,42                 | 0     |
| 86  | OHX  | 1     | 4024 | 7/7   | 0.88 | 0.18 | 119,119,119,119             | 0     |
| 85  | MG   | 7     | 208  | 1/1   | 0.88 | 0.19 | 54,54,54,54                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 7     | 213  | 1/1   | 0.88 | 0.12 | 70,70,70,70                 | 0     |
| 86  | OHX  | 1     | 4061 | 7/7   | 0.88 | 0.20 | 114,114,114,114             | 0     |
| 85  | MG   | 5     | 3500 | 1/1   | 0.88 | 0.27 | 37,37,37,37                 | 0     |
| 85  | MG   | 5     | 3702 | 1/1   | 0.88 | 0.12 | 60,60,60,60                 | 0     |
| 85  | MG   | 8     | 205  | 1/1   | 0.88 | 0.21 | 49,49,49,49                 | 0     |
| 85  | MG   | 2     | 2013 | 1/1   | 0.88 | 0.31 | 72,72,72,72                 | 0     |
| 86  | OHX  | 3     | 223  | 7/7   | 0.88 | 0.19 | 126,126,126,126             | 0     |
| 85  | MG   | 5     | 3707 | 1/1   | 0.88 | 0.18 | 50,50,50,50                 | 0     |
| 86  | OHX  | 5     | 4192 | 7/7   | 0.88 | 0.19 | 119,119,119,119             | 0     |
| 86  | OHX  | 5     | 4193 | 7/7   | 0.88 | 0.16 | 138,138,138,138             | 0     |
| 86  | OHX  | 5     | 4194 | 7/7   | 0.88 | 0.18 | 119,119,119,119             | 0     |
| 85  | MG   | 1     | 3637 | 1/1   | 0.88 | 0.14 | 42,42,42,42                 | 0     |
| 86  | OHX  | 5     | 4196 | 7/7   | 0.88 | 0.20 | 114,114,114,114             | 0     |
| 85  | MG   | 1     | 3723 | 1/1   | 0.88 | 0.16 | 45,45,45,45                 | 0     |
| 86  | OHX  | 1     | 4085 | 7/7   | 0.88 | 0.15 | 137,137,137,137             | 0     |
| 86  | OHX  | 1     | 4091 | 7/7   | 0.88 | 0.21 | 122,122,122,122             | 0     |
| 85  | MG   | 6     | 1970 | 1/1   | 0.88 | 0.18 | 60,60,60,60                 | 0     |
| 86  | OHX  | 5     | 4204 | 7/7   | 0.88 | 0.20 | 113,113,113,113             | 0     |
| 85  | MG   | 5     | 3519 | 1/1   | 0.88 | 0.26 | 25,25,25,25                 | 0     |
| 85  | MG   | 1     | 3670 | 1/1   | 0.88 | 0.39 | 82,82,82,82                 | 0     |
| 86  | OHX  | M8    | 201  | 7/7   | 0.88 | 0.18 | 134,134,134,134             | 0     |
| 86  | OHX  | 1     | 4101 | 7/7   | 0.88 | 0.15 | 144,144,144,144             | 0     |
| 86  | OHX  | 1     | 4103 | 7/7   | 0.88 | 0.18 | 113,113,113,113             | 0     |
| 85  | MG   | 1     | 3846 | 1/1   | 0.88 | 0.34 | 58,58,58,58                 | 0     |
| 85  | MG   | 1     | 3559 | 1/1   | 0.88 | 0.10 | 52,52,52,52                 | 0     |
| 86  | OHX  | 5     | 4212 | 7/7   | 0.88 | 0.19 | 137,137,137,137             | 0     |
| 85  | MG   | 5     | 3541 | 1/1   | 0.88 | 0.32 | 32,32,32,32                 | 0     |
| 85  | MG   | s8    | 301  | 1/1   | 0.88 | 0.23 | 51,51,51,51                 | 0     |
| 85  | MG   | n8    | 204  | 1/1   | 0.88 | 0.14 | 41,41,41,41                 | 0     |
| 85  | MG   | 1     | 3780 | 1/1   | 0.88 | 0.15 | 57,57,57,57                 | 0     |
| 85  | MG   | 5     | 3550 | 1/1   | 0.88 | 0.33 | 53,53,53,53                 | 0     |
| 86  | OHX  | 1     | 4117 | 7/7   | 0.88 | 0.12 | 163,163,163,163             | 0     |
| 85  | MG   | 5     | 3738 | 1/1   | 0.88 | 0.37 | 71,71,71,71                 | 0     |
| 86  | OHX  | 6     | 2160 | 7/7   | 0.88 | 0.15 | 135,135,135,135             | 0     |
| 86  | OHX  | 6     | 2162 | 7/7   | 0.88 | 0.20 | 124,124,124,124             | 0     |
| 86  | OHX  | 6     | 2163 | 7/7   | 0.88 | 0.17 | 124,124,124,124             | 0     |
| 86  | OHX  | 1     | 4122 | 7/7   | 0.88 | 0.17 | 124,124,124,124             | 0     |
| 86  | OHX  | 1     | 4124 | 7/7   | 0.88 | 0.18 | 129,129,129,129             | 0     |
| 86  | OHX  | 2     | 2079 | 7/7   | 0.88 | 0.12 | 167,167,167,167             | 0     |
| 86  | OHX  | 6     | 2170 | 7/7   | 0.88 | 0.23 | 114,114,114,114             | 0     |
| 86  | OHX  | 2     | 2087 | 7/7   | 0.88 | 0.16 | 130,130,130,130             | 0     |
| 85  | MG   | 1     | 3486 | 1/1   | 0.88 | 0.34 | 43,43,43,43                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 5     | 3556 | 1/1   | 0.88 | 0.25 | 36,36,36,36                 | 0     |
| 85  | MG   | 6     | 1932 | 1/1   | 0.88 | 0.24 | 45,45,45,45                 | 0     |
| 85  | MG   | 1     | 3785 | 1/1   | 0.88 | 0.26 | 47,47,47,47                 | 0     |
| 85  | MG   | 5     | 3569 | 1/1   | 0.88 | 0.28 | 36,36,36,36                 | 0     |
| 86  | OHX  | 1     | 4137 | 7/7   | 0.88 | 0.18 | 133,133,133,133             | 0     |
| 85  | MG   | 1     | 3788 | 1/1   | 0.88 | 0.29 | 54,54,54,54                 | 0     |
| 85  | MG   | 5     | 3403 | 1/1   | 0.88 | 0.33 | 49,49,49,49                 | 0     |
| 85  | MG   | 3     | 202  | 1/1   | 0.88 | 0.14 | 44,44,44,44                 | 0     |
| 86  | OHX  | 2     | 2121 | 7/7   | 0.88 | 0.15 | 141,141,141,141             | 0     |
| 85  | MG   | 5     | 3411 | 1/1   | 0.88 | 0.31 | 33,33,33,33                 | 0     |
| 85  | MG   | 5     | 3581 | 1/1   | 0.88 | 0.33 | 35,35,35,35                 | 0     |
| 85  | MG   | 5     | 3586 | 1/1   | 0.88 | 0.32 | 23,23,23,23                 | 0     |
| 86  | OHX  | 5     | 4245 | 7/7   | 0.88 | 0.20 | 100,100,100,100             | 0     |
| 85  | MG   | 1     | 3464 | 1/1   | 0.88 | 0.29 | 28,28,28,28                 | 0     |
| 86  | OHX  | 2     | 2133 | 7/7   | 0.88 | 0.13 | 154,154,154,154             | 0     |
| 85  | MG   | 1     | 3436 | 1/1   | 0.88 | 0.17 | 40,40,40,40                 | 0     |
| 86  | OHX  | 1     | 4152 | 7/7   | 0.88 | 0.15 | 135,135,135,135             | 0     |
| 85  | MG   | 5     | 3594 | 1/1   | 0.88 | 0.31 | 37,37,37,37                 | 0     |
| 85  | MG   | 5     | 3803 | 1/1   | 0.88 | 0.24 | 52,52,52,52                 | 0     |
| 86  | OHX  | 1     | 4157 | 7/7   | 0.88 | 0.19 | 128,128,128,128             | 0     |
| 85  | MG   | 5     | 3597 | 1/1   | 0.88 | 0.32 | 32,32,32,32                 | 0     |
| 86  | OHX  | 2     | 2138 | 7/7   | 0.88 | 0.15 | 139,139,139,139             | 0     |
| 85  | MG   | 1     | 3741 | 1/1   | 0.88 | 0.28 | 52,52,52,52                 | 0     |
| 86  | OHX  | 6     | 2199 | 7/7   | 0.88 | 0.19 | 132,132,132,132             | 0     |
| 86  | OHX  | 2     | 2140 | 7/7   | 0.88 | 0.16 | 154,154,154,154             | 0     |
| 86  | OHX  | 1     | 4166 | 7/7   | 0.88 | 0.14 | 141,141,141,141             | 0     |
| 85  | MG   | 5     | 3422 | 1/1   | 0.88 | 0.27 | 37,37,37,37                 | 0     |
| 85  | MG   | 5     | 3608 | 1/1   | 0.88 | 0.28 | 31,31,31,31                 | 0     |
| 85  | MG   | N8    | 201  | 1/1   | 0.88 | 0.11 | 29,29,29,29                 | 0     |
| 85  | MG   | 6     | 1944 | 1/1   | 0.88 | 0.42 | 72,72,72,72                 | 0     |
| 85  | MG   | S2    | 302  | 1/1   | 0.88 | 0.53 | 73,73,73,73                 | 0     |
| 86  | OHX  | l5    | 303  | 7/7   | 0.88 | 0.16 | 134,134,134,134             | 0     |
| 85  | MG   | 5     | 3817 | 1/1   | 0.88 | 0.09 | 44,44,44,44                 | 0     |
| 85  | MG   | 5     | 3631 | 1/1   | 0.88 | 0.14 | 43,43,43,43                 | 0     |
| 86  | OHX  | c5    | 201  | 7/7   | 0.88 | 0.12 | 155,155,155,155             | 0     |
| 85  | MG   | 5     | 3632 | 1/1   | 0.88 | 0.39 | 90,90,90,90                 | 0     |
| 85  | MG   | 5     | 3633 | 1/1   | 0.88 | 0.15 | 46,46,46,46                 | 0     |
| 85  | MG   | 5     | 3833 | 1/1   | 0.88 | 0.12 | 71,71,71,71                 | 0     |
| 85  | MG   | 1     | 3750 | 1/1   | 0.88 | 0.18 | 51,51,51,51                 | 0     |
| 85  | MG   | 1     | 3751 | 1/1   | 0.88 | 0.20 | 48,48,48,48                 | 0     |
| 85  | MG   | 2     | 1923 | 1/1   | 0.88 | 0.40 | 61,61,61,61                 | 0     |
| 86  | OHX  | 2     | 2157 | 7/7   | 0.88 | 0.22 | 113,113,113,113             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 6     | 2011 | 1/1   | 0.88 | 0.12 | 50,50,50,50                 | 0     |
| 85  | MG   | 6     | 1901 | 1/1   | 0.89 | 0.33 | 46,46,46,46                 | 0     |
| 85  | MG   | 1     | 3533 | 1/1   | 0.89 | 0.29 | 26,26,26,26                 | 0     |
| 86  | OHX  | 5     | 4165 | 7/7   | 0.89 | 0.20 | 115,115,115,115             | 0     |
| 86  | OHX  | 1     | 4141 | 7/7   | 0.89 | 0.18 | 117,117,117,117             | 0     |
| 86  | OHX  | 6     | 2129 | 7/7   | 0.89 | 0.18 | 113,113,113,113             | 0     |
| 86  | OHX  | 5     | 4171 | 7/7   | 0.89 | 0.18 | 126,126,126,126             | 0     |
| 85  | MG   | 1     | 3726 | 1/1   | 0.89 | 0.16 | 52,52,52,52                 | 0     |
| 85  | MG   | 5     | 3892 | 1/1   | 0.89 | 0.20 | 21,21,21,21                 | 0     |
| 85  | MG   | 5     | 3895 | 1/1   | 0.89 | 0.13 | 102,102,102,102             | 0     |
| 86  | OHX  | 2     | 2152 | 7/7   | 0.89 | 0.16 | 142,142,142,142             | 0     |
| 86  | OHX  | 6     | 2148 | 7/7   | 0.89 | 0.15 | 129,129,129,129             | 0     |
| 85  | MG   | 5     | 3730 | 1/1   | 0.89 | 0.12 | 47,47,47,47                 | 0     |
| 86  | OHX  | 6     | 2152 | 7/7   | 0.89 | 0.15 | 134,134,134,134             | 0     |
| 85  | MG   | 6     | 1906 | 1/1   | 0.89 | 0.30 | 44,44,44,44                 | 0     |
| 86  | OHX  | 6     | 2155 | 7/7   | 0.89 | 0.15 | 141,141,141,141             | 0     |
| 86  | OHX  | 6     | 2156 | 7/7   | 0.89 | 0.13 | 131,131,131,131             | 0     |
| 85  | MG   | 5     | 3736 | 1/1   | 0.89 | 0.14 | 50,50,50,50                 | 0     |
| 85  | MG   | 1     | 3669 | 1/1   | 0.89 | 0.18 | 39,39,39,39                 | 0     |
| 85  | MG   | 2     | 1980 | 1/1   | 0.89 | 0.36 | 66,66,66,66                 | 0     |
| 85  | MG   | 5     | 3477 | 1/1   | 0.89 | 0.30 | 34,34,34,34                 | 0     |
| 86  | OHX  | 6     | 2164 | 7/7   | 0.89 | 0.20 | 117,117,117,117             | 0     |
| 85  | MG   | 6     | 2025 | 1/1   | 0.89 | 0.19 | 56,56,56,56                 | 0     |
| 85  | MG   | 7     | 215  | 1/1   | 0.89 | 0.24 | 61,61,61,61                 | 0     |
| 86  | OHX  | 6     | 2168 | 7/7   | 0.89 | 0.13 | 147,147,147,147             | 0     |
| 85  | MG   | 5     | 3760 | 1/1   | 0.89 | 0.08 | 49,49,49,49                 | 0     |
| 85  | MG   | 4     | 201  | 1/1   | 0.89 | 0.36 | 55,55,55,55                 | 0     |
| 85  | MG   | 5     | 3629 | 1/1   | 0.89 | 0.23 | 62,62,62,62                 | 0     |
| 85  | MG   | 6     | 2029 | 1/1   | 0.89 | 0.20 | 88,88,88,88                 | 0     |
| 85  | MG   | 1     | 3636 | 1/1   | 0.89 | 0.28 | 56,56,56,56                 | 0     |
| 85  | MG   | 1     | 3676 | 1/1   | 0.89 | 0.39 | 65,65,65,65                 | 0     |
| 85  | MG   | 8     | 213  | 1/1   | 0.89 | 0.21 | 88,88,88,88                 | 0     |
| 86  | OHX  | 2     | 2171 | 7/7   | 0.89 | 0.16 | 141,141,141,141             | 0     |
| 86  | OHX  | 6     | 2179 | 7/7   | 0.89 | 0.21 | 112,112,112,112             | 0     |
| 85  | MG   | 5     | 3777 | 1/1   | 0.89 | 0.20 | 55,55,55,55                 | 0     |
| 85  | MG   | l3    | 401  | 1/1   | 0.89 | 0.39 | 24,24,24,24                 | 0     |
| 85  | MG   | 6     | 1915 | 1/1   | 0.89 | 0.35 | 56,56,56,56                 | 0     |
| 85  | MG   | 1     | 3505 | 1/1   | 0.89 | 0.32 | 40,40,40,40                 | 0     |
| 85  | MG   | 2     | 1925 | 1/1   | 0.89 | 0.48 | 67,67,67,67                 | 0     |
| 85  | MG   | 6     | 1918 | 1/1   | 0.89 | 0.38 | 69,69,69,69                 | 0     |
| 85  | MG   | 1     | 3438 | 1/1   | 0.89 | 0.22 | 33,33,33,33                 | 0     |
| 85  | MG   | m7    | 202  | 1/1   | 0.89 | 0.18 | 36,36,36,36                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 5     | 3795 | 1/1   | 0.89 | 0.12 | 55,55,55,55                 | 0     |
| 85  | MG   | 5     | 3796 | 1/1   | 0.89 | 0.25 | 53,53,53,53                 | 0     |
| 86  | OHX  | C3    | 201  | 7/7   | 0.89 | 0.12 | 151,151,151,151             | 0     |
| 86  | OHX  | 6     | 2191 | 7/7   | 0.89 | 0.15 | 129,129,129,129             | 0     |
| 85  | MG   | 1     | 3593 | 1/1   | 0.89 | 0.42 | 51,51,51,51                 | 0     |
| 86  | OHX  | 1     | 3896 | 7/7   | 0.89 | 0.19 | 101,101,101,101             | 0     |
| 85  | MG   | 1     | 3693 | 1/1   | 0.89 | 0.17 | 41,41,41,41                 | 0     |
| 85  | MG   | 1     | 3835 | 1/1   | 0.89 | 0.26 | 28,28,28,28                 | 0     |
| 85  | MG   | 1     | 3695 | 1/1   | 0.89 | 0.27 | 43,43,43,43                 | 0     |
| 85  | MG   | 5     | 3655 | 1/1   | 0.89 | 0.25 | 56,56,56,56                 | 0     |
| 85  | MG   | 1     | 3517 | 1/1   | 0.89 | 0.35 | 34,34,34,34                 | 0     |
| 85  | MG   | 5     | 3522 | 1/1   | 0.89 | 0.32 | 30,30,30,30                 | 0     |
| 85  | MG   | 1     | 3460 | 1/1   | 0.89 | 0.36 | 63,63,63,63                 | 0     |
| 85  | MG   | 1     | 3702 | 1/1   | 0.89 | 0.30 | 43,43,43,43                 | 0     |
| 85  | MG   | 5     | 3665 | 1/1   | 0.89 | 0.18 | 42,42,42,42                 | 0     |
| 86  | OHX  | 2     | 2103 | 7/7   | 0.89 | 0.11 | 195,195,195,195             | 0     |
| 85  | MG   | 1     | 3706 | 1/1   | 0.89 | 0.29 | 42,42,42,42                 | 0     |
| 85  | MG   | 5     | 3676 | 1/1   | 0.89 | 0.19 | 41,41,41,41                 | 0     |
| 86  | OHX  | 2     | 2113 | 7/7   | 0.89 | 0.14 | 154,154,154,154             | 0     |
| 85  | MG   | S4    | 301  | 1/1   | 0.89 | 0.29 | 70,70,70,70                 | 0     |
| 86  | OHX  | 1     | 4096 | 7/7   | 0.89 | 0.14 | 141,141,141,141             | 0     |
| 86  | OHX  | 2     | 2118 | 7/7   | 0.89 | 0.14 | 142,142,142,142             | 0     |
| 86  | OHX  | 1     | 4201 | 7/7   | 0.89 | 0.15 | 128,128,128,128             | 0     |
| 85  | MG   | 1     | 3853 | 1/1   | 0.89 | 0.51 | 56,56,56,56                 | 0     |
| 85  | MG   | 1     | 3441 | 1/1   | 0.89 | 0.19 | 36,36,36,36                 | 0     |
| 85  | MG   | 1     | 3429 | 1/1   | 0.89 | 0.23 | 50,50,50,50                 | 0     |
| 85  | MG   | 1     | 3861 | 1/1   | 0.89 | 0.13 | 64,64,64,64                 | 0     |
| 86  | OHX  | 1     | 4106 | 7/7   | 0.89 | 0.15 | 137,137,137,137             | 0     |
| 86  | OHX  | 2     | 2127 | 7/7   | 0.89 | 0.14 | 133,133,133,133             | 0     |
| 85  | MG   | 6     | 1996 | 1/1   | 0.89 | 0.07 | 43,43,43,43                 | 0     |
| 85  | MG   | 1     | 3569 | 1/1   | 0.89 | 0.30 | 29,29,29,29                 | 0     |
| 85  | MG   | 5     | 3560 | 1/1   | 0.89 | 0.30 | 33,33,33,33                 | 0     |
| 86  | OHX  | 1     | 4114 | 7/7   | 0.89 | 0.21 | 106,106,106,106             | 0     |
| 85  | MG   | 1     | 3404 | 1/1   | 0.89 | 0.42 | 62,62,62,62                 | 0     |
| 85  | MG   | 5     | 3860 | 1/1   | 0.89 | 0.20 | 39,39,39,39                 | 0     |
| 85  | MG   | 1     | 3720 | 1/1   | 0.89 | 0.23 | 72,72,72,72                 | 0     |
| 86  | OHX  | 5     | 4131 | 7/7   | 0.89 | 0.14 | 144,144,144,144             | 0     |
| 85  | MG   | 1     | 3453 | 1/1   | 0.89 | 0.21 | 35,35,35,35                 | 0     |
| 86  | OHX  | 5     | 4139 | 7/7   | 0.89 | 0.21 | 126,126,126,126             | 0     |
| 86  | OHX  | 1     | 4216 | 7/7   | 0.89 | 0.18 | 141,141,141,141             | 0     |
| 85  | MG   | 5     | 3866 | 1/1   | 0.89 | 0.30 | 56,56,56,56                 | 0     |
| 86  | OHX  | 1     | 4123 | 7/7   | 0.89 | 0.21 | 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  | OHX  | 3     | 224  | 7/7   | 0.89 | 0.16 | 136,136,136,136             | 0     |
| 85  | MG   | 5     | 3427 | 1/1   | 0.89 | 0.17 | 40,40,40,40                 | 0     |
| 86  | OHX  | 5     | 4146 | 7/7   | 0.89 | 0.18 | 110,110,110,110             | 0     |
| 85  | MG   | 3     | 203  | 1/1   | 0.89 | 0.16 | 96,96,96,96                 | 0     |
| 86  | OHX  | 4     | 236  | 7/7   | 0.89 | 0.16 | 131,131,131,131             | 0     |
| 86  | OHX  | 1     | 4126 | 7/7   | 0.89 | 0.23 | 103,103,103,103             | 0     |
| 86  | OHX  | 2     | 2141 | 7/7   | 0.89 | 0.13 | 160,160,160,160             | 0     |
| 86  | OHX  | 1     | 4130 | 7/7   | 0.89 | 0.15 | 143,143,143,143             | 0     |
| 85  | MG   | 5     | 3434 | 1/1   | 0.89 | 0.27 | 79,79,79,79                 | 0     |
| 86  | OHX  | 1     | 4132 | 7/7   | 0.89 | 0.17 | 118,118,118,118             | 0     |
| 85  | MG   | 6     | 2008 | 1/1   | 0.89 | 0.19 | 56,56,56,56                 | 0     |
| 85  | MG   | 3     | 206  | 1/1   | 0.89 | 0.38 | 31,31,31,31                 | 0     |
| 85  | MG   | 1     | 3787 | 1/1   | 0.89 | 0.12 | 43,43,43,43                 | 0     |
| 87  | ZN   | q2    | 501  | 1/1   | 0.89 | 0.31 | 82,82,82,82                 | 0     |
| 85  | MG   | 6     | 1926 | 1/1   | 0.90 | 0.38 | 49,49,49,49                 | 0     |
| 86  | OHX  | 5     | 4019 | 7/7   | 0.90 | 0.14 | 145,145,145,145             | 0     |
| 86  | OHX  | 5     | 4088 | 7/7   | 0.90 | 0.14 | 126,126,126,126             | 0     |
| 85  | MG   | 5     | 3624 | 1/1   | 0.90 | 0.28 | 38,38,38,38                 | 0     |
| 85  | MG   | 5     | 3626 | 1/1   | 0.90 | 0.28 | 28,28,28,28                 | 0     |
| 85  | MG   | 1     | 3807 | 1/1   | 0.90 | 0.17 | 37,37,37,37                 | 0     |
| 85  | MG   | 1     | 3448 | 1/1   | 0.90 | 0.27 | 45,45,45,45                 | 0     |
| 85  | MG   | 5     | 3437 | 1/1   | 0.90 | 0.36 | 45,45,45,45                 | 0     |
| 85  | MG   | 5     | 3439 | 1/1   | 0.90 | 0.39 | 62,62,62,62                 | 0     |
| 86  | OHX  | 5     | 4110 | 7/7   | 0.90 | 0.16 | 119,119,119,119             | 0     |
| 85  | MG   | 5     | 3442 | 1/1   | 0.90 | 0.25 | 32,32,32,32                 | 0     |
| 85  | MG   | 1     | 3513 | 1/1   | 0.90 | 0.25 | 41,41,41,41                 | 0     |
| 86  | OHX  | 5     | 4115 | 7/7   | 0.90 | 0.22 | 105,105,105,105             | 0     |
| 86  | OHX  | 5     | 4118 | 7/7   | 0.90 | 0.13 | 141,141,141,141             | 0     |
| 85  | MG   | 1     | 3514 | 1/1   | 0.90 | 0.36 | 27,27,27,27                 | 0     |
| 86  | OHX  | 5     | 4121 | 7/7   | 0.90 | 0.20 | 107,107,107,107             | 0     |
| 85  | MG   | 6     | 2002 | 1/1   | 0.90 | 0.11 | 94,94,94,94                 | 0     |
| 86  | OHX  | 5     | 4124 | 7/7   | 0.90 | 0.15 | 132,132,132,132             | 0     |
| 86  | OHX  | 5     | 4127 | 7/7   | 0.90 | 0.13 | 144,144,144,144             | 0     |
| 85  | MG   | 5     | 3640 | 1/1   | 0.90 | 0.18 | 37,37,37,37                 | 0     |
| 85  | MG   | 5     | 3850 | 1/1   | 0.90 | 0.23 | 54,54,54,54                 | 0     |
| 85  | MG   | 6     | 2003 | 1/1   | 0.90 | 0.15 | 54,54,54,54                 | 0     |
| 86  | OHX  | 5     | 4135 | 7/7   | 0.90 | 0.18 | 114,114,114,114             | 0     |
| 86  | OHX  | 5     | 4138 | 7/7   | 0.90 | 0.14 | 133,133,133,133             | 0     |
| 85  | MG   | 5     | 3859 | 1/1   | 0.90 | 0.27 | 69,69,69,69                 | 0     |
| 85  | MG   | 1     | 3450 | 1/1   | 0.90 | 0.19 | 37,37,37,37                 | 0     |
| 86  | OHX  | 2     | 2166 | 7/7   | 0.90 | 0.12 | 155,155,155,155             | 0     |
| 85  | MG   | 5     | 3647 | 1/1   | 0.90 | 0.25 | 52,52,52,52                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 6     | 2005 | 1/1   | 0.90 | 0.14 | 73,73,73,73                 | 0     |
| 85  | MG   | 5     | 3468 | 1/1   | 0.90 | 0.09 | 35,35,35,35                 | 0     |
| 85  | MG   | 5     | 3867 | 1/1   | 0.90 | 0.32 | 55,55,55,55                 | 0     |
| 86  | OHX  | 5     | 4147 | 7/7   | 0.90 | 0.19 | 126,126,126,126             | 0     |
| 85  | MG   | 1     | 3646 | 1/1   | 0.90 | 0.18 | 46,46,46,46                 | 0     |
| 85  | MG   | 5     | 3654 | 1/1   | 0.90 | 0.10 | 61,61,61,61                 | 0     |
| 86  | OHX  | 5     | 4151 | 7/7   | 0.90 | 0.17 | 129,129,129,129             | 0     |
| 85  | MG   | 6     | 2007 | 1/1   | 0.90 | 0.13 | 58,58,58,58                 | 0     |
| 85  | MG   | 1     | 3478 | 1/1   | 0.90 | 0.10 | 48,48,48,48                 | 0     |
| 85  | MG   | 6     | 2009 | 1/1   | 0.90 | 0.21 | 51,51,51,51                 | 0     |
| 85  | MG   | 5     | 3881 | 1/1   | 0.90 | 0.28 | 34,34,34,34                 | 0     |
| 85  | MG   | L3    | 401  | 1/1   | 0.90 | 0.22 | 70,70,70,70                 | 0     |
| 86  | OHX  | 5     | 4159 | 7/7   | 0.90 | 0.15 | 129,129,129,129             | 0     |
| 85  | MG   | 1     | 3823 | 1/1   | 0.90 | 0.09 | 59,59,59,59                 | 0     |
| 85  | MG   | 1     | 3479 | 1/1   | 0.90 | 0.26 | 38,38,38,38                 | 0     |
| 85  | MG   | 5     | 3667 | 1/1   | 0.90 | 0.21 | 31,31,31,31                 | 0     |
| 85  | MG   | 5     | 3891 | 1/1   | 0.90 | 0.11 | 34,34,34,34                 | 0     |
| 85  | MG   | 5     | 3668 | 1/1   | 0.90 | 0.08 | 27,27,27,27                 | 0     |
| 85  | MG   | 5     | 3894 | 1/1   | 0.90 | 0.34 | 66,66,66,66                 | 0     |
| 85  | MG   | 5     | 3670 | 1/1   | 0.90 | 0.23 | 36,36,36,36                 | 0     |
| 85  | MG   | 1     | 3728 | 1/1   | 0.90 | 0.16 | 62,62,62,62                 | 0     |
| 86  | OHX  | 5     | 4169 | 7/7   | 0.90 | 0.18 | 124,124,124,124             | 0     |
| 86  | OHX  | 5     | 4170 | 7/7   | 0.90 | 0.13 | 139,139,139,139             | 0     |
| 85  | MG   | 1     | 3452 | 1/1   | 0.90 | 0.32 | 44,44,44,44                 | 0     |
| 86  | OHX  | 5     | 4172 | 7/7   | 0.90 | 0.18 | 128,128,128,128             | 0     |
| 86  | OHX  | 1     | 4065 | 7/7   | 0.90 | 0.13 | 144,144,144,144             | 0     |
| 86  | OHX  | 3     | 220  | 7/7   | 0.90 | 0.14 | 137,137,137,137             | 0     |
| 86  | OHX  | 5     | 4178 | 7/7   | 0.90 | 0.19 | 134,134,134,134             | 0     |
| 86  | OHX  | 3     | 221  | 7/7   | 0.90 | 0.20 | 115,115,115,115             | 0     |
| 85  | MG   | 1     | 3411 | 1/1   | 0.90 | 0.26 | 43,43,43,43                 | 0     |
| 85  | MG   | 6     | 2019 | 1/1   | 0.90 | 0.09 | 41,41,41,41                 | 0     |
| 86  | OHX  | 1     | 4070 | 7/7   | 0.90 | 0.21 | 107,107,107,107             | 0     |
| 85  | MG   | 1     | 3401 | 1/1   | 0.90 | 0.34 | 41,41,41,41                 | 0     |
| 85  | MG   | 1     | 3657 | 1/1   | 0.90 | 0.14 | 32,32,32,32                 | 0     |
| 85  | MG   | 5     | 3687 | 1/1   | 0.90 | 0.11 | 44,44,44,44                 | 0     |
| 86  | OHX  | 1     | 4081 | 7/7   | 0.90 | 0.20 | 113,113,113,113             | 0     |
| 86  | OHX  | 1     | 4082 | 7/7   | 0.90 | 0.18 | 116,116,116,116             | 0     |
| 85  | MG   | 5     | 3688 | 1/1   | 0.90 | 0.07 | 42,42,42,42                 | 0     |
| 85  | MG   | 1     | 3528 | 1/1   | 0.90 | 0.35 | 28,28,28,28                 | 0     |
| 85  | MG   | 1     | 3843 | 1/1   | 0.90 | 0.23 | 43,43,43,43                 | 0     |
| 86  | OHX  | 1     | 4087 | 7/7   | 0.90 | 0.13 | 138,138,138,138             | 0     |
| 85  | MG   | 8     | 203  | 1/1   | 0.90 | 0.22 | 55,55,55,55                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 2     | 1913 | 1/1   | 0.90 | 0.39 | 82,82,82,82                 | 0     |
| 86  | OHX  | O3    | 202  | 7/7   | 0.90 | 0.20 | 106,106,106,106             | 0     |
| 85  | MG   | 6     | 2030 | 1/1   | 0.90 | 0.34 | 66,66,66,66                 | 0     |
| 86  | OHX  | 6     | 2105 | 7/7   | 0.90 | 0.19 | 117,117,117,117             | 0     |
| 85  | MG   | 8     | 208  | 1/1   | 0.90 | 0.10 | 59,59,59,59                 | 0     |
| 85  | MG   | 5     | 3696 | 1/1   | 0.90 | 0.09 | 41,41,41,41                 | 0     |
| 86  | OHX  | 5     | 4202 | 7/7   | 0.90 | 0.18 | 110,110,110,110             | 0     |
| 86  | OHX  | 6     | 2126 | 7/7   | 0.90 | 0.18 | 130,130,130,130             | 0     |
| 86  | OHX  | 6     | 2127 | 7/7   | 0.90 | 0.17 | 131,131,131,131             | 0     |
| 86  | OHX  | 1     | 4100 | 7/7   | 0.90 | 0.14 | 137,137,137,137             | 0     |
| 86  | OHX  | 6     | 2130 | 7/7   | 0.90 | 0.17 | 145,145,145,145             | 0     |
| 86  | OHX  | 6     | 2134 | 7/7   | 0.90 | 0.21 | 123,123,123,123             | 0     |
| 85  | MG   | 5     | 3700 | 1/1   | 0.90 | 0.19 | 54,54,54,54                 | 0     |
| 86  | OHX  | 6     | 2137 | 7/7   | 0.90 | 0.13 | 136,136,136,136             | 0     |
| 85  | MG   | 8     | 212  | 1/1   | 0.90 | 0.21 | 56,56,56,56                 | 0     |
| 86  | OHX  | 6     | 2140 | 7/7   | 0.90 | 0.17 | 116,116,116,116             | 0     |
| 85  | MG   | 6     | 1957 | 1/1   | 0.90 | 0.47 | 58,58,58,58                 | 0     |
| 86  | OHX  | 5     | 4214 | 7/7   | 0.90 | 0.15 | 132,132,132,132             | 0     |
| 85  | MG   | 1     | 3488 | 1/1   | 0.90 | 0.25 | 30,30,30,30                 | 0     |
| 85  | MG   | 5     | 3520 | 1/1   | 0.90 | 0.30 | 34,34,34,34                 | 0     |
| 86  | OHX  | 5     | 4217 | 7/7   | 0.90 | 0.10 | 185,185,185,185             | 0     |
| 85  | MG   | 5     | 3521 | 1/1   | 0.90 | 0.30 | 41,41,41,41                 | 0     |
| 85  | MG   | 1     | 3597 | 1/1   | 0.90 | 0.38 | 24,24,24,24                 | 0     |
| 86  | OHX  | 6     | 2153 | 7/7   | 0.90 | 0.21 | 110,110,110,110             | 0     |
| 85  | MG   | 5     | 3711 | 1/1   | 0.90 | 0.10 | 40,40,40,40                 | 0     |
| 85  | MG   | 5     | 3712 | 1/1   | 0.90 | 0.10 | 68,68,68,68                 | 0     |
| 85  | MG   | 6     | 2034 | 1/1   | 0.90 | 0.23 | 66,66,66,66                 | 0     |
| 85  | MG   | 5     | 3714 | 1/1   | 0.90 | 0.16 | 45,45,45,45                 | 0     |
| 85  | MG   | 1     | 3599 | 1/1   | 0.90 | 0.38 | 42,42,42,42                 | 0     |
| 85  | MG   | n6    | 202  | 1/1   | 0.90 | 0.23 | 44,44,44,44                 | 0     |
| 85  | MG   | 5     | 3716 | 1/1   | 0.90 | 0.22 | 63,63,63,63                 | 0     |
| 85  | MG   | 1     | 3674 | 1/1   | 0.90 | 0.16 | 49,49,49,49                 | 0     |
| 85  | MG   | 1     | 3858 | 1/1   | 0.90 | 0.14 | 88,88,88,88                 | 0     |
| 85  | MG   | 1     | 3860 | 1/1   | 0.90 | 0.14 | 61,61,61,61                 | 0     |
| 85  | MG   | 1     | 3493 | 1/1   | 0.90 | 0.17 | 62,62,62,62                 | 0     |
| 86  | OHX  | 1     | 4127 | 7/7   | 0.90 | 0.15 | 133,133,133,133             | 0     |
| 86  | OHX  | 1     | 4128 | 7/7   | 0.90 | 0.13 | 144,144,144,144             | 0     |
| 85  | MG   | 5     | 3727 | 1/1   | 0.90 | 0.23 | 29,29,29,29                 | 0     |
| 85  | MG   | 1     | 3536 | 1/1   | 0.90 | 0.36 | 29,29,29,29                 | 0     |
| 85  | MG   | 5     | 3551 | 1/1   | 0.90 | 0.27 | 30,30,30,30                 | 0     |
| 85  | MG   | 1     | 3423 | 1/1   | 0.90 | 0.18 | 32,32,32,32                 | 0     |
| 85  | MG   | 5     | 3733 | 1/1   | 0.90 | 0.29 | 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  | MG   | s1    | 301  | 1/1   | 0.90 | 0.21 | 74,74,74,74                 | 0     |
| 85  | MG   | 5     | 3558 | 1/1   | 0.90 | 0.20 | 46,46,46,46                 | 0     |
| 86  | OHX  | 2     | 2104 | 7/7   | 0.90 | 0.15 | 120,120,120,120             | 0     |
| 85  | MG   | s4    | 301  | 1/1   | 0.90 | 0.30 | 58,58,58,58                 | 0     |
| 86  | OHX  | 1     | 4139 | 7/7   | 0.90 | 0.20 | 110,110,110,110             | 0     |
| 85  | MG   | 1     | 3417 | 1/1   | 0.90 | 0.15 | 32,32,32,32                 | 0     |
| 85  | MG   | 5     | 3561 | 1/1   | 0.90 | 0.31 | 31,31,31,31                 | 0     |
| 85  | MG   | 5     | 3750 | 1/1   | 0.90 | 0.21 | 40,40,40,40                 | 0     |
| 86  | OHX  | 2     | 2117 | 7/7   | 0.90 | 0.13 | 152,152,152,152             | 0     |
| 85  | MG   | 1     | 3545 | 1/1   | 0.90 | 0.28 | 37,37,37,37                 | 0     |
| 85  | MG   | 5     | 3761 | 1/1   | 0.90 | 0.20 | 63,63,63,63                 | 0     |
| 85  | MG   | 1     | 3768 | 1/1   | 0.90 | 0.12 | 52,52,52,52                 | 0     |
| 85  | MG   | 1     | 3461 | 1/1   | 0.90 | 0.31 | 30,30,30,30                 | 0     |
| 85  | MG   | 1     | 3771 | 1/1   | 0.90 | 0.16 | 83,83,83,83                 | 0     |
| 85  | MG   | 1     | 3625 | 1/1   | 0.90 | 0.23 | 49,49,49,49                 | 0     |
| 85  | MG   | 5     | 3576 | 1/1   | 0.90 | 0.33 | 45,45,45,45                 | 0     |
| 85  | MG   | 1     | 3696 | 1/1   | 0.90 | 0.38 | 53,53,53,53                 | 0     |
| 85  | MG   | 1     | 3555 | 1/1   | 0.90 | 0.35 | 49,49,49,49                 | 0     |
| 85  | MG   | 5     | 3583 | 1/1   | 0.90 | 0.36 | 38,38,38,38                 | 0     |
| 85  | MG   | 1     | 3463 | 1/1   | 0.90 | 0.29 | 28,28,28,28                 | 0     |
| 85  | MG   | 5     | 3407 | 1/1   | 0.90 | 0.15 | 37,37,37,37                 | 0     |
| 85  | MG   | 1     | 3557 | 1/1   | 0.90 | 0.41 | 28,28,28,28                 | 0     |
| 86  | OHX  | 6     | 2200 | 7/7   | 0.90 | 0.17 | 133,133,133,133             | 0     |
| 85  | MG   | 5     | 3415 | 1/1   | 0.90 | 0.18 | 51,51,51,51                 | 0     |
| 85  | MG   | 5     | 3596 | 1/1   | 0.90 | 0.28 | 26,26,26,26                 | 0     |
| 85  | MG   | 6     | 1986 | 1/1   | 0.90 | 0.30 | 82,82,82,82                 | 0     |
| 85  | MG   | 5     | 3604 | 1/1   | 0.90 | 0.20 | 40,40,40,40                 | 0     |
| 85  | MG   | 1     | 3427 | 1/1   | 0.90 | 0.16 | 59,59,59,59                 | 0     |
| 85  | MG   | 1     | 3428 | 1/1   | 0.90 | 0.31 | 42,42,42,42                 | 0     |
| 86  | OHX  | s4    | 302  | 7/7   | 0.90 | 0.14 | 142,142,142,142             | 0     |
| 86  | OHX  | 1     | 4170 | 7/7   | 0.90 | 0.32 | 98,98,98,98                 | 0     |
| 85  | MG   | 1     | 3709 | 1/1   | 0.90 | 0.11 | 40,40,40,40                 | 0     |
| 85  | MG   | 5     | 3808 | 1/1   | 0.90 | 0.16 | 38,38,38,38                 | 0     |
| 85  | MG   | 2     | 1995 | 1/1   | 0.90 | 0.25 | 96,96,96,96                 | 0     |
| 85  | MG   | 5     | 3426 | 1/1   | 0.90 | 0.18 | 41,41,41,41                 | 0     |
| 85  | MG   | 5     | 3620 | 1/1   | 0.90 | 0.14 | 41,41,41,41                 | 0     |
| 86  | OHX  | 5     | 4084 | 7/7   | 0.91 | 0.20 | 103,103,103,103             | 0     |
| 85  | MG   | 6     | 1994 | 1/1   | 0.91 | 0.22 | 53,53,53,53                 | 0     |
| 86  | OHX  | 5     | 4089 | 7/7   | 0.91 | 0.22 | 108,108,108,108             | 0     |
| 85  | MG   | 5     | 3627 | 1/1   | 0.91 | 0.24 | 58,58,58,58                 | 0     |
| 86  | OHX  | 5     | 4093 | 7/7   | 0.91 | 0.19 | 111,111,111,111             | 0     |
| 85  | MG   | 6     | 1995 | 1/1   | 0.91 | 0.31 | 56,56,56,56                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 5     | 3444 | 1/1   | 0.91 | 0.22 | 25,25,25,25                 | 0     |
| 85  | MG   | 1     | 3626 | 1/1   | 0.91 | 0.21 | 55,55,55,55                 | 0     |
| 85  | MG   | 1     | 3862 | 1/1   | 0.91 | 0.12 | 115,115,115,115             | 0     |
| 85  | MG   | 5     | 3452 | 1/1   | 0.91 | 0.19 | 40,40,40,40                 | 0     |
| 86  | OHX  | 5     | 4109 | 7/7   | 0.91 | 0.17 | 114,114,114,114             | 0     |
| 85  | MG   | 1     | 3767 | 1/1   | 0.91 | 0.11 | 42,42,42,42                 | 0     |
| 85  | MG   | 5     | 3824 | 1/1   | 0.91 | 0.18 | 64,64,64,64                 | 0     |
| 85  | MG   | 1     | 3483 | 1/1   | 0.91 | 0.27 | 31,31,31,31                 | 0     |
| 85  | MG   | 5     | 3832 | 1/1   | 0.91 | 0.12 | 51,51,51,51                 | 0     |
| 85  | MG   | 1     | 3451 | 1/1   | 0.91 | 0.26 | 36,36,36,36                 | 0     |
| 85  | MG   | 1     | 3485 | 1/1   | 0.91 | 0.11 | 42,42,42,42                 | 0     |
| 85  | MG   | 1     | 3634 | 1/1   | 0.91 | 0.09 | 33,33,33,33                 | 0     |
| 85  | MG   | 5     | 3469 | 1/1   | 0.91 | 0.17 | 34,34,34,34                 | 0     |
| 85  | MG   | 3     | 205  | 1/1   | 0.91 | 0.31 | 44,44,44,44                 | 0     |
| 86  | OHX  | 5     | 4126 | 7/7   | 0.91 | 0.14 | 140,140,140,140             | 0     |
| 85  | MG   | 1     | 3700 | 1/1   | 0.91 | 0.17 | 55,55,55,55                 | 0     |
| 85  | MG   | 1     | 3776 | 1/1   | 0.91 | 0.13 | 53,53,53,53                 | 0     |
| 85  | MG   | 5     | 3652 | 1/1   | 0.91 | 0.23 | 27,27,27,27                 | 0     |
| 85  | MG   | 5     | 3858 | 1/1   | 0.91 | 0.17 | 45,45,45,45                 | 0     |
| 85  | MG   | 1     | 3778 | 1/1   | 0.91 | 0.23 | 61,61,61,61                 | 0     |
| 85  | MG   | 1     | 3779 | 1/1   | 0.91 | 0.15 | 75,75,75,75                 | 0     |
| 85  | MG   | 2     | 1984 | 1/1   | 0.91 | 0.25 | 62,62,62,62                 | 0     |
| 85  | MG   | 2     | 1991 | 1/1   | 0.91 | 0.16 | 55,55,55,55                 | 0     |
| 85  | MG   | 5     | 3657 | 1/1   | 0.91 | 0.22 | 47,47,47,47                 | 0     |
| 86  | OHX  | 2     | 2168 | 7/7   | 0.91 | 0.19 | 118,118,118,118             | 0     |
| 85  | MG   | 1     | 3489 | 1/1   | 0.91 | 0.18 | 36,36,36,36                 | 0     |
| 85  | MG   | 1     | 3587 | 1/1   | 0.91 | 0.34 | 53,53,53,53                 | 0     |
| 85  | MG   | 4     | 203  | 1/1   | 0.91 | 0.37 | 55,55,55,55                 | 0     |
| 85  | MG   | 5     | 3872 | 1/1   | 0.91 | 0.33 | 38,38,38,38                 | 0     |
| 85  | MG   | 5     | 3875 | 1/1   | 0.91 | 0.28 | 41,41,41,41                 | 0     |
| 85  | MG   | 1     | 3546 | 1/1   | 0.91 | 0.22 | 34,34,34,34                 | 0     |
| 85  | MG   | 5     | 3877 | 1/1   | 0.91 | 0.31 | 47,47,47,47                 | 0     |
| 85  | MG   | 6     | 2018 | 1/1   | 0.91 | 0.13 | 68,68,68,68                 | 0     |
| 85  | MG   | 1     | 3793 | 1/1   | 0.91 | 0.17 | 81,81,81,81                 | 0     |
| 85  | MG   | 5     | 3494 | 1/1   | 0.91 | 0.11 | 45,45,45,45                 | 0     |
| 85  | MG   | 5     | 3496 | 1/1   | 0.91 | 0.23 | 26,26,26,26                 | 0     |
| 85  | MG   | 5     | 3499 | 1/1   | 0.91 | 0.18 | 31,31,31,31                 | 0     |
| 85  | MG   | 4     | 206  | 1/1   | 0.91 | 0.36 | 39,39,39,39                 | 0     |
| 85  | MG   | 1     | 3590 | 1/1   | 0.91 | 0.27 | 30,30,30,30                 | 0     |
| 86  | OHX  | C5    | 201  | 7/7   | 0.91 | 0.11 | 155,155,155,155             | 0     |
| 85  | MG   | 5     | 3683 | 1/1   | 0.91 | 0.09 | 27,27,27,27                 | 0     |
| 85  | MG   | 4     | 211  | 1/1   | 0.91 | 0.10 | 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  | OHX  | 1     | 3968 | 7/7   | 0.91 | 0.12 | 116,116,116,116             | 0     |
| 86  | OHX  | 1     | 3987 | 7/7   | 0.91 | 0.19 | 102,102,102,102             | 0     |
| 86  | OHX  | 1     | 4004 | 7/7   | 0.91 | 0.17 | 110,110,110,110             | 0     |
| 85  | MG   | 6     | 1943 | 1/1   | 0.91 | 0.34 | 40,40,40,40                 | 0     |
| 86  | OHX  | 5     | 4168 | 7/7   | 0.91 | 0.18 | 128,128,128,128             | 0     |
| 85  | MG   | 2     | 1918 | 1/1   | 0.91 | 0.46 | 57,57,57,57                 | 0     |
| 85  | MG   | 5     | 3509 | 1/1   | 0.91 | 0.34 | 35,35,35,35                 | 0     |
| 86  | OHX  | 1     | 4045 | 7/7   | 0.91 | 0.16 | 121,121,121,121             | 0     |
| 86  | OHX  | 1     | 4053 | 7/7   | 0.91 | 0.19 | 110,110,110,110             | 0     |
| 85  | MG   | 5     | 3513 | 1/1   | 0.91 | 0.31 | 61,61,61,61                 | 0     |
| 86  | OHX  | 1     | 4062 | 7/7   | 0.91 | 0.12 | 166,166,166,166             | 0     |
| 85  | MG   | 5     | 3899 | 1/1   | 0.91 | 0.25 | 52,52,52,52                 | 0     |
| 85  | MG   | 7     | 201  | 1/1   | 0.91 | 0.34 | 45,45,45,45                 | 0     |
| 86  | OHX  | 5     | 4180 | 7/7   | 0.91 | 0.16 | 120,120,120,120             | 0     |
| 85  | MG   | 5     | 3516 | 1/1   | 0.91 | 0.23 | 28,28,28,28                 | 0     |
| 85  | MG   | 5     | 3517 | 1/1   | 0.91 | 0.24 | 36,36,36,36                 | 0     |
| 85  | MG   | 6     | 1945 | 1/1   | 0.91 | 0.41 | 52,52,52,52                 | 0     |
| 85  | MG   | 1     | 3643 | 1/1   | 0.91 | 0.11 | 67,67,67,67                 | 0     |
| 85  | MG   | 7     | 209  | 1/1   | 0.91 | 0.22 | 65,65,65,65                 | 0     |
| 86  | OHX  | 1     | 4080 | 7/7   | 0.91 | 0.13 | 130,130,130,130             | 0     |
| 86  | OHX  | 6     | 2107 | 7/7   | 0.91 | 0.16 | 116,116,116,116             | 0     |
| 85  | MG   | 5     | 3697 | 1/1   | 0.91 | 0.23 | 54,54,54,54                 | 0     |
| 85  | MG   | 4     | 214  | 1/1   | 0.91 | 0.11 | 37,37,37,37                 | 0     |
| 86  | OHX  | 6     | 2122 | 7/7   | 0.91 | 0.19 | 107,107,107,107             | 0     |
| 85  | MG   | 1     | 3644 | 1/1   | 0.91 | 0.20 | 42,42,42,42                 | 0     |
| 85  | MG   | 1     | 3810 | 1/1   | 0.91 | 0.11 | 49,49,49,49                 | 0     |
| 85  | MG   | 8     | 202  | 1/1   | 0.91 | 0.27 | 39,39,39,39                 | 0     |
| 85  | MG   | 5     | 3704 | 1/1   | 0.91 | 0.07 | 51,51,51,51                 | 0     |
| 86  | OHX  | 6     | 2133 | 7/7   | 0.91 | 0.13 | 139,139,139,139             | 0     |
| 86  | OHX  | 1     | 4088 | 7/7   | 0.91 | 0.16 | 124,124,124,124             | 0     |
| 86  | OHX  | 1     | 4090 | 7/7   | 0.91 | 0.15 | 127,127,127,127             | 0     |
| 86  | OHX  | 6     | 2136 | 7/7   | 0.91 | 0.15 | 129,129,129,129             | 0     |
| 85  | MG   | 1     | 3549 | 1/1   | 0.91 | 0.24 | 40,40,40,40                 | 0     |
| 85  | MG   | 6     | 1953 | 1/1   | 0.91 | 0.43 | 63,63,63,63                 | 0     |
| 86  | OHX  | 1     | 4095 | 7/7   | 0.91 | 0.19 | 113,113,113,113             | 0     |
| 86  | OHX  | 6     | 2142 | 7/7   | 0.91 | 0.16 | 130,130,130,130             | 0     |
| 85  | MG   | 5     | 3540 | 1/1   | 0.91 | 0.31 | 27,27,27,27                 | 0     |
| 86  | OHX  | 6     | 2145 | 7/7   | 0.91 | 0.13 | 138,138,138,138             | 0     |
| 85  | MG   | 1     | 3554 | 1/1   | 0.91 | 0.38 | 38,38,38,38                 | 0     |
| 85  | MG   | 6     | 2039 | 1/1   | 0.91 | 0.28 | 58,58,58,58                 | 0     |
| 85  | MG   | 1     | 3442 | 1/1   | 0.91 | 0.09 | 44,44,44,44                 | 0     |
| 85  | MG   | 1     | 3598 | 1/1   | 0.91 | 0.38 | 26,26,26,26                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 1     | 3727 | 1/1   | 0.91 | 0.11 | 47,47,47,47                 | 0     |
| 85  | MG   | 5     | 3552 | 1/1   | 0.91 | 0.23 | 45,45,45,45                 | 0     |
| 86  | OHX  | 1     | 4105 | 7/7   | 0.91 | 0.14 | 136,136,136,136             | 0     |
| 85  | MG   | 1     | 3820 | 1/1   | 0.91 | 0.10 | 39,39,39,39                 | 0     |
| 85  | MG   | 6     | 2047 | 1/1   | 0.91 | 0.35 | 76,76,76,76                 | 0     |
| 85  | MG   | 1     | 3822 | 1/1   | 0.91 | 0.10 | 47,47,47,47                 | 0     |
| 85  | MG   | 1     | 3520 | 1/1   | 0.91 | 0.34 | 30,30,30,30                 | 0     |
| 85  | MG   | 1     | 3825 | 1/1   | 0.91 | 0.18 | 60,60,60,60                 | 0     |
| 85  | MG   | m7    | 201  | 1/1   | 0.91 | 0.30 | 31,31,31,31                 | 0     |
| 86  | OHX  | 6     | 2165 | 7/7   | 0.91 | 0.14 | 127,127,127,127             | 0     |
| 85  | MG   | 1     | 3729 | 1/1   | 0.91 | 0.35 | 35,35,35,35                 | 0     |
| 85  | MG   | m7    | 204  | 1/1   | 0.91 | 0.14 | 34,34,34,34                 | 0     |
| 85  | MG   | n3    | 201  | 1/1   | 0.91 | 0.28 | 24,24,24,24                 | 0     |
| 85  | MG   | 1     | 3605 | 1/1   | 0.91 | 0.21 | 35,35,35,35                 | 0     |
| 86  | OHX  | 1     | 4120 | 7/7   | 0.91 | 0.16 | 122,122,122,122             | 0     |
| 85  | MG   | 5     | 3567 | 1/1   | 0.91 | 0.25 | 25,25,25,25                 | 0     |
| 85  | MG   | M7    | 201  | 1/1   | 0.91 | 0.22 | 33,33,33,33                 | 0     |
| 85  | MG   | n8    | 203  | 1/1   | 0.91 | 0.28 | 45,45,45,45                 | 0     |
| 85  | MG   | 1     | 3495 | 1/1   | 0.91 | 0.19 | 43,43,43,43                 | 0     |
| 85  | MG   | 1     | 3660 | 1/1   | 0.91 | 0.27 | 39,39,39,39                 | 0     |
| 85  | MG   | 1     | 3608 | 1/1   | 0.91 | 0.47 | 53,53,53,53                 | 0     |
| 85  | MG   | 5     | 3739 | 1/1   | 0.91 | 0.28 | 35,35,35,35                 | 0     |
| 86  | OHX  | 2     | 2075 | 7/7   | 0.91 | 0.19 | 126,126,126,126             | 0     |
| 85  | MG   | 5     | 3744 | 1/1   | 0.91 | 0.26 | 41,41,41,41                 | 0     |
| 86  | OHX  | 2     | 2080 | 7/7   | 0.91 | 0.15 | 132,132,132,132             | 0     |
| 85  | MG   | sM    | 302  | 1/1   | 0.91 | 0.10 | 43,43,43,43                 | 0     |
| 85  | MG   | 1     | 3609 | 1/1   | 0.91 | 0.25 | 65,65,65,65                 | 0     |
| 85  | MG   | 1     | 3558 | 1/1   | 0.91 | 0.31 | 38,38,38,38                 | 0     |
| 85  | MG   | 5     | 3758 | 1/1   | 0.91 | 0.27 | 64,64,64,64                 | 0     |
| 86  | OHX  | 2     | 2100 | 7/7   | 0.91 | 0.13 | 139,139,139,139             | 0     |
| 85  | MG   | 2     | 1919 | 1/1   | 0.91 | 0.46 | 71,71,71,71                 | 0     |
| 85  | MG   | 5     | 3409 | 1/1   | 0.91 | 0.29 | 48,48,48,48                 | 0     |
| 85  | MG   | 1     | 3524 | 1/1   | 0.91 | 0.35 | 36,36,36,36                 | 0     |
| 85  | MG   | 2     | 1921 | 1/1   | 0.91 | 0.41 | 56,56,56,56                 | 0     |
| 85  | MG   | 5     | 3417 | 1/1   | 0.91 | 0.24 | 25,25,25,25                 | 0     |
| 85  | MG   | 1     | 3847 | 1/1   | 0.91 | 0.44 | 51,51,51,51                 | 0     |
| 85  | MG   | 1     | 3848 | 1/1   | 0.91 | 0.18 | 42,42,42,42                 | 0     |
| 86  | OHX  | 2     | 2116 | 7/7   | 0.91 | 0.17 | 139,139,139,139             | 0     |
| 85  | MG   | 5     | 3598 | 1/1   | 0.91 | 0.42 | 28,28,28,28                 | 0     |
| 85  | MG   | 5     | 3602 | 1/1   | 0.91 | 0.12 | 58,58,58,58                 | 0     |
| 85  | MG   | 1     | 3851 | 1/1   | 0.91 | 0.26 | 57,57,57,57                 | 0     |
| 85  | MG   | 1     | 3617 | 1/1   | 0.91 | 0.21 | 36,36,36,36                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 5     | 3606 | 1/1   | 0.91 | 0.17 | 35,35,35,35                 | 0     |
| 85  | MG   | 5     | 3786 | 1/1   | 0.91 | 0.44 | 81,81,81,81                 | 0     |
| 86  | OHX  | 2     | 2125 | 7/7   | 0.91 | 0.14 | 125,125,125,125             | 0     |
| 85  | MG   | 5     | 3790 | 1/1   | 0.91 | 0.12 | 55,55,55,55                 | 0     |
| 86  | OHX  | 8     | 228  | 7/7   | 0.91 | 0.13 | 135,135,135,135             | 0     |
| 85  | MG   | 1     | 3414 | 1/1   | 0.91 | 0.49 | 58,58,58,58                 | 0     |
| 85  | MG   | 6     | 1989 | 1/1   | 0.91 | 0.12 | 46,46,46,46                 | 0     |
| 86  | OHX  | 13    | 406  | 7/7   | 0.91 | 0.14 | 131,131,131,131             | 0     |
| 86  | OHX  | 2     | 2132 | 7/7   | 0.91 | 0.13 | 150,150,150,150             | 0     |
| 85  | MG   | 1     | 3621 | 1/1   | 0.91 | 0.30 | 57,57,57,57                 | 0     |
| 86  | OHX  | 15    | 302  | 7/7   | 0.91 | 0.13 | 128,128,128,128             | 0     |
| 85  | MG   | 1     | 3685 | 1/1   | 0.91 | 0.15 | 45,45,45,45                 | 0     |
| 86  | OHX  | 1     | 4165 | 7/7   | 0.91 | 0.18 | 134,134,134,134             | 0     |
| 85  | MG   | 5     | 3432 | 1/1   | 0.91 | 0.11 | 35,35,35,35                 | 0     |
| 85  | MG   | 5     | 3801 | 1/1   | 0.91 | 0.09 | 31,31,31,31                 | 0     |
| 85  | MG   | 2     | 1911 | 1/1   | 0.91 | 0.47 | 60,60,60,60                 | 0     |
| 85  | MG   | 5     | 3622 | 1/1   | 0.91 | 0.24 | 35,35,35,35                 | 0     |
| 85  | MG   | 6     | 1993 | 1/1   | 0.91 | 0.13 | 51,51,51,51                 | 0     |
| 85  | MG   | 5     | 3625 | 1/1   | 0.91 | 0.33 | 40,40,40,40                 | 0     |
| 86  | OHX  | 5     | 4028 | 7/7   | 0.91 | 0.20 | 102,102,102,102             | 0     |
| 86  | OHX  | 5     | 4044 | 7/7   | 0.91 | 0.15 | 127,127,127,127             | 0     |
| 86  | OHX  | 5     | 4064 | 7/7   | 0.91 | 0.15 | 125,125,125,125             | 0     |
| 86  | OHX  | 5     | 4065 | 7/7   | 0.91 | 0.14 | 122,122,122,122             | 0     |
| 86  | OHX  | 5     | 4077 | 7/7   | 0.91 | 0.20 | 117,117,117,117             | 0     |
| 85  | MG   | 5     | 3510 | 1/1   | 0.92 | 0.36 | 29,29,29,29                 | 0     |
| 85  | MG   | 2     | 1973 | 1/1   | 0.92 | 0.17 | 73,73,73,73                 | 0     |
| 86  | OHX  | 5     | 4123 | 7/7   | 0.92 | 0.12 | 140,140,140,140             | 0     |
| 85  | MG   | 5     | 3645 | 1/1   | 0.92 | 0.10 | 44,44,44,44                 | 0     |
| 86  | OHX  | 5     | 4125 | 7/7   | 0.92 | 0.15 | 127,127,127,127             | 0     |
| 85  | MG   | 5     | 3646 | 1/1   | 0.92 | 0.29 | 34,34,34,34                 | 0     |
| 86  | OHX  | 1     | 4078 | 7/7   | 0.92 | 0.16 | 117,117,117,117             | 0     |
| 86  | OHX  | 1     | 4079 | 7/7   | 0.92 | 0.15 | 117,117,117,117             | 0     |
| 85  | MG   | 1     | 3529 | 1/1   | 0.92 | 0.37 | 32,32,32,32                 | 0     |
| 85  | MG   | 5     | 3401 | 1/1   | 0.92 | 0.14 | 59,59,59,59                 | 0     |
| 85  | MG   | 1     | 3504 | 1/1   | 0.92 | 0.23 | 28,28,28,28                 | 0     |
| 86  | OHX  | 5     | 4136 | 7/7   | 0.92 | 0.17 | 120,120,120,120             | 0     |
| 85  | MG   | 1     | 3691 | 1/1   | 0.92 | 0.15 | 39,39,39,39                 | 0     |
| 85  | MG   | 1     | 3409 | 1/1   | 0.92 | 0.25 | 34,34,34,34                 | 0     |
| 85  | MG   | q1    | 101  | 1/1   | 0.92 | 0.32 | 42,42,42,42                 | 0     |
| 86  | OHX  | 2     | 2067 | 7/7   | 0.92 | 0.11 | 153,153,153,153             | 0     |
| 85  | MG   | 1     | 3601 | 1/1   | 0.92 | 0.23 | 36,36,36,36                 | 0     |
| 85  | MG   | 5     | 3410 | 1/1   | 0.92 | 0.27 | 55,55,55,55                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 5     | 3527 | 1/1   | 0.92 | 0.24 | 30,30,30,30                 | 0     |
| 86  | OHX  | 2     | 2083 | 7/7   | 0.92 | 0.17 | 121,121,121,121             | 0     |
| 86  | OHX  | 1     | 4094 | 7/7   | 0.92 | 0.11 | 151,151,151,151             | 0     |
| 86  | OHX  | 2     | 2084 | 7/7   | 0.92 | 0.12 | 141,141,141,141             | 0     |
| 85  | MG   | 4     | 208  | 1/1   | 0.92 | 0.18 | 27,27,27,27                 | 0     |
| 86  | OHX  | 2     | 2088 | 7/7   | 0.92 | 0.17 | 108,108,108,108             | 0     |
| 86  | OHX  | 6     | 2097 | 7/7   | 0.92 | 0.14 | 127,127,127,127             | 0     |
| 86  | OHX  | 5     | 4153 | 7/7   | 0.92 | 0.21 | 110,110,110,110             | 0     |
| 86  | OHX  | 6     | 2102 | 7/7   | 0.92 | 0.11 | 169,169,169,169             | 0     |
| 85  | MG   | 5     | 3534 | 1/1   | 0.92 | 0.29 | 37,37,37,37                 | 0     |
| 85  | MG   | 5     | 3811 | 1/1   | 0.92 | 0.22 | 67,67,67,67                 | 0     |
| 85  | MG   | 1     | 3756 | 1/1   | 0.92 | 0.13 | 43,43,43,43                 | 0     |
| 86  | OHX  | 1     | 4102 | 7/7   | 0.92 | 0.20 | 107,107,107,107             | 0     |
| 85  | MG   | 5     | 3662 | 1/1   | 0.92 | 0.25 | 47,47,47,47                 | 0     |
| 85  | MG   | 6     | 1998 | 1/1   | 0.92 | 0.13 | 52,52,52,52                 | 0     |
| 85  | MG   | 1     | 3831 | 1/1   | 0.92 | 0.20 | 22,22,22,22                 | 0     |
| 86  | OHX  | 6     | 2128 | 7/7   | 0.92 | 0.35 | 99,99,99,99                 | 0     |
| 85  | MG   | 5     | 3819 | 1/1   | 0.92 | 0.06 | 63,63,63,63                 | 0     |
| 86  | OHX  | 2     | 2105 | 7/7   | 0.92 | 0.15 | 132,132,132,132             | 0     |
| 86  | OHX  | 1     | 4110 | 7/7   | 0.92 | 0.16 | 114,114,114,114             | 0     |
| 85  | MG   | 5     | 3542 | 1/1   | 0.92 | 0.27 | 31,31,31,31                 | 0     |
| 85  | MG   | 5     | 3419 | 1/1   | 0.92 | 0.16 | 33,33,33,33                 | 0     |
| 85  | MG   | 5     | 3669 | 1/1   | 0.92 | 0.16 | 38,38,38,38                 | 0     |
| 85  | MG   | 5     | 3545 | 1/1   | 0.92 | 0.44 | 50,50,50,50                 | 0     |
| 85  | MG   | 5     | 3672 | 1/1   | 0.92 | 0.35 | 57,57,57,57                 | 0     |
| 85  | MG   | 1     | 3603 | 1/1   | 0.92 | 0.27 | 31,31,31,31                 | 0     |
| 85  | MG   | 2     | 1920 | 1/1   | 0.92 | 0.22 | 65,65,65,65                 | 0     |
| 85  | MG   | 5     | 3839 | 1/1   | 0.92 | 0.26 | 43,43,43,43                 | 0     |
| 86  | OHX  | 5     | 4175 | 7/7   | 0.92 | 0.38 | 95,95,95,95                 | 0     |
| 86  | OHX  | 2     | 2120 | 7/7   | 0.92 | 0.14 | 147,147,147,147             | 0     |
| 85  | MG   | 4     | 216  | 1/1   | 0.92 | 0.07 | 52,52,52,52                 | 0     |
| 85  | MG   | 5     | 3680 | 1/1   | 0.92 | 0.21 | 41,41,41,41                 | 0     |
| 85  | MG   | 1     | 3760 | 1/1   | 0.92 | 0.07 | 47,47,47,47                 | 0     |
| 86  | OHX  | 2     | 2124 | 7/7   | 0.92 | 0.14 | 136,136,136,136             | 0     |
| 85  | MG   | 1     | 3454 | 1/1   | 0.92 | 0.30 | 44,44,44,44                 | 0     |
| 86  | OHX  | 2     | 2126 | 7/7   | 0.92 | 0.14 | 135,135,135,135             | 0     |
| 85  | MG   | 5     | 3684 | 1/1   | 0.92 | 0.17 | 33,33,33,33                 | 0     |
| 86  | OHX  | 2     | 2128 | 7/7   | 0.92 | 0.14 | 147,147,147,147             | 0     |
| 85  | MG   | 5     | 3851 | 1/1   | 0.92 | 0.17 | 45,45,45,45                 | 0     |
| 86  | OHX  | 6     | 2159 | 7/7   | 0.92 | 0.20 | 139,139,139,139             | 0     |
| 85  | MG   | 5     | 3555 | 1/1   | 0.92 | 0.26 | 40,40,40,40                 | 0     |
| 86  | OHX  | 6     | 2161 | 7/7   | 0.92 | 0.17 | 107,107,107,107             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 5     | 3856 | 1/1   | 0.92 | 0.12 | 71,71,71,71                 | 0     |
| 85  | MG   | 5     | 3857 | 1/1   | 0.92 | 0.15 | 56,56,56,56                 | 0     |
| 85  | MG   | 4     | 221  | 1/1   | 0.92 | 0.29 | 52,52,52,52                 | 0     |
| 85  | MG   | 1     | 3537 | 1/1   | 0.92 | 0.28 | 47,47,47,47                 | 0     |
| 85  | MG   | 1     | 3491 | 1/1   | 0.92 | 0.24 | 49,49,49,49                 | 0     |
| 85  | MG   | 1     | 3703 | 1/1   | 0.92 | 0.20 | 44,44,44,44                 | 0     |
| 85  | MG   | 1     | 3402 | 1/1   | 0.92 | 0.34 | 52,52,52,52                 | 0     |
| 85  | MG   | 1     | 3574 | 1/1   | 0.92 | 0.27 | 33,33,33,33                 | 0     |
| 85  | MG   | 1     | 3650 | 1/1   | 0.92 | 0.21 | 39,39,39,39                 | 0     |
| 85  | MG   | 1     | 3651 | 1/1   | 0.92 | 0.17 | 46,46,46,46                 | 0     |
| 86  | OHX  | 5     | 4203 | 7/7   | 0.92 | 0.14 | 117,117,117,117             | 0     |
| 85  | MG   | 5     | 3446 | 1/1   | 0.92 | 0.25 | 42,42,42,42                 | 0     |
| 86  | OHX  | 6     | 2173 | 7/7   | 0.92 | 0.20 | 106,106,106,106             | 0     |
| 85  | MG   | 5     | 3699 | 1/1   | 0.92 | 0.12 | 33,33,33,33                 | 0     |
| 85  | MG   | 1     | 3652 | 1/1   | 0.92 | 0.20 | 46,46,46,46                 | 0     |
| 85  | MG   | 1     | 3543 | 1/1   | 0.92 | 0.22 | 25,25,25,25                 | 0     |
| 85  | MG   | 1     | 3579 | 1/1   | 0.92 | 0.23 | 27,27,27,27                 | 0     |
| 85  | MG   | 5     | 3578 | 1/1   | 0.92 | 0.46 | 44,44,44,44                 | 0     |
| 85  | MG   | 5     | 3579 | 1/1   | 0.92 | 0.18 | 28,28,28,28                 | 0     |
| 85  | MG   | M3    | 201  | 1/1   | 0.92 | 0.13 | 44,44,44,44                 | 0     |
| 85  | MG   | 5     | 3459 | 1/1   | 0.92 | 0.17 | 65,65,65,65                 | 0     |
| 85  | MG   | 5     | 3886 | 1/1   | 0.92 | 0.32 | 57,57,57,57                 | 0     |
| 86  | OHX  | 1     | 4154 | 7/7   | 0.92 | 0.16 | 108,108,108,108             | 0     |
| 85  | MG   | 1     | 3856 | 1/1   | 0.92 | 0.17 | 69,69,69,69                 | 0     |
| 85  | MG   | 6     | 1954 | 1/1   | 0.92 | 0.28 | 47,47,47,47                 | 0     |
| 85  | MG   | 1     | 3580 | 1/1   | 0.92 | 0.28 | 26,26,26,26                 | 0     |
| 85  | MG   | M7    | 204  | 1/1   | 0.92 | 0.12 | 39,39,39,39                 | 0     |
| 85  | MG   | 1     | 3722 | 1/1   | 0.92 | 0.35 | 54,54,54,54                 | 0     |
| 85  | MG   | 5     | 3893 | 1/1   | 0.92 | 0.08 | 82,82,82,82                 | 0     |
| 85  | MG   | 1     | 3859 | 1/1   | 0.92 | 0.34 | 58,58,58,58                 | 0     |
| 85  | MG   | N3    | 201  | 1/1   | 0.92 | 0.31 | 32,32,32,32                 | 0     |
| 85  | MG   | 5     | 3719 | 1/1   | 0.92 | 0.11 | 61,61,61,61                 | 0     |
| 85  | MG   | 1     | 3457 | 1/1   | 0.92 | 0.45 | 58,58,58,58                 | 0     |
| 85  | MG   | 5     | 3599 | 1/1   | 0.92 | 0.18 | 37,37,37,37                 | 0     |
| 85  | MG   | 1     | 3403 | 1/1   | 0.92 | 0.29 | 37,37,37,37                 | 0     |
| 85  | MG   | 5     | 3478 | 1/1   | 0.92 | 0.19 | 26,26,26,26                 | 0     |
| 85  | MG   | 1     | 3622 | 1/1   | 0.92 | 0.17 | 69,69,69,69                 | 0     |
| 86  | OHX  | 2     | 2167 | 7/7   | 0.92 | 0.11 | 153,153,153,153             | 0     |
| 85  | MG   | N8    | 203  | 1/1   | 0.92 | 0.13 | 48,48,48,48                 | 0     |
| 85  | MG   | 1     | 3863 | 1/1   | 0.92 | 0.27 | 42,42,42,42                 | 0     |
| 85  | MG   | O4    | 201  | 1/1   | 0.92 | 0.18 | 60,60,60,60                 | 0     |
| 85  | MG   | 7     | 211  | 1/1   | 0.92 | 0.26 | 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  | MG   | 7     | 212  | 1/1   | 0.92 | 0.20 | 61,61,61,61                 | 0     |
| 85  | MG   | 5     | 3735 | 1/1   | 0.92 | 0.13 | 38,38,38,38                 | 0     |
| 85  | MG   | 2     | 1996 | 1/1   | 0.92 | 0.12 | 83,83,83,83                 | 0     |
| 85  | MG   | 5     | 3614 | 1/1   | 0.92 | 0.21 | 31,31,31,31                 | 0     |
| 85  | MG   | 5     | 3486 | 1/1   | 0.92 | 0.20 | 45,45,45,45                 | 0     |
| 85  | MG   | 5     | 3487 | 1/1   | 0.92 | 0.21 | 35,35,35,35                 | 0     |
| 85  | MG   | 2     | 1956 | 1/1   | 0.92 | 0.35 | 60,60,60,60                 | 0     |
| 85  | MG   | 8     | 204  | 1/1   | 0.92 | 0.34 | 48,48,48,48                 | 0     |
| 85  | MG   | 1     | 3797 | 1/1   | 0.92 | 0.12 | 26,26,26,26                 | 0     |
| 85  | MG   | 1     | 3798 | 1/1   | 0.92 | 0.21 | 51,51,51,51                 | 0     |
| 86  | OHX  | sR    | 401  | 7/7   | 0.92 | 0.11 | 156,156,156,156             | 0     |
| 85  | MG   | 8     | 207  | 1/1   | 0.92 | 0.13 | 53,53,53,53                 | 0     |
| 85  | MG   | 5     | 3491 | 1/1   | 0.92 | 0.18 | 40,40,40,40                 | 0     |
| 85  | MG   | 5     | 3757 | 1/1   | 0.92 | 0.13 | 50,50,50,50                 | 0     |
| 85  | MG   | 1     | 3799 | 1/1   | 0.92 | 0.08 | 31,31,31,31                 | 0     |
| 85  | MG   | 1     | 3551 | 1/1   | 0.92 | 0.15 | 34,34,34,34                 | 0     |
| 85  | MG   | 5     | 3628 | 1/1   | 0.92 | 0.10 | 52,52,52,52                 | 0     |
| 86  | OHX  | 5     | 4071 | 7/7   | 0.92 | 0.11 | 137,137,137,137             | 0     |
| 86  | OHX  | 5     | 4072 | 7/7   | 0.92 | 0.16 | 130,130,130,130             | 0     |
| 86  | OHX  | 1     | 4196 | 7/7   | 0.92 | 0.11 | 168,168,168,168             | 0     |
| 86  | OHX  | 5     | 4078 | 7/7   | 0.92 | 0.17 | 119,119,119,119             | 0     |
| 85  | MG   | 1     | 3806 | 1/1   | 0.92 | 0.21 | 59,59,59,59                 | 0     |
| 86  | OHX  | 5     | 4086 | 7/7   | 0.92 | 0.15 | 113,113,113,113             | 0     |
| 86  | OHX  | 1     | 4015 | 7/7   | 0.92 | 0.14 | 125,125,125,125             | 0     |
| 85  | MG   | 3     | 207  | 1/1   | 0.92 | 0.35 | 66,66,66,66                 | 0     |
| 86  | OHX  | 1     | 4027 | 7/7   | 0.92 | 0.12 | 143,143,143,143             | 0     |
| 85  | MG   | 1     | 3628 | 1/1   | 0.92 | 0.23 | 30,30,30,30                 | 0     |
| 86  | OHX  | 5     | 4094 | 7/7   | 0.92 | 0.18 | 107,107,107,107             | 0     |
| 86  | OHX  | 5     | 4097 | 7/7   | 0.92 | 0.14 | 127,127,127,127             | 0     |
| 86  | OHX  | 1     | 4035 | 7/7   | 0.92 | 0.15 | 128,128,128,128             | 0     |
| 85  | MG   | 2     | 1935 | 1/1   | 0.92 | 0.38 | 60,60,60,60                 | 0     |
| 86  | OHX  | 5     | 4100 | 7/7   | 0.92 | 0.14 | 130,130,130,130             | 0     |
| 85  | MG   | 2     | 1906 | 1/1   | 0.92 | 0.24 | 54,54,54,54                 | 0     |
| 85  | MG   | 19    | 201  | 1/1   | 0.92 | 0.12 | 42,42,42,42                 | 0     |
| 86  | OHX  | 5     | 4105 | 7/7   | 0.92 | 0.11 | 143,143,143,143             | 0     |
| 86  | OHX  | 1     | 4055 | 7/7   | 0.92 | 0.12 | 136,136,136,136             | 0     |
| 86  | OHX  | 1     | 4058 | 7/7   | 0.92 | 0.20 | 102,102,102,102             | 0     |
| 86  | OHX  | 1     | 4060 | 7/7   | 0.92 | 0.34 | 94,94,94,94                 | 0     |
| 86  | OHX  | n3    | 204  | 7/7   | 0.92 | 0.17 | 105,105,105,105             | 0     |
| 85  | MG   | 5     | 3635 | 1/1   | 0.92 | 0.41 | 74,74,74,74                 | 0     |
| 85  | MG   | 1     | 3502 | 1/1   | 0.92 | 0.34 | 28,28,28,28                 | 0     |
| 85  | MG   | 1     | 3635 | 1/1   | 0.92 | 0.19 | 56,56,56,56                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 5     | 3507 | 1/1   | 0.92 | 0.40 | 35,35,35,35                 | 0     |
| 85  | MG   | 1     | 3743 | 1/1   | 0.92 | 0.28 | 67,67,67,67                 | 0     |
| 86  | OHX  | 1     | 3985 | 7/7   | 0.93 | 0.15 | 104,104,104,104             | 0     |
| 85  | MG   | 1     | 3470 | 1/1   | 0.93 | 0.28 | 48,48,48,48                 | 0     |
| 85  | MG   | 1     | 3827 | 1/1   | 0.93 | 0.08 | 43,43,43,43                 | 0     |
| 86  | OHX  | 1     | 4008 | 7/7   | 0.93 | 0.14 | 120,120,120,120             | 0     |
| 86  | OHX  | 1     | 4013 | 7/7   | 0.93 | 0.13 | 125,125,125,125             | 0     |
| 86  | OHX  | 1     | 4014 | 7/7   | 0.93 | 0.15 | 121,121,121,121             | 0     |
| 85  | MG   | 5     | 3779 | 1/1   | 0.93 | 0.14 | 44,44,44,44                 | 0     |
| 86  | OHX  | 5     | 4103 | 7/7   | 0.93 | 0.12 | 140,140,140,140             | 0     |
| 86  | OHX  | 1     | 4020 | 7/7   | 0.93 | 0.09 | 153,153,153,153             | 0     |
| 86  | OHX  | 1     | 4022 | 7/7   | 0.93 | 0.12 | 128,128,128,128             | 0     |
| 85  | MG   | 1     | 3830 | 1/1   | 0.93 | 0.31 | 48,48,48,48                 | 0     |
| 86  | OHX  | 1     | 4025 | 7/7   | 0.93 | 0.13 | 113,113,113,113             | 0     |
| 85  | MG   | 1     | 3672 | 1/1   | 0.93 | 0.19 | 41,41,41,41                 | 0     |
| 85  | MG   | 5     | 3782 | 1/1   | 0.93 | 0.10 | 77,77,77,77                 | 0     |
| 85  | MG   | 17    | 303  | 1/1   | 0.93 | 0.22 | 39,39,39,39                 | 0     |
| 86  | OHX  | 5     | 4117 | 7/7   | 0.93 | 0.17 | 112,112,112,112             | 0     |
| 85  | MG   | 5     | 3783 | 1/1   | 0.93 | 0.23 | 59,59,59,59                 | 0     |
| 86  | OHX  | 1     | 4040 | 7/7   | 0.93 | 0.12 | 140,140,140,140             | 0     |
| 86  | OHX  | 1     | 4042 | 7/7   | 0.93 | 0.16 | 114,114,114,114             | 0     |
| 85  | MG   | 1     | 3582 | 1/1   | 0.93 | 0.31 | 37,37,37,37                 | 0     |
| 86  | OHX  | 1     | 4048 | 7/7   | 0.93 | 0.16 | 105,105,105,105             | 0     |
| 86  | OHX  | 1     | 4049 | 7/7   | 0.93 | 0.19 | 104,104,104,104             | 0     |
| 86  | OHX  | 1     | 4052 | 7/7   | 0.93 | 0.13 | 134,134,134,134             | 0     |
| 85  | MG   | 5     | 3785 | 1/1   | 0.93 | 0.08 | 36,36,36,36                 | 0     |
| 85  | MG   | 1     | 3770 | 1/1   | 0.93 | 0.29 | 65,65,65,65                 | 0     |
| 86  | OHX  | 5     | 4129 | 7/7   | 0.93 | 0.15 | 121,121,121,121             | 0     |
| 86  | OHX  | 3     | 219  | 7/7   | 0.93 | 0.14 | 124,124,124,124             | 0     |
| 85  | MG   | 1     | 3471 | 1/1   | 0.93 | 0.18 | 39,39,39,39                 | 0     |
| 85  | MG   | 5     | 3791 | 1/1   | 0.93 | 0.12 | 35,35,35,35                 | 0     |
| 85  | MG   | 6     | 1921 | 1/1   | 0.93 | 0.36 | 44,44,44,44                 | 0     |
| 85  | MG   | n3    | 202  | 1/1   | 0.93 | 0.10 | 44,44,44,44                 | 0     |
| 86  | OHX  | 5     | 4137 | 7/7   | 0.93 | 0.17 | 113,113,113,113             | 0     |
| 86  | OHX  | 1     | 4063 | 7/7   | 0.93 | 0.13 | 121,121,121,121             | 0     |
| 85  | MG   | 5     | 3793 | 1/1   | 0.93 | 0.20 | 42,42,42,42                 | 0     |
| 85  | MG   | 5     | 3794 | 1/1   | 0.93 | 0.09 | 48,48,48,48                 | 0     |
| 85  | MG   | 1     | 3675 | 1/1   | 0.93 | 0.37 | 57,57,57,57                 | 0     |
| 85  | MG   | n8    | 202  | 1/1   | 0.93 | 0.09 | 35,35,35,35                 | 0     |
| 85  | MG   | 1     | 3584 | 1/1   | 0.93 | 0.28 | 39,39,39,39                 | 0     |
| 86  | OHX  | 1     | 4072 | 7/7   | 0.93 | 0.17 | 117,117,117,117             | 0     |
| 85  | MG   | 5     | 3535 | 1/1   | 0.93 | 0.42 | 38,38,38,38                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 1     | 3677 | 1/1   | 0.93 | 0.22 | 24,24,24,24                 | 0     |
| 86  | OHX  | 1     | 4075 | 7/7   | 0.93 | 0.15 | 139,139,139,139             | 0     |
| 86  | OHX  | 1     | 4076 | 7/7   | 0.93 | 0.36 | 97,97,97,97                 | 0     |
| 85  | MG   | 4     | 217  | 1/1   | 0.93 | 0.23 | 65,65,65,65                 | 0     |
| 85  | MG   | 6     | 1999 | 1/1   | 0.93 | 0.34 | 60,60,60,60                 | 0     |
| 85  | MG   | o7    | 502  | 1/1   | 0.93 | 0.24 | 34,34,34,34                 | 0     |
| 86  | OHX  | 6     | 2087 | 7/7   | 0.93 | 0.10 | 128,128,128,128             | 0     |
| 85  | MG   | 5     | 3804 | 1/1   | 0.93 | 0.08 | 47,47,47,47                 | 0     |
| 86  | OHX  | 2     | 2061 | 7/7   | 0.93 | 0.14 | 131,131,131,131             | 0     |
| 85  | MG   | 5     | 3659 | 1/1   | 0.93 | 0.20 | 30,30,30,30                 | 0     |
| 86  | OHX  | 2     | 2074 | 7/7   | 0.93 | 0.13 | 139,139,139,139             | 0     |
| 86  | OHX  | 6     | 2108 | 7/7   | 0.93 | 0.17 | 111,111,111,111             | 0     |
| 85  | MG   | 1     | 3777 | 1/1   | 0.93 | 0.23 | 53,53,53,53                 | 0     |
| 86  | OHX  | 6     | 2118 | 7/7   | 0.93 | 0.14 | 132,132,132,132             | 0     |
| 85  | MG   | 5     | 3423 | 1/1   | 0.93 | 0.14 | 39,39,39,39                 | 0     |
| 85  | MG   | 5     | 3544 | 1/1   | 0.93 | 0.21 | 30,30,30,30                 | 0     |
| 86  | OHX  | 6     | 2123 | 7/7   | 0.93 | 0.11 | 140,140,140,140             | 0     |
| 85  | MG   | 1     | 3510 | 1/1   | 0.93 | 0.31 | 25,25,25,25                 | 0     |
| 85  | MG   | 4     | 220  | 1/1   | 0.93 | 0.10 | 37,37,37,37                 | 0     |
| 85  | MG   | 5     | 3666 | 1/1   | 0.93 | 0.27 | 53,53,53,53                 | 0     |
| 85  | MG   | 1     | 3681 | 1/1   | 0.93 | 0.24 | 46,46,46,46                 | 0     |
| 85  | MG   | 6     | 1931 | 1/1   | 0.93 | 0.39 | 59,59,59,59                 | 0     |
| 85  | MG   | 1     | 3511 | 1/1   | 0.93 | 0.27 | 45,45,45,45                 | 0     |
| 86  | OHX  | 1     | 4097 | 7/7   | 0.93 | 0.11 | 141,141,141,141             | 0     |
| 86  | OHX  | 2     | 2095 | 7/7   | 0.93 | 0.14 | 134,134,134,134             | 0     |
| 86  | OHX  | 2     | 2097 | 7/7   | 0.93 | 0.11 | 157,157,157,157             | 0     |
| 85  | MG   | 5     | 3433 | 1/1   | 0.93 | 0.23 | 42,42,42,42                 | 0     |
| 85  | MG   | 1     | 3544 | 1/1   | 0.93 | 0.28 | 32,32,32,32                 | 0     |
| 86  | OHX  | 6     | 2139 | 7/7   | 0.93 | 0.16 | 118,118,118,118             | 0     |
| 86  | OHX  | 2     | 2101 | 7/7   | 0.93 | 0.12 | 144,144,144,144             | 0     |
| 86  | OHX  | 6     | 2141 | 7/7   | 0.93 | 0.15 | 129,129,129,129             | 0     |
| 85  | MG   | 1     | 3849 | 1/1   | 0.93 | 0.26 | 50,50,50,50                 | 0     |
| 86  | OHX  | 5     | 4183 | 7/7   | 0.93 | 0.10 | 148,148,148,148             | 0     |
| 85  | MG   | 5     | 3438 | 1/1   | 0.93 | 0.19 | 52,52,52,52                 | 0     |
| 85  | MG   | 5     | 3677 | 1/1   | 0.93 | 0.15 | 41,41,41,41                 | 0     |
| 85  | MG   | 5     | 3827 | 1/1   | 0.93 | 0.13 | 41,41,41,41                 | 0     |
| 86  | OHX  | 1     | 4107 | 7/7   | 0.93 | 0.15 | 119,119,119,119             | 0     |
| 85  | MG   | 1     | 3687 | 1/1   | 0.93 | 0.18 | 46,46,46,46                 | 0     |
| 85  | MG   | 1     | 3733 | 1/1   | 0.93 | 0.25 | 41,41,41,41                 | 0     |
| 85  | MG   | 1     | 3512 | 1/1   | 0.93 | 0.29 | 31,31,31,31                 | 0     |
| 85  | MG   | 5     | 3838 | 1/1   | 0.93 | 0.23 | 33,33,33,33                 | 0     |
| 85  | MG   | 1     | 3790 | 1/1   | 0.93 | 0.14 | 38,38,38,38                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | L7    | 302  | 1/1   | 0.93 | 0.09 | 40,40,40,40                 | 0     |
| 85  | MG   | 5     | 3568 | 1/1   | 0.93 | 0.24 | 27,27,27,27                 | 0     |
| 85  | MG   | 5     | 3846 | 1/1   | 0.93 | 0.16 | 32,32,32,32                 | 0     |
| 85  | MG   | 1     | 3736 | 1/1   | 0.93 | 0.14 | 60,60,60,60                 | 0     |
| 85  | MG   | L7    | 304  | 1/1   | 0.93 | 0.15 | 36,36,36,36                 | 0     |
| 85  | MG   | 1     | 3589 | 1/1   | 0.93 | 0.26 | 29,29,29,29                 | 0     |
| 85  | MG   | 5     | 3573 | 1/1   | 0.93 | 0.28 | 31,31,31,31                 | 0     |
| 85  | MG   | 5     | 3853 | 1/1   | 0.93 | 0.17 | 62,62,62,62                 | 0     |
| 85  | MG   | 5     | 3854 | 1/1   | 0.93 | 0.12 | 46,46,46,46                 | 0     |
| 85  | MG   | 1     | 3490 | 1/1   | 0.93 | 0.13 | 52,52,52,52                 | 0     |
| 85  | MG   | 6     | 1947 | 1/1   | 0.93 | 0.36 | 50,50,50,50                 | 0     |
| 85  | MG   | 6     | 2020 | 1/1   | 0.93 | 0.34 | 53,53,53,53                 | 0     |
| 85  | MG   | 5     | 3466 | 1/1   | 0.93 | 0.22 | 51,51,51,51                 | 0     |
| 85  | MG   | M1    | 202  | 1/1   | 0.93 | 0.12 | 75,75,75,75                 | 0     |
| 85  | MG   | 1     | 3740 | 1/1   | 0.93 | 0.22 | 67,67,67,67                 | 0     |
| 85  | MG   | 1     | 3435 | 1/1   | 0.93 | 0.13 | 46,46,46,46                 | 0     |
| 85  | MG   | 1     | 3592 | 1/1   | 0.93 | 0.30 | 35,35,35,35                 | 0     |
| 85  | MG   | 5     | 3471 | 1/1   | 0.93 | 0.25 | 35,35,35,35                 | 0     |
| 85  | MG   | M7    | 202  | 1/1   | 0.93 | 0.24 | 29,29,29,29                 | 0     |
| 85  | MG   | 5     | 3705 | 1/1   | 0.93 | 0.21 | 46,46,46,46                 | 0     |
| 85  | MG   | 5     | 3706 | 1/1   | 0.93 | 0.20 | 39,39,39,39                 | 0     |
| 86  | OHX  | 6     | 2178 | 7/7   | 0.93 | 0.26 | 99,99,99,99                 | 0     |
| 85  | MG   | 5     | 3592 | 1/1   | 0.93 | 0.26 | 26,26,26,26                 | 0     |
| 86  | OHX  | 1     | 4138 | 7/7   | 0.93 | 0.20 | 101,101,101,101             | 0     |
| 85  | MG   | 5     | 3874 | 1/1   | 0.93 | 0.42 | 54,54,54,54                 | 0     |
| 86  | OHX  | 1     | 4140 | 7/7   | 0.93 | 0.14 | 104,104,104,104             | 0     |
| 85  | MG   | 1     | 3802 | 1/1   | 0.93 | 0.18 | 88,88,88,88                 | 0     |
| 85  | MG   | 5     | 3709 | 1/1   | 0.93 | 0.16 | 42,42,42,42                 | 0     |
| 85  | MG   | 1     | 3805 | 1/1   | 0.93 | 0.18 | 60,60,60,60                 | 0     |
| 85  | MG   | 1     | 3746 | 1/1   | 0.93 | 0.18 | 44,44,44,44                 | 0     |
| 85  | MG   | 1     | 3866 | 1/1   | 0.93 | 0.26 | 29,29,29,29                 | 0     |
| 86  | OHX  | 2     | 2146 | 7/7   | 0.93 | 0.13 | 132,132,132,132             | 0     |
| 85  | MG   | 1     | 3567 | 1/1   | 0.93 | 0.21 | 36,36,36,36                 | 0     |
| 85  | MG   | 5     | 3882 | 1/1   | 0.93 | 0.17 | 34,34,34,34                 | 0     |
| 85  | MG   | 2     | 1987 | 1/1   | 0.93 | 0.31 | 80,80,80,80                 | 0     |
| 85  | MG   | 5     | 3603 | 1/1   | 0.93 | 0.20 | 38,38,38,38                 | 0     |
| 85  | MG   | 1     | 3596 | 1/1   | 0.93 | 0.27 | 25,25,25,25                 | 0     |
| 85  | MG   | 5     | 3717 | 1/1   | 0.93 | 0.25 | 47,47,47,47                 | 0     |
| 85  | MG   | 1     | 3814 | 1/1   | 0.93 | 0.12 | 39,39,39,39                 | 0     |
| 85  | MG   | 1     | 3570 | 1/1   | 0.93 | 0.24 | 29,29,29,29                 | 0     |
| 85  | MG   | O2    | 201  | 1/1   | 0.93 | 0.08 | 34,34,34,34                 | 0     |
| 85  | MG   | O3    | 201  | 1/1   | 0.93 | 0.07 | 38,38,38,38                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 1     | 4158 | 7/7   | 0.93 | 0.18 | 125,125,125,125             | 0     |
| 85  | MG   | 1     | 3516 | 1/1   | 0.93 | 0.25 | 28,28,28,28                 | 0     |
| 85  | MG   | 5     | 3612 | 1/1   | 0.93 | 0.23 | 49,49,49,49                 | 0     |
| 85  | MG   | 6     | 2043 | 1/1   | 0.93 | 0.39 | 75,75,75,75                 | 0     |
| 85  | MG   | 6     | 2044 | 1/1   | 0.93 | 0.30 | 47,47,47,47                 | 0     |
| 85  | MG   | 5     | 3618 | 1/1   | 0.93 | 0.16 | 43,43,43,43                 | 0     |
| 85  | MG   | 5     | 3619 | 1/1   | 0.93 | 0.25 | 43,43,43,43                 | 0     |
| 85  | MG   | 5     | 3492 | 1/1   | 0.93 | 0.20 | 52,52,52,52                 | 0     |
| 85  | MG   | 6     | 2045 | 1/1   | 0.93 | 0.23 | 58,58,58,58                 | 0     |
| 85  | MG   | 1     | 3552 | 1/1   | 0.93 | 0.26 | 43,43,43,43                 | 0     |
| 85  | MG   | 7     | 206  | 1/1   | 0.93 | 0.34 | 27,27,27,27                 | 0     |
| 85  | MG   | 1     | 3705 | 1/1   | 0.93 | 0.31 | 45,45,45,45                 | 0     |
| 85  | MG   | 5     | 3497 | 1/1   | 0.93 | 0.14 | 33,33,33,33                 | 0     |
| 86  | OHX  | c8    | 201  | 7/7   | 0.93 | 0.10 | 142,142,142,142             | 0     |
| 85  | MG   | 6     | 1971 | 1/1   | 0.93 | 0.22 | 63,63,63,63                 | 0     |
| 85  | MG   | 3     | 210  | 1/1   | 0.93 | 0.23 | 67,67,67,67                 | 0     |
| 85  | MG   | 1     | 3663 | 1/1   | 0.93 | 0.17 | 34,34,34,34                 | 0     |
| 85  | MG   | 7     | 214  | 1/1   | 0.93 | 0.06 | 41,41,41,41                 | 0     |
| 86  | OHX  | 5     | 3997 | 7/7   | 0.93 | 0.13 | 104,104,104,104             | 0     |
| 85  | MG   | 1     | 3445 | 1/1   | 0.93 | 0.34 | 63,63,63,63                 | 0     |
| 86  | OHX  | 8     | 222  | 7/7   | 0.93 | 0.17 | 111,111,111,111             | 0     |
| 85  | MG   | 5     | 3630 | 1/1   | 0.93 | 0.15 | 40,40,40,40                 | 0     |
| 86  | OHX  | 5     | 4034 | 7/7   | 0.93 | 0.17 | 107,107,107,107             | 0     |
| 86  | OHX  | 5     | 4039 | 7/7   | 0.93 | 0.12 | 115,115,115,115             | 0     |
| 85  | MG   | 1     | 3578 | 1/1   | 0.93 | 0.27 | 29,29,29,29                 | 0     |
| 86  | OHX  | 5     | 4058 | 7/7   | 0.93 | 0.16 | 105,105,105,105             | 0     |
| 86  | OHX  | 5     | 4063 | 7/7   | 0.93 | 0.17 | 104,104,104,104             | 0     |
| 85  | MG   | 1     | 3446 | 1/1   | 0.93 | 0.33 | 47,47,47,47                 | 0     |
| 85  | MG   | 1     | 3824 | 1/1   | 0.93 | 0.09 | 36,36,36,36                 | 0     |
| 85  | MG   | 6     | 1910 | 1/1   | 0.93 | 0.26 | 48,48,48,48                 | 0     |
| 85  | MG   | 5     | 3764 | 1/1   | 0.93 | 0.31 | 41,41,41,41                 | 0     |
| 86  | OHX  | 5     | 4073 | 7/7   | 0.93 | 0.16 | 124,124,124,124             | 0     |
| 86  | OHX  | 5     | 4075 | 7/7   | 0.93 | 0.15 | 107,107,107,107             | 0     |
| 85  | MG   | 5     | 3765 | 1/1   | 0.93 | 0.08 | 57,57,57,57                 | 0     |
| 85  | MG   | 1     | 3711 | 1/1   | 0.93 | 0.11 | 51,51,51,51                 | 0     |
| 86  | OHX  | 5     | 4081 | 7/7   | 0.93 | 0.16 | 121,121,121,121             | 0     |
| 85  | MG   | 6     | 1913 | 1/1   | 0.93 | 0.29 | 39,39,39,39                 | 0     |
| 86  | OHX  | 5     | 4085 | 7/7   | 0.93 | 0.11 | 134,134,134,134             | 0     |
| 85  | MG   | 5     | 3514 | 1/1   | 0.93 | 0.32 | 27,27,27,27                 | 0     |
| 85  | MG   | 5     | 3774 | 1/1   | 0.93 | 0.10 | 32,32,32,32                 | 0     |
| 85  | MG   | 8     | 211  | 1/1   | 0.93 | 0.09 | 38,38,38,38                 | 0     |
| 85  | MG   | 5     | 3515 | 1/1   | 0.93 | 0.29 | 37,37,37,37                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 5     | 4091 | 7/7   | 0.93 | 0.29 | 98,98,98,98                 | 0     |
| 86  | OHX  | 1     | 3975 | 7/7   | 0.93 | 0.15 | 103,103,103,103             | 0     |
| 86  | OHX  | 5     | 4107 | 7/7   | 0.94 | 0.27 | 100,100,100,100             | 0     |
| 85  | MG   | 1     | 3684 | 1/1   | 0.94 | 0.18 | 63,63,63,63                 | 0     |
| 85  | MG   | 2     | 2002 | 1/1   | 0.94 | 0.20 | 83,83,83,83                 | 0     |
| 85  | MG   | 5     | 3571 | 1/1   | 0.94 | 0.35 | 23,23,23,23                 | 0     |
| 85  | MG   | 1     | 3474 | 1/1   | 0.94 | 0.27 | 29,29,29,29                 | 0     |
| 86  | OHX  | 6     | 2079 | 7/7   | 0.94 | 0.13 | 110,110,110,110             | 0     |
| 86  | OHX  | 5     | 4114 | 7/7   | 0.94 | 0.16 | 120,120,120,120             | 0     |
| 85  | MG   | 7     | 203  | 1/1   | 0.94 | 0.13 | 26,26,26,26                 | 0     |
| 86  | OHX  | 5     | 4116 | 7/7   | 0.94 | 0.17 | 108,108,108,108             | 0     |
| 85  | MG   | 1     | 3732 | 1/1   | 0.94 | 0.27 | 24,24,24,24                 | 0     |
| 85  | MG   | d6    | 102  | 1/1   | 0.94 | 0.19 | 55,55,55,55                 | 0     |
| 85  | MG   | 5     | 3575 | 1/1   | 0.94 | 0.30 | 24,24,24,24                 | 0     |
| 85  | MG   | 1     | 3832 | 1/1   | 0.94 | 0.26 | 26,26,26,26                 | 0     |
| 85  | MG   | 1     | 3620 | 1/1   | 0.94 | 0.21 | 51,51,51,51                 | 0     |
| 85  | MG   | 1     | 3734 | 1/1   | 0.94 | 0.10 | 54,54,54,54                 | 0     |
| 86  | OHX  | 6     | 2110 | 7/7   | 0.94 | 0.17 | 108,108,108,108             | 0     |
| 86  | OHX  | 6     | 2117 | 7/7   | 0.94 | 0.12 | 124,124,124,124             | 0     |
| 85  | MG   | N8    | 206  | 1/1   | 0.94 | 0.07 | 34,34,34,34                 | 0     |
| 85  | MG   | 5     | 3675 | 1/1   | 0.94 | 0.26 | 44,44,44,44                 | 0     |
| 86  | OHX  | 6     | 2120 | 7/7   | 0.94 | 0.12 | 138,138,138,138             | 0     |
| 85  | MG   | 1     | 3836 | 1/1   | 0.94 | 0.21 | 43,43,43,43                 | 0     |
| 85  | MG   | 1     | 3783 | 1/1   | 0.94 | 0.11 | 43,43,43,43                 | 0     |
| 86  | OHX  | 5     | 4133 | 7/7   | 0.94 | 0.13 | 108,108,108,108             | 0     |
| 86  | OHX  | 6     | 2124 | 7/7   | 0.94 | 0.12 | 136,136,136,136             | 0     |
| 85  | MG   | 1     | 3838 | 1/1   | 0.94 | 0.33 | 34,34,34,34                 | 0     |
| 85  | MG   | 5     | 3587 | 1/1   | 0.94 | 0.22 | 27,27,27,27                 | 0     |
| 85  | MG   | 1     | 3413 | 1/1   | 0.94 | 0.23 | 39,39,39,39                 | 0     |
| 85  | MG   | 5     | 3589 | 1/1   | 0.94 | 0.28 | 25,25,25,25                 | 0     |
| 85  | MG   | 1     | 3506 | 1/1   | 0.94 | 0.19 | 36,36,36,36                 | 0     |
| 86  | OHX  | 6     | 2131 | 7/7   | 0.94 | 0.12 | 134,134,134,134             | 0     |
| 85  | MG   | 5     | 3591 | 1/1   | 0.94 | 0.25 | 43,43,43,43                 | 0     |
| 85  | MG   | 1     | 3841 | 1/1   | 0.94 | 0.20 | 29,29,29,29                 | 0     |
| 86  | OHX  | 1     | 4121 | 7/7   | 0.94 | 0.16 | 118,118,118,118             | 0     |
| 85  | MG   | 5     | 3593 | 1/1   | 0.94 | 0.27 | 30,30,30,30                 | 0     |
| 86  | OHX  | 5     | 4145 | 7/7   | 0.94 | 0.12 | 128,128,128,128             | 0     |
| 85  | MG   | 1     | 3786 | 1/1   | 0.94 | 0.34 | 33,33,33,33                 | 0     |
| 85  | MG   | 5     | 3595 | 1/1   | 0.94 | 0.37 | 34,34,34,34                 | 0     |
| 85  | MG   | 5     | 3498 | 1/1   | 0.94 | 0.33 | 31,31,31,31                 | 0     |
| 85  | MG   | 1     | 3525 | 1/1   | 0.94 | 0.20 | 25,25,25,25                 | 0     |
| 85  | MG   | 5     | 3694 | 1/1   | 0.94 | 0.09 | 43,43,43,43                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 6     | 1905 | 1/1   | 0.94 | 0.40 | 53,53,53,53                 | 0     |
| 85  | MG   | 5     | 3812 | 1/1   | 0.94 | 0.13 | 28,28,28,28                 | 0     |
| 85  | MG   | 8     | 215  | 1/1   | 0.94 | 0.30 | 36,36,36,36                 | 0     |
| 85  | MG   | 12    | 301  | 1/1   | 0.94 | 0.39 | 49,49,49,49                 | 0     |
| 85  | MG   | 12    | 302  | 1/1   | 0.94 | 0.15 | 40,40,40,40                 | 0     |
| 86  | OHX  | 5     | 4157 | 7/7   | 0.94 | 0.16 | 112,112,112,112             | 0     |
| 86  | OHX  | 6     | 2149 | 7/7   | 0.94 | 0.16 | 105,105,105,105             | 0     |
| 85  | MG   | 5     | 3813 | 1/1   | 0.94 | 0.06 | 39,39,39,39                 | 0     |
| 85  | MG   | 5     | 3501 | 1/1   | 0.94 | 0.23 | 26,26,26,26                 | 0     |
| 85  | MG   | 1     | 3595 | 1/1   | 0.94 | 0.31 | 30,30,30,30                 | 0     |
| 85  | MG   | 1     | 3789 | 1/1   | 0.94 | 0.07 | 40,40,40,40                 | 0     |
| 85  | MG   | 6     | 1960 | 1/1   | 0.94 | 0.37 | 41,41,41,41                 | 0     |
| 85  | MG   | 1     | 3437 | 1/1   | 0.94 | 0.20 | 40,40,40,40                 | 0     |
| 85  | MG   | m0    | 301  | 1/1   | 0.94 | 0.27 | 28,28,28,28                 | 0     |
| 85  | MG   | 1     | 3656 | 1/1   | 0.94 | 0.18 | 39,39,39,39                 | 0     |
| 85  | MG   | 1     | 3527 | 1/1   | 0.94 | 0.27 | 28,28,28,28                 | 0     |
| 85  | MG   | 1     | 3577 | 1/1   | 0.94 | 0.26 | 19,19,19,19                 | 0     |
| 85  | MG   | 5     | 3429 | 1/1   | 0.94 | 0.20 | 27,27,27,27                 | 0     |
| 85  | MG   | m7    | 203  | 1/1   | 0.94 | 0.11 | 41,41,41,41                 | 0     |
| 85  | MG   | 1     | 3661 | 1/1   | 0.94 | 0.28 | 26,26,26,26                 | 0     |
| 85  | MG   | 5     | 3829 | 1/1   | 0.94 | 0.21 | 27,27,27,27                 | 0     |
| 85  | MG   | 2     | 2010 | 1/1   | 0.94 | 0.28 | 61,61,61,61                 | 0     |
| 85  | MG   | 6     | 2023 | 1/1   | 0.94 | 0.13 | 81,81,81,81                 | 0     |
| 85  | MG   | 1     | 3704 | 1/1   | 0.94 | 0.08 | 42,42,42,42                 | 0     |
| 85  | MG   | 5     | 3836 | 1/1   | 0.94 | 0.14 | 39,39,39,39                 | 0     |
| 85  | MG   | 5     | 3518 | 1/1   | 0.94 | 0.36 | 22,22,22,22                 | 0     |
| 85  | MG   | 1     | 3664 | 1/1   | 0.94 | 0.11 | 33,33,33,33                 | 0     |
| 85  | MG   | 1     | 3553 | 1/1   | 0.94 | 0.35 | 32,32,32,32                 | 0     |
| 86  | OHX  | 1     | 3952 | 7/7   | 0.94 | 0.13 | 119,119,119,119             | 0     |
| 86  | OHX  | 1     | 3955 | 7/7   | 0.94 | 0.18 | 96,96,96,96                 | 0     |
| 86  | OHX  | 1     | 3965 | 7/7   | 0.94 | 0.17 | 94,94,94,94                 | 0     |
| 85  | MG   | 5     | 3844 | 1/1   | 0.94 | 0.18 | 47,47,47,47                 | 0     |
| 86  | OHX  | 1     | 4160 | 7/7   | 0.94 | 0.14 | 110,110,110,110             | 0     |
| 85  | MG   | o3    | 201  | 1/1   | 0.94 | 0.19 | 45,45,45,45                 | 0     |
| 85  | MG   | 1     | 3667 | 1/1   | 0.94 | 0.07 | 52,52,52,52                 | 0     |
| 85  | MG   | 5     | 3623 | 1/1   | 0.94 | 0.18 | 68,68,68,68                 | 0     |
| 85  | MG   | 5     | 3440 | 1/1   | 0.94 | 0.27 | 33,33,33,33                 | 0     |
| 86  | OHX  | 1     | 4005 | 7/7   | 0.94 | 0.22 | 97,97,97,97                 | 0     |
| 85  | MG   | 5     | 3524 | 1/1   | 0.94 | 0.31 | 34,34,34,34                 | 0     |
| 86  | OHX  | 1     | 4009 | 7/7   | 0.94 | 0.15 | 112,112,112,112             | 0     |
| 86  | OHX  | 1     | 4012 | 7/7   | 0.94 | 0.15 | 120,120,120,120             | 0     |
| 86  | OHX  | 2     | 2039 | 7/7   | 0.94 | 0.14 | 102,102,102,102             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 2     | 2053 | 7/7   | 0.94 | 0.11 | 133,133,133,133             | 0     |
| 86  | OHX  | 2     | 2054 | 7/7   | 0.94 | 0.13 | 112,112,112,112             | 0     |
| 86  | OHX  | 1     | 4018 | 7/7   | 0.94 | 0.13 | 121,121,121,121             | 0     |
| 86  | OHX  | 1     | 4019 | 7/7   | 0.94 | 0.14 | 107,107,107,107             | 0     |
| 85  | MG   | 1     | 3424 | 1/1   | 0.94 | 0.27 | 44,44,44,44                 | 0     |
| 86  | OHX  | 2     | 2064 | 7/7   | 0.94 | 0.18 | 107,107,107,107             | 0     |
| 86  | OHX  | 2     | 2066 | 7/7   | 0.94 | 0.10 | 138,138,138,138             | 0     |
| 85  | MG   | 1     | 3455 | 1/1   | 0.94 | 0.33 | 32,32,32,32                 | 0     |
| 86  | OHX  | 1     | 4026 | 7/7   | 0.94 | 0.11 | 135,135,135,135             | 0     |
| 86  | OHX  | 2     | 2068 | 7/7   | 0.94 | 0.15 | 111,111,111,111             | 0     |
| 85  | MG   | 5     | 3532 | 1/1   | 0.94 | 0.25 | 33,33,33,33                 | 0     |
| 86  | OHX  | 1     | 4032 | 7/7   | 0.94 | 0.12 | 130,130,130,130             | 0     |
| 85  | MG   | 5     | 3445 | 1/1   | 0.94 | 0.08 | 33,33,33,33                 | 0     |
| 86  | OHX  | 2     | 2076 | 7/7   | 0.94 | 0.12 | 118,118,118,118             | 0     |
| 85  | MG   | 6     | 1974 | 1/1   | 0.94 | 0.28 | 52,52,52,52                 | 0     |
| 85  | MG   | 5     | 3447 | 1/1   | 0.94 | 0.10 | 38,38,38,38                 | 0     |
| 86  | OHX  | 2     | 2081 | 7/7   | 0.94 | 0.10 | 147,147,147,147             | 0     |
| 86  | OHX  | 1     | 4047 | 7/7   | 0.94 | 0.15 | 106,106,106,106             | 0     |
| 85  | MG   | 1     | 3606 | 1/1   | 0.94 | 0.15 | 39,39,39,39                 | 0     |
| 85  | MG   | 5     | 3539 | 1/1   | 0.94 | 0.23 | 25,25,25,25                 | 0     |
| 86  | OHX  | 1     | 4050 | 7/7   | 0.94 | 0.15 | 111,111,111,111             | 0     |
| 86  | OHX  | 2     | 2085 | 7/7   | 0.94 | 0.14 | 111,111,111,111             | 0     |
| 85  | MG   | 6     | 1978 | 1/1   | 0.94 | 0.18 | 42,42,42,42                 | 0     |
| 85  | MG   | 5     | 3451 | 1/1   | 0.94 | 0.22 | 30,30,30,30                 | 0     |
| 86  | OHX  | 1     | 4056 | 7/7   | 0.94 | 0.10 | 139,139,139,139             | 0     |
| 86  | OHX  | 1     | 4057 | 7/7   | 0.94 | 0.14 | 128,128,128,128             | 0     |
| 85  | MG   | 1     | 3482 | 1/1   | 0.94 | 0.37 | 41,41,41,41                 | 0     |
| 85  | MG   | 5     | 3455 | 1/1   | 0.94 | 0.17 | 41,41,41,41                 | 0     |
| 85  | MG   | 1     | 3466 | 1/1   | 0.94 | 0.30 | 48,48,48,48                 | 0     |
| 85  | MG   | 1     | 3534 | 1/1   | 0.94 | 0.29 | 37,37,37,37                 | 0     |
| 85  | MG   | 5     | 3641 | 1/1   | 0.94 | 0.22 | 47,47,47,47                 | 0     |
| 86  | OHX  | 5     | 4001 | 7/7   | 0.94 | 0.12 | 107,107,107,107             | 0     |
| 86  | OHX  | 5     | 4008 | 7/7   | 0.94 | 0.13 | 109,109,109,109             | 0     |
| 86  | OHX  | 5     | 4014 | 7/7   | 0.94 | 0.15 | 103,103,103,103             | 0     |
| 86  | OHX  | 1     | 4064 | 7/7   | 0.94 | 0.10 | 147,147,147,147             | 0     |
| 86  | OHX  | 5     | 4024 | 7/7   | 0.94 | 0.14 | 108,108,108,108             | 0     |
| 85  | MG   | 5     | 3869 | 1/1   | 0.94 | 0.20 | 28,28,28,28                 | 0     |
| 86  | OHX  | 5     | 4029 | 7/7   | 0.94 | 0.17 | 98,98,98,98                 | 0     |
| 86  | OHX  | 5     | 4033 | 7/7   | 0.94 | 0.12 | 129,129,129,129             | 0     |
| 85  | MG   | 5     | 3742 | 1/1   | 0.94 | 0.27 | 33,33,33,33                 | 0     |
| 86  | OHX  | 5     | 4037 | 7/7   | 0.94 | 0.12 | 119,119,119,119             | 0     |
| 86  | OHX  | 5     | 4038 | 7/7   | 0.94 | 0.11 | 127,127,127,127             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 5     | 3871 | 1/1   | 0.94 | 0.21 | 27,27,27,27                 | 0     |
| 85  | MG   | 5     | 3642 | 1/1   | 0.94 | 0.11 | 38,38,38,38                 | 0     |
| 86  | OHX  | 5     | 4047 | 7/7   | 0.94 | 0.14 | 119,119,119,119             | 0     |
| 86  | OHX  | 5     | 4050 | 7/7   | 0.94 | 0.13 | 114,114,114,114             | 0     |
| 86  | OHX  | 5     | 4053 | 7/7   | 0.94 | 0.32 | 100,100,100,100             | 0     |
| 86  | OHX  | 5     | 4054 | 7/7   | 0.94 | 0.29 | 95,95,95,95                 | 0     |
| 85  | MG   | 1     | 3765 | 1/1   | 0.94 | 0.30 | 49,49,49,49                 | 0     |
| 86  | OHX  | 5     | 4060 | 7/7   | 0.94 | 0.12 | 136,136,136,136             | 0     |
| 85  | MG   | 5     | 3463 | 1/1   | 0.94 | 0.28 | 33,33,33,33                 | 0     |
| 85  | MG   | 5     | 3749 | 1/1   | 0.94 | 0.08 | 50,50,50,50                 | 0     |
| 85  | MG   | 6     | 1983 | 1/1   | 0.94 | 0.09 | 46,46,46,46                 | 0     |
| 86  | OHX  | 5     | 4067 | 7/7   | 0.94 | 0.15 | 108,108,108,108             | 0     |
| 86  | OHX  | 5     | 4069 | 7/7   | 0.94 | 0.12 | 122,122,122,122             | 0     |
| 86  | OHX  | 5     | 4070 | 7/7   | 0.94 | 0.16 | 105,105,105,105             | 0     |
| 86  | OHX  | 7     | 224  | 7/7   | 0.94 | 0.12 | 127,127,127,127             | 0     |
| 86  | OHX  | 2     | 2112 | 7/7   | 0.94 | 0.13 | 128,128,128,128             | 0     |
| 85  | MG   | 5     | 3754 | 1/1   | 0.94 | 0.19 | 50,50,50,50                 | 0     |
| 86  | OHX  | 1     | 4077 | 7/7   | 0.94 | 0.11 | 119,119,119,119             | 0     |
| 85  | MG   | 1     | 3766 | 1/1   | 0.94 | 0.26 | 41,41,41,41                 | 0     |
| 86  | OHX  | 8     | 224  | 7/7   | 0.94 | 0.10 | 138,138,138,138             | 0     |
| 86  | OHX  | 8     | 225  | 7/7   | 0.94 | 0.14 | 119,119,119,119             | 0     |
| 85  | MG   | 1     | 3447 | 1/1   | 0.94 | 0.05 | 46,46,46,46                 | 0     |
| 85  | MG   | 1     | 3611 | 1/1   | 0.94 | 0.14 | 42,42,42,42                 | 0     |
| 85  | MG   | D3    | 201  | 1/1   | 0.94 | 0.14 | 57,57,57,57                 | 0     |
| 86  | OHX  | 5     | 4082 | 7/7   | 0.94 | 0.13 | 113,113,113,113             | 0     |
| 85  | MG   | M5    | 302  | 1/1   | 0.94 | 0.33 | 50,50,50,50                 | 0     |
| 85  | MG   | 1     | 3501 | 1/1   | 0.94 | 0.40 | 77,77,77,77                 | 0     |
| 85  | MG   | 6     | 1933 | 1/1   | 0.94 | 0.45 | 65,65,65,65                 | 0     |
| 85  | MG   | 5     | 3889 | 1/1   | 0.94 | 0.30 | 53,53,53,53                 | 0     |
| 86  | OHX  | 4     | 231  | 7/7   | 0.94 | 0.12 | 114,114,114,114             | 0     |
| 86  | OHX  | 4     | 232  | 7/7   | 0.94 | 0.10 | 142,142,142,142             | 0     |
| 86  | OHX  | 1     | 4086 | 7/7   | 0.94 | 0.16 | 119,119,119,119             | 0     |
| 86  | OHX  | 5     | 4092 | 7/7   | 0.94 | 0.33 | 103,103,103,103             | 0     |
| 85  | MG   | 5     | 3766 | 1/1   | 0.94 | 0.16 | 40,40,40,40                 | 0     |
| 85  | MG   | 5     | 3475 | 1/1   | 0.94 | 0.37 | 51,51,51,51                 | 0     |
| 86  | OHX  | 5     | 4096 | 7/7   | 0.94 | 0.11 | 126,126,126,126             | 0     |
| 85  | MG   | 5     | 3563 | 1/1   | 0.94 | 0.43 | 34,34,34,34                 | 0     |
| 85  | MG   | 1     | 3645 | 1/1   | 0.94 | 0.26 | 38,38,38,38                 | 0     |
| 85  | MG   | M7    | 203  | 1/1   | 0.94 | 0.24 | 33,33,33,33                 | 0     |
| 85  | MG   | 5     | 3775 | 1/1   | 0.94 | 0.10 | 27,27,27,27                 | 0     |
| 86  | OHX  | M0    | 304  | 7/7   | 0.94 | 0.13 | 108,108,108,108             | 0     |
| 87  | ZN   | Q2    | 501  | 1/1   | 0.94 | 0.22 | 82,82,82,82                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | M5    | 303  | 7/7   | 0.94 | 0.15 | 113,113,113,113             | 0     |
| 85  | MG   | 1     | 3449 | 1/1   | 0.94 | 0.15 | 29,29,29,29                 | 0     |
| 85  | MG   | 5     | 3897 | 1/1   | 0.94 | 0.20 | 58,58,58,58                 | 0     |
| 85  | MG   | 1     | 3850 | 1/1   | 0.95 | 0.35 | 58,58,58,58                 | 0     |
| 85  | MG   | 1     | 3757 | 1/1   | 0.95 | 0.16 | 24,24,24,24                 | 0     |
| 85  | MG   | 5     | 3755 | 1/1   | 0.95 | 0.23 | 57,57,57,57                 | 0     |
| 86  | OHX  | 2     | 2036 | 7/7   | 0.95 | 0.12 | 128,128,128,128             | 0     |
| 85  | MG   | 5     | 3865 | 1/1   | 0.95 | 0.10 | 42,42,42,42                 | 0     |
| 86  | OHX  | 2     | 2042 | 7/7   | 0.95 | 0.12 | 114,114,114,114             | 0     |
| 86  | OHX  | 2     | 2052 | 7/7   | 0.95 | 0.09 | 131,131,131,131             | 0     |
| 85  | MG   | 5     | 3756 | 1/1   | 0.95 | 0.06 | 41,41,41,41                 | 0     |
| 85  | MG   | 5     | 3413 | 1/1   | 0.95 | 0.25 | 43,43,43,43                 | 0     |
| 86  | OHX  | 2     | 2055 | 7/7   | 0.95 | 0.10 | 127,127,127,127             | 0     |
| 86  | OHX  | 2     | 2056 | 7/7   | 0.95 | 0.10 | 140,140,140,140             | 0     |
| 85  | MG   | 5     | 3414 | 1/1   | 0.95 | 0.28 | 30,30,30,30                 | 0     |
| 86  | OHX  | 2     | 2062 | 7/7   | 0.95 | 0.10 | 129,129,129,129             | 0     |
| 86  | OHX  | 1     | 3921 | 7/7   | 0.95 | 0.14 | 114,114,114,114             | 0     |
| 86  | OHX  | 1     | 3929 | 7/7   | 0.95 | 0.13 | 99,99,99,99                 | 0     |
| 86  | OHX  | 5     | 4128 | 7/7   | 0.95 | 0.10 | 133,133,133,133             | 0     |
| 86  | OHX  | 1     | 3948 | 7/7   | 0.95 | 0.15 | 85,85,85,85                 | 0     |
| 85  | MG   | 1     | 3852 | 1/1   | 0.95 | 0.18 | 36,36,36,36                 | 0     |
| 86  | OHX  | 1     | 3954 | 7/7   | 0.95 | 0.11 | 107,107,107,107             | 0     |
| 85  | MG   | 1     | 3535 | 1/1   | 0.95 | 0.10 | 31,31,31,31                 | 0     |
| 86  | OHX  | 1     | 3964 | 7/7   | 0.95 | 0.10 | 118,118,118,118             | 0     |
| 86  | OHX  | 6     | 2147 | 7/7   | 0.95 | 0.13 | 129,129,129,129             | 0     |
| 85  | MG   | 1     | 3803 | 1/1   | 0.95 | 0.11 | 55,55,55,55                 | 0     |
| 85  | MG   | 1     | 3519 | 1/1   | 0.95 | 0.30 | 34,34,34,34                 | 0     |
| 86  | OHX  | 1     | 3971 | 7/7   | 0.95 | 0.12 | 102,102,102,102             | 0     |
| 85  | MG   | 6     | 2017 | 1/1   | 0.95 | 0.19 | 42,42,42,42                 | 0     |
| 85  | MG   | 5     | 3582 | 1/1   | 0.95 | 0.30 | 30,30,30,30                 | 0     |
| 85  | MG   | 5     | 3767 | 1/1   | 0.95 | 0.10 | 39,39,39,39                 | 0     |
| 86  | OHX  | 1     | 3988 | 7/7   | 0.95 | 0.12 | 116,116,116,116             | 0     |
| 86  | OHX  | 1     | 3993 | 7/7   | 0.95 | 0.27 | 101,101,101,101             | 0     |
| 86  | OHX  | 6     | 2157 | 7/7   | 0.95 | 0.14 | 108,108,108,108             | 0     |
| 86  | OHX  | 1     | 3994 | 7/7   | 0.95 | 0.14 | 118,118,118,118             | 0     |
| 86  | OHX  | 2     | 2077 | 7/7   | 0.95 | 0.10 | 126,126,126,126             | 0     |
| 86  | OHX  | 2     | 2078 | 7/7   | 0.95 | 0.16 | 117,117,117,117             | 0     |
| 86  | OHX  | 5     | 4148 | 7/7   | 0.95 | 0.16 | 111,111,111,111             | 0     |
| 86  | OHX  | 1     | 4006 | 7/7   | 0.95 | 0.11 | 116,116,116,116             | 0     |
| 86  | OHX  | 1     | 4007 | 7/7   | 0.95 | 0.23 | 103,103,103,103             | 0     |
| 85  | MG   | 1     | 3602 | 1/1   | 0.95 | 0.16 | 28,28,28,28                 | 0     |
| 85  | MG   | 1     | 3440 | 1/1   | 0.95 | 0.27 | 32,32,32,32                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 1     | 4155 | 7/7   | 0.95 | 0.12 | 124,124,124,124             | 0     |
| 85  | MG   | 5     | 3772 | 1/1   | 0.95 | 0.11 | 31,31,31,31                 | 0     |
| 85  | MG   | 5     | 3880 | 1/1   | 0.95 | 0.27 | 24,24,24,24                 | 0     |
| 85  | MG   | 1     | 3808 | 1/1   | 0.95 | 0.10 | 34,34,34,34                 | 0     |
| 85  | MG   | C8    | 201  | 1/1   | 0.95 | 0.10 | 106,106,106,106             | 0     |
| 86  | OHX  | 1     | 4016 | 7/7   | 0.95 | 0.10 | 133,133,133,133             | 0     |
| 85  | MG   | 1     | 3725 | 1/1   | 0.95 | 0.09 | 56,56,56,56                 | 0     |
| 85  | MG   | 5     | 3885 | 1/1   | 0.95 | 0.17 | 28,28,28,28                 | 0     |
| 85  | MG   | 1     | 3811 | 1/1   | 0.95 | 0.16 | 38,38,38,38                 | 0     |
| 86  | OHX  | 1     | 4021 | 7/7   | 0.95 | 0.12 | 114,114,114,114             | 0     |
| 85  | MG   | 6     | 2024 | 1/1   | 0.95 | 0.29 | 61,61,61,61                 | 0     |
| 86  | OHX  | 1     | 4023 | 7/7   | 0.95 | 0.12 | 108,108,108,108             | 0     |
| 85  | MG   | 1     | 3508 | 1/1   | 0.95 | 0.24 | 37,37,37,37                 | 0     |
| 86  | OHX  | 2     | 2096 | 7/7   | 0.95 | 0.09 | 163,163,163,163             | 0     |
| 85  | MG   | 1     | 3467 | 1/1   | 0.95 | 0.27 | 59,59,59,59                 | 0     |
| 85  | MG   | 6     | 1975 | 1/1   | 0.95 | 0.25 | 51,51,51,51                 | 0     |
| 86  | OHX  | 1     | 4029 | 7/7   | 0.95 | 0.11 | 124,124,124,124             | 0     |
| 85  | MG   | 6     | 1976 | 1/1   | 0.95 | 0.19 | 60,60,60,60                 | 0     |
| 85  | MG   | 1     | 3692 | 1/1   | 0.95 | 0.34 | 60,60,60,60                 | 0     |
| 86  | OHX  | 1     | 4033 | 7/7   | 0.95 | 0.12 | 125,125,125,125             | 0     |
| 85  | MG   | 1     | 3662 | 1/1   | 0.95 | 0.30 | 42,42,42,42                 | 0     |
| 86  | OHX  | 1     | 4037 | 7/7   | 0.95 | 0.15 | 104,104,104,104             | 0     |
| 85  | MG   | 1     | 3561 | 1/1   | 0.95 | 0.18 | 26,26,26,26                 | 0     |
| 86  | OHX  | 5     | 4177 | 7/7   | 0.95 | 0.15 | 111,111,111,111             | 0     |
| 85  | MG   | 6     | 1927 | 1/1   | 0.95 | 0.27 | 47,47,47,47                 | 0     |
| 86  | OHX  | 1     | 4041 | 7/7   | 0.95 | 0.16 | 111,111,111,111             | 0     |
| 85  | MG   | 5     | 3600 | 1/1   | 0.95 | 0.20 | 39,39,39,39                 | 0     |
| 86  | OHX  | 1     | 4043 | 7/7   | 0.95 | 0.14 | 105,105,105,105             | 0     |
| 86  | OHX  | 2     | 2106 | 7/7   | 0.95 | 0.12 | 111,111,111,111             | 0     |
| 86  | OHX  | 1     | 4185 | 7/7   | 0.95 | 0.27 | 99,99,99,99                 | 0     |
| 85  | MG   | 5     | 3441 | 1/1   | 0.95 | 0.26 | 36,36,36,36                 | 0     |
| 86  | OHX  | 2     | 2108 | 7/7   | 0.95 | 0.10 | 149,149,149,149             | 0     |
| 86  | OHX  | 2     | 2110 | 7/7   | 0.95 | 0.14 | 114,114,114,114             | 0     |
| 85  | MG   | 1     | 3731 | 1/1   | 0.95 | 0.18 | 32,32,32,32                 | 0     |
| 86  | OHX  | 1     | 4051 | 7/7   | 0.95 | 0.12 | 116,116,116,116             | 0     |
| 85  | MG   | M3    | 203  | 1/1   | 0.95 | 0.11 | 32,32,32,32                 | 0     |
| 85  | MG   | 1     | 3772 | 1/1   | 0.95 | 0.20 | 28,28,28,28                 | 0     |
| 86  | OHX  | 1     | 4054 | 7/7   | 0.95 | 0.15 | 109,109,109,109             | 0     |
| 85  | MG   | 5     | 3692 | 1/1   | 0.95 | 0.11 | 48,48,48,48                 | 0     |
| 85  | MG   | 1     | 3773 | 1/1   | 0.95 | 0.16 | 66,66,66,66                 | 0     |
| 86  | OHX  | 6     | 2204 | 7/7   | 0.95 | 0.07 | 185,185,185,185             | 0     |
| 85  | MG   | 1     | 3468 | 1/1   | 0.95 | 0.19 | 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  | MG   | 5     | 3448 | 1/1   | 0.95 | 0.11 | 42,42,42,42                 | 0     |
| 85  | MG   | 5     | 3609 | 1/1   | 0.95 | 0.24 | 29,29,29,29                 | 0     |
| 85  | MG   | 5     | 3525 | 1/1   | 0.95 | 0.28 | 27,27,27,27                 | 0     |
| 85  | MG   | 1     | 3563 | 1/1   | 0.95 | 0.39 | 41,41,41,41                 | 0     |
| 85  | MG   | 1     | 3564 | 1/1   | 0.95 | 0.28 | 26,26,26,26                 | 0     |
| 85  | MG   | 1     | 3434 | 1/1   | 0.95 | 0.14 | 34,34,34,34                 | 0     |
| 85  | MG   | 5     | 3806 | 1/1   | 0.95 | 0.11 | 34,34,34,34                 | 0     |
| 85  | MG   | 5     | 3617 | 1/1   | 0.95 | 0.22 | 39,39,39,39                 | 0     |
| 85  | MG   | 2     | 1903 | 1/1   | 0.95 | 0.36 | 50,50,50,50                 | 0     |
| 86  | OHX  | 1     | 4069 | 7/7   | 0.95 | 0.09 | 143,143,143,143             | 0     |
| 85  | MG   | 5     | 3453 | 1/1   | 0.95 | 0.06 | 34,34,34,34                 | 0     |
| 85  | MG   | 5     | 3454 | 1/1   | 0.95 | 0.35 | 45,45,45,45                 | 0     |
| 86  | OHX  | 5     | 3978 | 7/7   | 0.95 | 0.13 | 93,93,93,93                 | 0     |
| 86  | OHX  | 5     | 3980 | 7/7   | 0.95 | 0.14 | 96,96,96,96                 | 0     |
| 86  | OHX  | 5     | 3995 | 7/7   | 0.95 | 0.30 | 93,93,93,93                 | 0     |
| 86  | OHX  | 5     | 3996 | 7/7   | 0.95 | 0.11 | 128,128,128,128             | 0     |
| 85  | MG   | 1     | 3737 | 1/1   | 0.95 | 0.14 | 36,36,36,36                 | 0     |
| 86  | OHX  | 2     | 2130 | 7/7   | 0.95 | 0.17 | 113,113,113,113             | 0     |
| 86  | OHX  | 5     | 4006 | 7/7   | 0.95 | 0.16 | 100,100,100,100             | 0     |
| 85  | MG   | 5     | 3537 | 1/1   | 0.95 | 0.28 | 34,34,34,34                 | 0     |
| 85  | MG   | 1     | 3547 | 1/1   | 0.95 | 0.25 | 52,52,52,52                 | 0     |
| 85  | MG   | 1     | 3616 | 1/1   | 0.95 | 0.21 | 38,38,38,38                 | 0     |
| 85  | MG   | 1     | 3568 | 1/1   | 0.95 | 0.36 | 34,34,34,34                 | 0     |
| 86  | OHX  | 5     | 4027 | 7/7   | 0.95 | 0.14 | 103,103,103,103             | 0     |
| 85  | MG   | 5     | 3461 | 1/1   | 0.95 | 0.11 | 27,27,27,27                 | 0     |
| 85  | MG   | 5     | 3462 | 1/1   | 0.95 | 0.12 | 38,38,38,38                 | 0     |
| 86  | OHX  | 5     | 4031 | 7/7   | 0.95 | 0.22 | 93,93,93,93                 | 0     |
| 86  | OHX  | 3     | 215  | 7/7   | 0.95 | 0.16 | 107,107,107,107             | 0     |
| 86  | OHX  | 3     | 216  | 7/7   | 0.95 | 0.13 | 105,105,105,105             | 0     |
| 85  | MG   | 2     | 2014 | 1/1   | 0.95 | 0.51 | 65,65,65,65                 | 0     |
| 85  | MG   | 1     | 3430 | 1/1   | 0.95 | 0.46 | 41,41,41,41                 | 0     |
| 85  | MG   | 5     | 3547 | 1/1   | 0.95 | 0.30 | 47,47,47,47                 | 0     |
| 86  | OHX  | 5     | 4040 | 7/7   | 0.95 | 0.09 | 126,126,126,126             | 0     |
| 86  | OHX  | 5     | 4042 | 7/7   | 0.95 | 0.14 | 117,117,117,117             | 0     |
| 85  | MG   | 1     | 3744 | 1/1   | 0.95 | 0.22 | 46,46,46,46                 | 0     |
| 86  | OHX  | 5     | 4045 | 7/7   | 0.95 | 0.14 | 105,105,105,105             | 0     |
| 85  | MG   | s8    | 302  | 1/1   | 0.95 | 0.17 | 50,50,50,50                 | 0     |
| 86  | OHX  | 5     | 4049 | 7/7   | 0.95 | 0.13 | 122,122,122,122             | 0     |
| 86  | OHX  | 5     | 4236 | 7/7   | 0.95 | 0.25 | 97,97,97,97                 | 0     |
| 85  | MG   | 5     | 3826 | 1/1   | 0.95 | 0.12 | 36,36,36,36                 | 0     |
| 85  | MG   | 1     | 3473 | 1/1   | 0.95 | 0.23 | 39,39,39,39                 | 0     |
| 85  | MG   | 5     | 3828 | 1/1   | 0.95 | 0.12 | 34,34,34,34                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 4     | 233  | 7/7   | 0.95 | 0.11 | 129,129,129,129             | 0     |
| 86  | OHX  | 5     | 4059 | 7/7   | 0.95 | 0.11 | 122,122,122,122             | 0     |
| 85  | MG   | 2     | 1957 | 1/1   | 0.95 | 0.45 | 72,72,72,72                 | 0     |
| 86  | OHX  | 1     | 4089 | 7/7   | 0.95 | 0.08 | 189,189,189,189             | 0     |
| 85  | MG   | 5     | 3830 | 1/1   | 0.95 | 0.18 | 50,50,50,50                 | 0     |
| 85  | MG   | l3    | 402  | 1/1   | 0.95 | 0.34 | 24,24,24,24                 | 0     |
| 86  | OHX  | 5     | 4066 | 7/7   | 0.95 | 0.09 | 142,142,142,142             | 0     |
| 85  | MG   | 1     | 3432 | 1/1   | 0.95 | 0.23 | 45,45,45,45                 | 0     |
| 86  | OHX  | L3    | 404  | 7/7   | 0.95 | 0.13 | 106,106,106,106             | 0     |
| 85  | MG   | 1     | 3792 | 1/1   | 0.95 | 0.10 | 67,67,67,67                 | 0     |
| 85  | MG   | d3    | 201  | 1/1   | 0.95 | 0.23 | 47,47,47,47                 | 0     |
| 85  | MG   | 1     | 3680 | 1/1   | 0.95 | 0.19 | 47,47,47,47                 | 0     |
| 85  | MG   | 5     | 3729 | 1/1   | 0.95 | 0.13 | 51,51,51,51                 | 0     |
| 86  | OHX  | 5     | 4074 | 7/7   | 0.95 | 0.14 | 108,108,108,108             | 0     |
| 85  | MG   | 1     | 3715 | 1/1   | 0.95 | 0.10 | 54,54,54,54                 | 0     |
| 86  | OHX  | 5     | 4076 | 7/7   | 0.95 | 0.14 | 108,108,108,108             | 0     |
| 85  | MG   | 5     | 3840 | 1/1   | 0.95 | 0.14 | 59,59,59,59                 | 0     |
| 85  | MG   | 5     | 3842 | 1/1   | 0.95 | 0.10 | 38,38,38,38                 | 0     |
| 86  | OHX  | 5     | 4079 | 7/7   | 0.95 | 0.10 | 150,150,150,150             | 0     |
| 86  | OHX  | 8     | 220  | 7/7   | 0.95 | 0.11 | 126,126,126,126             | 0     |
| 85  | MG   | 6     | 1903 | 1/1   | 0.95 | 0.33 | 44,44,44,44                 | 0     |
| 86  | OHX  | 8     | 223  | 7/7   | 0.95 | 0.12 | 118,118,118,118             | 0     |
| 85  | MG   | 5     | 3732 | 1/1   | 0.95 | 0.07 | 38,38,38,38                 | 0     |
| 85  | MG   | 1     | 3796 | 1/1   | 0.95 | 0.17 | 40,40,40,40                 | 0     |
| 86  | OHX  | 6     | 2066 | 7/7   | 0.95 | 0.13 | 94,94,94,94                 | 0     |
| 86  | OHX  | 6     | 2075 | 7/7   | 0.95 | 0.11 | 137,137,137,137             | 0     |
| 85  | MG   | 5     | 3562 | 1/1   | 0.95 | 0.36 | 26,26,26,26                 | 0     |
| 85  | MG   | n0    | 202  | 1/1   | 0.95 | 0.17 | 41,41,41,41                 | 0     |
| 86  | OHX  | 6     | 2088 | 7/7   | 0.95 | 0.12 | 102,102,102,102             | 0     |
| 86  | OHX  | 6     | 2093 | 7/7   | 0.95 | 0.16 | 111,111,111,111             | 0     |
| 85  | MG   | 1     | 3477 | 1/1   | 0.95 | 0.18 | 34,34,34,34                 | 0     |
| 85  | MG   | 5     | 3404 | 1/1   | 0.95 | 0.10 | 45,45,45,45                 | 0     |
| 85  | MG   | 5     | 3565 | 1/1   | 0.95 | 0.17 | 25,25,25,25                 | 0     |
| 86  | OHX  | 5     | 4095 | 7/7   | 0.95 | 0.13 | 109,109,109,109             | 0     |
| 85  | MG   | 5     | 3566 | 1/1   | 0.95 | 0.38 | 47,47,47,47                 | 0     |
| 85  | MG   | 5     | 3741 | 1/1   | 0.95 | 0.22 | 25,25,25,25                 | 0     |
| 85  | MG   | 1     | 3717 | 1/1   | 0.95 | 0.10 | 32,32,32,32                 | 0     |
| 85  | MG   | 5     | 3406 | 1/1   | 0.95 | 0.18 | 36,36,36,36                 | 0     |
| 86  | OHX  | 6     | 2114 | 7/7   | 0.95 | 0.12 | 115,115,115,115             | 0     |
| 86  | OHX  | m5    | 301  | 7/7   | 0.95 | 0.12 | 126,126,126,126             | 0     |
| 86  | OHX  | 6     | 2116 | 7/7   | 0.95 | 0.14 | 123,123,123,123             | 0     |
| 85  | MG   | 1     | 3718 | 1/1   | 0.95 | 0.08 | 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  | MG   | 5     | 3746 | 1/1   | 0.95 | 0.17 | 60,60,60,60                 | 0     |
| 86  | OHX  | 5     | 4104 | 7/7   | 0.95 | 0.26 | 95,95,95,95                 | 0     |
| 85  | MG   | 5     | 3408 | 1/1   | 0.95 | 0.10 | 26,26,26,26                 | 0     |
| 85  | MG   | o3    | 202  | 1/1   | 0.95 | 0.32 | 31,31,31,31                 | 0     |
| 86  | OHX  | 6     | 2121 | 7/7   | 0.95 | 0.12 | 113,113,113,113             | 0     |
| 86  | OHX  | 1     | 4118 | 7/7   | 0.95 | 0.15 | 113,113,113,113             | 0     |
| 85  | MG   | 1     | 3800 | 1/1   | 0.95 | 0.16 | 48,48,48,48                 | 0     |
| 85  | MG   | 1     | 3507 | 1/1   | 0.96 | 0.35 | 37,37,37,37                 | 0     |
| 85  | MG   | 5     | 3788 | 1/1   | 0.96 | 0.10 | 45,45,45,45                 | 0     |
| 85  | MG   | 5     | 3789 | 1/1   | 0.96 | 0.20 | 23,23,23,23                 | 0     |
| 86  | OHX  | 5     | 4132 | 7/7   | 0.96 | 0.09 | 133,133,133,133             | 0     |
| 85  | MG   | 5     | 3464 | 1/1   | 0.96 | 0.29 | 51,51,51,51                 | 0     |
| 85  | MG   | L8    | 301  | 1/1   | 0.96 | 0.29 | 53,53,53,53                 | 0     |
| 85  | MG   | M0    | 301  | 1/1   | 0.96 | 0.18 | 40,40,40,40                 | 0     |
| 85  | MG   | M0    | 302  | 1/1   | 0.96 | 0.07 | 46,46,46,46                 | 0     |
| 85  | MG   | 5     | 3585 | 1/1   | 0.96 | 0.35 | 30,30,30,30                 | 0     |
| 85  | MG   | 5     | 3883 | 1/1   | 0.96 | 0.23 | 50,50,50,50                 | 0     |
| 86  | OHX  | 2     | 2048 | 7/7   | 0.96 | 0.09 | 126,126,126,126             | 0     |
| 86  | OHX  | 2     | 2049 | 7/7   | 0.96 | 0.10 | 116,116,116,116             | 0     |
| 85  | MG   | 1     | 3623 | 1/1   | 0.96 | 0.26 | 42,42,42,42                 | 0     |
| 85  | MG   | 1     | 3712 | 1/1   | 0.96 | 0.26 | 34,34,34,34                 | 0     |
| 85  | MG   | 5     | 3797 | 1/1   | 0.96 | 0.18 | 38,38,38,38                 | 0     |
| 85  | MG   | 5     | 3648 | 1/1   | 0.96 | 0.11 | 46,46,46,46                 | 0     |
| 85  | MG   | 1     | 3828 | 1/1   | 0.96 | 0.10 | 61,61,61,61                 | 0     |
| 85  | MG   | 6     | 2035 | 1/1   | 0.96 | 0.09 | 52,52,52,52                 | 0     |
| 85  | MG   | 5     | 3802 | 1/1   | 0.96 | 0.18 | 49,49,49,49                 | 0     |
| 85  | MG   | 5     | 3528 | 1/1   | 0.96 | 0.15 | 26,26,26,26                 | 0     |
| 85  | MG   | 5     | 3720 | 1/1   | 0.96 | 0.12 | 42,42,42,42                 | 0     |
| 85  | MG   | 5     | 3472 | 1/1   | 0.96 | 0.08 | 43,43,43,43                 | 0     |
| 85  | MG   | 6     | 1912 | 1/1   | 0.96 | 0.39 | 51,51,51,51                 | 0     |
| 86  | OHX  | 2     | 2070 | 7/7   | 0.96 | 0.12 | 127,127,127,127             | 0     |
| 86  | OHX  | 2     | 2071 | 7/7   | 0.96 | 0.11 | 117,117,117,117             | 0     |
| 86  | OHX  | 2     | 2073 | 7/7   | 0.96 | 0.13 | 111,111,111,111             | 0     |
| 85  | MG   | 5     | 3723 | 1/1   | 0.96 | 0.11 | 40,40,40,40                 | 0     |
| 85  | MG   | 1     | 3829 | 1/1   | 0.96 | 0.15 | 27,27,27,27                 | 0     |
| 85  | MG   | 1     | 3624 | 1/1   | 0.96 | 0.07 | 38,38,38,38                 | 0     |
| 85  | MG   | 1     | 3755 | 1/1   | 0.96 | 0.17 | 59,59,59,59                 | 0     |
| 85  | MG   | 5     | 3658 | 1/1   | 0.96 | 0.17 | 44,44,44,44                 | 0     |
| 85  | MG   | 5     | 3900 | 1/1   | 0.96 | 0.16 | 36,36,36,36                 | 0     |
| 85  | MG   | M5    | 301  | 1/1   | 0.96 | 0.10 | 45,45,45,45                 | 0     |
| 85  | MG   | 1     | 3550 | 1/1   | 0.96 | 0.22 | 41,41,41,41                 | 0     |
| 85  | MG   | 1     | 3697 | 1/1   | 0.96 | 0.20 | 39,39,39,39                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 2     | 1902 | 1/1   | 0.96 | 0.23 | 36,36,36,36                 | 0     |
| 86  | OHX  | 3     | 217  | 7/7   | 0.96 | 0.10 | 118,118,118,118             | 0     |
| 86  | OHX  | 3     | 218  | 7/7   | 0.96 | 0.11 | 119,119,119,119             | 0     |
| 85  | MG   | 5     | 3734 | 1/1   | 0.96 | 0.12 | 43,43,43,43                 | 0     |
| 86  | OHX  | 2     | 2086 | 7/7   | 0.96 | 0.14 | 122,122,122,122             | 0     |
| 86  | OHX  | SR    | 401  | 7/7   | 0.96 | 0.08 | 164,164,164,164             | 0     |
| 85  | MG   | 1     | 3781 | 1/1   | 0.96 | 0.17 | 32,32,32,32                 | 0     |
| 86  | OHX  | 1     | 3905 | 7/7   | 0.96 | 0.17 | 81,81,81,81                 | 0     |
| 86  | OHX  | 1     | 3911 | 7/7   | 0.96 | 0.17 | 83,83,83,83                 | 0     |
| 86  | OHX  | 4     | 229  | 7/7   | 0.96 | 0.11 | 118,118,118,118             | 0     |
| 86  | OHX  | 4     | 230  | 7/7   | 0.96 | 0.20 | 103,103,103,103             | 0     |
| 85  | MG   | 7     | 207  | 1/1   | 0.96 | 0.12 | 44,44,44,44                 | 0     |
| 85  | MG   | 5     | 3601 | 1/1   | 0.96 | 0.11 | 41,41,41,41                 | 0     |
| 86  | OHX  | 1     | 3936 | 7/7   | 0.96 | 0.12 | 100,100,100,100             | 0     |
| 86  | OHX  | 5     | 3963 | 7/7   | 0.96 | 0.12 | 71,71,71,71                 | 0     |
| 86  | OHX  | 5     | 3969 | 7/7   | 0.96 | 0.11 | 101,101,101,101             | 0     |
| 86  | OHX  | 5     | 3977 | 7/7   | 0.96 | 0.10 | 103,103,103,103             | 0     |
| 86  | OHX  | 1     | 3938 | 7/7   | 0.96 | 0.12 | 95,95,95,95                 | 0     |
| 86  | OHX  | 1     | 3941 | 7/7   | 0.96 | 0.10 | 101,101,101,101             | 0     |
| 86  | OHX  | 5     | 3983 | 7/7   | 0.96 | 0.12 | 103,103,103,103             | 0     |
| 86  | OHX  | 1     | 3947 | 7/7   | 0.96 | 0.11 | 102,102,102,102             | 0     |
| 86  | OHX  | 2     | 2091 | 7/7   | 0.96 | 0.18 | 111,111,111,111             | 0     |
| 86  | OHX  | 1     | 3951 | 7/7   | 0.96 | 0.10 | 122,122,122,122             | 0     |
| 85  | MG   | 5     | 3484 | 1/1   | 0.96 | 0.31 | 26,26,26,26                 | 0     |
| 86  | OHX  | 5     | 4002 | 7/7   | 0.96 | 0.10 | 111,111,111,111             | 0     |
| 86  | OHX  | 5     | 4004 | 7/7   | 0.96 | 0.27 | 75,75,75,75                 | 0     |
| 86  | OHX  | 5     | 4005 | 7/7   | 0.96 | 0.11 | 105,105,105,105             | 0     |
| 86  | OHX  | 2     | 2094 | 7/7   | 0.96 | 0.09 | 146,146,146,146             | 0     |
| 86  | OHX  | 1     | 4109 | 7/7   | 0.96 | 0.09 | 138,138,138,138             | 0     |
| 86  | OHX  | 5     | 4013 | 7/7   | 0.96 | 0.27 | 100,100,100,100             | 0     |
| 85  | MG   | 7     | 210  | 1/1   | 0.96 | 0.20 | 45,45,45,45                 | 0     |
| 86  | OHX  | 5     | 4017 | 7/7   | 0.96 | 0.13 | 103,103,103,103             | 0     |
| 86  | OHX  | 1     | 3959 | 7/7   | 0.96 | 0.20 | 92,92,92,92                 | 0     |
| 85  | MG   | 6     | 1962 | 1/1   | 0.96 | 0.21 | 45,45,45,45                 | 0     |
| 85  | MG   | 1     | 3782 | 1/1   | 0.96 | 0.28 | 62,62,62,62                 | 0     |
| 86  | OHX  | 2     | 2098 | 7/7   | 0.96 | 0.12 | 116,116,116,116             | 0     |
| 85  | MG   | 5     | 3740 | 1/1   | 0.96 | 0.09 | 55,55,55,55                 | 0     |
| 86  | OHX  | O2    | 202  | 7/7   | 0.96 | 0.23 | 94,94,94,94                 | 0     |
| 86  | OHX  | 1     | 3973 | 7/7   | 0.96 | 0.16 | 110,110,110,110             | 0     |
| 85  | MG   | 5     | 3546 | 1/1   | 0.96 | 0.35 | 43,43,43,43                 | 0     |
| 86  | OHX  | 1     | 3976 | 7/7   | 0.96 | 0.09 | 121,121,121,121             | 0     |
| 86  | OHX  | 1     | 3980 | 7/7   | 0.96 | 0.30 | 87,87,87,87                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 1     | 3981 | 7/7   | 0.96 | 0.10 | 104,104,104,104             | 0     |
| 86  | OHX  | 1     | 3982 | 7/7   | 0.96 | 0.13 | 100,100,100,100             | 0     |
| 85  | MG   | M7    | 205  | 1/1   | 0.96 | 0.10 | 39,39,39,39                 | 0     |
| 86  | OHX  | 5     | 4043 | 7/7   | 0.96 | 0.09 | 151,151,151,151             | 0     |
| 85  | MG   | 5     | 3671 | 1/1   | 0.96 | 0.19 | 31,31,31,31                 | 0     |
| 86  | OHX  | 6     | 2096 | 7/7   | 0.96 | 0.09 | 133,133,133,133             | 0     |
| 86  | OHX  | 5     | 4046 | 7/7   | 0.96 | 0.24 | 98,98,98,98                 | 0     |
| 85  | MG   | 5     | 3548 | 1/1   | 0.96 | 0.32 | 45,45,45,45                 | 0     |
| 86  | OHX  | 6     | 2099 | 7/7   | 0.96 | 0.07 | 152,152,152,152             | 0     |
| 86  | OHX  | 6     | 2101 | 7/7   | 0.96 | 0.09 | 155,155,155,155             | 0     |
| 86  | OHX  | 5     | 4051 | 7/7   | 0.96 | 0.21 | 102,102,102,102             | 0     |
| 86  | OHX  | 5     | 4219 | 7/7   | 0.96 | 0.27 | 99,99,99,99                 | 0     |
| 86  | OHX  | 5     | 4052 | 7/7   | 0.96 | 0.10 | 128,128,128,128             | 0     |
| 86  | OHX  | 1     | 3990 | 7/7   | 0.96 | 0.13 | 114,114,114,114             | 0     |
| 86  | OHX  | 6     | 2104 | 7/7   | 0.96 | 0.10 | 114,114,114,114             | 0     |
| 85  | MG   | 5     | 3673 | 1/1   | 0.96 | 0.27 | 28,28,28,28                 | 0     |
| 85  | MG   | 5     | 3831 | 1/1   | 0.96 | 0.11 | 72,72,72,72                 | 0     |
| 86  | OHX  | 1     | 3995 | 7/7   | 0.96 | 0.10 | 127,127,127,127             | 0     |
| 86  | OHX  | 1     | 3998 | 7/7   | 0.96 | 0.10 | 125,125,125,125             | 0     |
| 86  | OHX  | 1     | 4000 | 7/7   | 0.96 | 0.09 | 157,157,157,157             | 0     |
| 86  | OHX  | 6     | 2112 | 7/7   | 0.96 | 0.14 | 105,105,105,105             | 0     |
| 86  | OHX  | 6     | 2113 | 7/7   | 0.96 | 0.12 | 124,124,124,124             | 0     |
| 86  | OHX  | 1     | 4002 | 7/7   | 0.96 | 0.15 | 104,104,104,104             | 0     |
| 85  | MG   | 5     | 3435 | 1/1   | 0.96 | 0.21 | 29,29,29,29                 | 0     |
| 85  | MG   | M9    | 201  | 1/1   | 0.96 | 0.05 | 61,61,61,61                 | 0     |
| 85  | MG   | 1     | 3665 | 1/1   | 0.96 | 0.15 | 45,45,45,45                 | 0     |
| 85  | MG   | 5     | 3751 | 1/1   | 0.96 | 0.21 | 49,49,49,49                 | 0     |
| 85  | MG   | 5     | 3752 | 1/1   | 0.96 | 0.23 | 36,36,36,36                 | 0     |
| 85  | MG   | 5     | 3753 | 1/1   | 0.96 | 0.13 | 46,46,46,46                 | 0     |
| 86  | OHX  | 1     | 4010 | 7/7   | 0.96 | 0.20 | 103,103,103,103             | 0     |
| 86  | OHX  | 1     | 4011 | 7/7   | 0.96 | 0.13 | 103,103,103,103             | 0     |
| 85  | MG   | 1     | 3539 | 1/1   | 0.96 | 0.45 | 37,37,37,37                 | 0     |
| 86  | OHX  | 6     | 2125 | 7/7   | 0.96 | 0.24 | 101,101,101,101             | 0     |
| 86  | OHX  | 2     | 2114 | 7/7   | 0.96 | 0.13 | 120,120,120,120             | 0     |
| 85  | MG   | 5     | 3841 | 1/1   | 0.96 | 0.11 | 68,68,68,68                 | 0     |
| 85  | MG   | 5     | 3553 | 1/1   | 0.96 | 0.41 | 47,47,47,47                 | 0     |
| 86  | OHX  | 5     | 4083 | 7/7   | 0.96 | 0.21 | 98,98,98,98                 | 0     |
| 85  | MG   | 1     | 3761 | 1/1   | 0.96 | 0.22 | 37,37,37,37                 | 0     |
| 86  | OHX  | 1     | 4017 | 7/7   | 0.96 | 0.12 | 115,115,115,115             | 0     |
| 85  | MG   | 5     | 3681 | 1/1   | 0.96 | 0.08 | 33,33,33,33                 | 0     |
| 86  | OHX  | 5     | 4087 | 7/7   | 0.96 | 0.12 | 112,112,112,112             | 0     |
| 86  | OHX  | 6     | 2132 | 7/7   | 0.96 | 0.13 | 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  | MG   | 1     | 3475 | 1/1   | 0.96 | 0.22 | 23,23,23,23                 | 0     |
| 85  | MG   | 1     | 3721 | 1/1   | 0.96 | 0.06 | 34,34,34,34                 | 0     |
| 85  | MG   | 5     | 3847 | 1/1   | 0.96 | 0.08 | 32,32,32,32                 | 0     |
| 85  | MG   | 3     | 204  | 1/1   | 0.96 | 0.34 | 59,59,59,59                 | 0     |
| 85  | MG   | 1     | 3619 | 1/1   | 0.96 | 0.15 | 55,55,55,55                 | 0     |
| 86  | OHX  | 7     | 223  | 7/7   | 0.96 | 0.14 | 101,101,101,101             | 0     |
| 85  | MG   | N8    | 205  | 1/1   | 0.96 | 0.24 | 28,28,28,28                 | 0     |
| 86  | OHX  | 7     | 225  | 7/7   | 0.96 | 0.13 | 102,102,102,102             | 0     |
| 85  | MG   | c9    | 202  | 1/1   | 0.96 | 0.27 | 66,66,66,66                 | 0     |
| 85  | MG   | 1     | 3581 | 1/1   | 0.96 | 0.36 | 34,34,34,34                 | 0     |
| 85  | MG   | L2    | 301  | 1/1   | 0.96 | 0.18 | 29,29,29,29                 | 0     |
| 86  | OHX  | 8     | 219  | 7/7   | 0.96 | 0.12 | 105,105,105,105             | 0     |
| 86  | OHX  | 1     | 4028 | 7/7   | 0.96 | 0.11 | 107,107,107,107             | 0     |
| 86  | OHX  | 8     | 221  | 7/7   | 0.96 | 0.10 | 112,112,112,112             | 0     |
| 85  | MG   | 1     | 3845 | 1/1   | 0.96 | 0.32 | 36,36,36,36                 | 0     |
| 86  | OHX  | 6     | 2144 | 7/7   | 0.96 | 0.13 | 127,127,127,127             | 0     |
| 86  | OHX  | 1     | 4030 | 7/7   | 0.96 | 0.09 | 124,124,124,124             | 0     |
| 85  | MG   | 5     | 3691 | 1/1   | 0.96 | 0.17 | 43,43,43,43                 | 0     |
| 85  | MG   | 5     | 3771 | 1/1   | 0.96 | 0.11 | 66,66,66,66                 | 0     |
| 85  | MG   | 1     | 3633 | 1/1   | 0.96 | 0.11 | 33,33,33,33                 | 0     |
| 86  | OHX  | 1     | 4034 | 7/7   | 0.96 | 0.13 | 103,103,103,103             | 0     |
| 86  | OHX  | 5     | 4106 | 7/7   | 0.96 | 0.12 | 126,126,126,126             | 0     |
| 85  | MG   | 5     | 3504 | 1/1   | 0.96 | 0.32 | 31,31,31,31                 | 0     |
| 86  | OHX  | l3    | 405  | 7/7   | 0.96 | 0.12 | 113,113,113,113             | 0     |
| 86  | OHX  | 6     | 2151 | 7/7   | 0.96 | 0.17 | 106,106,106,106             | 0     |
| 85  | MG   | 1     | 3671 | 1/1   | 0.96 | 0.20 | 53,53,53,53                 | 0     |
| 86  | OHX  | 1     | 4038 | 7/7   | 0.96 | 0.08 | 146,146,146,146             | 0     |
| 85  | MG   | 5     | 3402 | 1/1   | 0.96 | 0.20 | 25,25,25,25                 | 0     |
| 85  | MG   | 6     | 1937 | 1/1   | 0.96 | 0.29 | 43,43,43,43                 | 0     |
| 85  | MG   | m7    | 205  | 1/1   | 0.96 | 0.09 | 35,35,35,35                 | 0     |
| 85  | MG   | 2     | 1967 | 1/1   | 0.96 | 0.39 | 52,52,52,52                 | 0     |
| 86  | OHX  | m0    | 302  | 7/7   | 0.96 | 0.10 | 117,117,117,117             | 0     |
| 85  | MG   | 1     | 3708 | 1/1   | 0.96 | 0.16 | 54,54,54,54                 | 0     |
| 86  | OHX  | 1     | 4044 | 7/7   | 0.96 | 0.10 | 126,126,126,126             | 0     |
| 85  | MG   | 5     | 3511 | 1/1   | 0.96 | 0.29 | 25,25,25,25                 | 0     |
| 86  | OHX  | 5     | 4119 | 7/7   | 0.96 | 0.31 | 95,95,95,95                 | 0     |
| 86  | OHX  | 1     | 4046 | 7/7   | 0.96 | 0.26 | 96,96,96,96                 | 0     |
| 85  | MG   | 5     | 3458 | 1/1   | 0.96 | 0.23 | 34,34,34,34                 | 0     |
| 85  | MG   | L6    | 201  | 1/1   | 0.96 | 0.08 | 47,47,47,47                 | 0     |
| 85  | MG   | 1     | 3748 | 1/1   | 0.96 | 0.20 | 29,29,29,29                 | 0     |
| 85  | MG   | 1     | 3659 | 1/1   | 0.96 | 0.18 | 32,32,32,32                 | 0     |
| 85  | MG   | 6     | 2026 | 1/1   | 0.96 | 0.23 | 42,42,42,42                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 5     | 3873 | 1/1   | 0.96 | 0.23 | 25,25,25,25                 | 0     |
| 85  | MG   | n8    | 205  | 1/1   | 0.96 | 0.10 | 36,36,36,36                 | 0     |
| 85  | MG   | 5     | 3639 | 1/1   | 0.96 | 0.25 | 40,40,40,40                 | 0     |
| 88  | HMT  | 1     | 4217 | 39/39 | 0.96 | 0.09 | 30,30,30,30                 | 0     |
| 88  | HMT  | 5     | 4255 | 39/39 | 0.96 | 0.08 | 28,28,28,28                 | 0     |
| 86  | OHX  | 6     | 2076 | 7/7   | 0.97 | 0.08 | 136,136,136,136             | 0     |
| 86  | OHX  | 2     | 2093 | 7/7   | 0.97 | 0.07 | 149,149,149,149             | 0     |
| 86  | OHX  | 6     | 2085 | 7/7   | 0.97 | 0.10 | 112,112,112,112             | 0     |
| 86  | OHX  | 6     | 2086 | 7/7   | 0.97 | 0.09 | 113,113,113,113             | 0     |
| 85  | MG   | 17    | 301  | 1/1   | 0.97 | 0.05 | 32,32,32,32                 | 0     |
| 85  | MG   | 5     | 3416 | 1/1   | 0.97 | 0.07 | 34,34,34,34                 | 0     |
| 86  | OHX  | 6     | 2090 | 7/7   | 0.97 | 0.09 | 117,117,117,117             | 0     |
| 86  | OHX  | 5     | 3929 | 7/7   | 0.97 | 0.14 | 70,70,70,70                 | 0     |
| 86  | OHX  | 6     | 2091 | 7/7   | 0.97 | 0.08 | 130,130,130,130             | 0     |
| 86  | OHX  | 5     | 3943 | 7/7   | 0.97 | 0.10 | 84,84,84,84                 | 0     |
| 86  | OHX  | 5     | 3952 | 7/7   | 0.97 | 0.11 | 99,99,99,99                 | 0     |
| 86  | OHX  | 5     | 3954 | 7/7   | 0.97 | 0.14 | 106,106,106,106             | 0     |
| 86  | OHX  | 5     | 3955 | 7/7   | 0.97 | 0.10 | 101,101,101,101             | 0     |
| 86  | OHX  | 5     | 3961 | 7/7   | 0.97 | 0.12 | 88,88,88,88                 | 0     |
| 86  | OHX  | 6     | 2092 | 7/7   | 0.97 | 0.12 | 111,111,111,111             | 0     |
| 86  | OHX  | 5     | 3966 | 7/7   | 0.97 | 0.09 | 94,94,94,94                 | 0     |
| 85  | MG   | 5     | 3679 | 1/1   | 0.97 | 0.19 | 40,40,40,40                 | 0     |
| 86  | OHX  | 5     | 3972 | 7/7   | 0.97 | 0.12 | 98,98,98,98                 | 0     |
| 86  | OHX  | 5     | 3976 | 7/7   | 0.97 | 0.17 | 91,91,91,91                 | 0     |
| 86  | OHX  | 6     | 2094 | 7/7   | 0.97 | 0.09 | 112,112,112,112             | 0     |
| 86  | OHX  | 6     | 2095 | 7/7   | 0.97 | 0.16 | 102,102,102,102             | 0     |
| 85  | MG   | 1     | 3698 | 1/1   | 0.97 | 0.11 | 44,44,44,44                 | 0     |
| 86  | OHX  | 5     | 3982 | 7/7   | 0.97 | 0.10 | 88,88,88,88                 | 0     |
| 85  | MG   | 5     | 3512 | 1/1   | 0.97 | 0.21 | 29,29,29,29                 | 0     |
| 86  | OHX  | 5     | 3987 | 7/7   | 0.97 | 0.25 | 90,90,90,90                 | 0     |
| 86  | OHX  | 5     | 3991 | 7/7   | 0.97 | 0.07 | 116,116,116,116             | 0     |
| 86  | OHX  | 5     | 3994 | 7/7   | 0.97 | 0.10 | 101,101,101,101             | 0     |
| 86  | OHX  | 6     | 2098 | 7/7   | 0.97 | 0.08 | 123,123,123,123             | 0     |
| 85  | MG   | 1     | 3487 | 1/1   | 0.97 | 0.37 | 41,41,41,41                 | 0     |
| 86  | OHX  | 6     | 2100 | 7/7   | 0.97 | 0.10 | 117,117,117,117             | 0     |
| 86  | OHX  | 5     | 3998 | 7/7   | 0.97 | 0.21 | 91,91,91,91                 | 0     |
| 85  | MG   | 1     | 3426 | 1/1   | 0.97 | 0.11 | 29,29,29,29                 | 0     |
| 85  | MG   | m6    | 201  | 1/1   | 0.97 | 0.16 | 35,35,35,35                 | 0     |
| 86  | OHX  | 5     | 4003 | 7/7   | 0.97 | 0.24 | 94,94,94,94                 | 0     |
| 86  | OHX  | 6     | 2103 | 7/7   | 0.97 | 0.09 | 162,162,162,162             | 0     |
| 85  | MG   | N8    | 202  | 1/1   | 0.97 | 0.17 | 30,30,30,30                 | 0     |
| 86  | OHX  | C8    | 202  | 7/7   | 0.97 | 0.09 | 121,121,121,121             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 5     | 3748 | 1/1   | 0.97 | 0.20 | 46,46,46,46                 | 0     |
| 86  | OHX  | 5     | 4176 | 7/7   | 0.97 | 0.26 | 87,87,87,87                 | 0     |
| 85  | MG   | 1     | 3422 | 1/1   | 0.97 | 0.25 | 39,39,39,39                 | 0     |
| 85  | MG   | L4    | 401  | 1/1   | 0.97 | 0.09 | 32,32,32,32                 | 0     |
| 86  | OHX  | 5     | 4015 | 7/7   | 0.97 | 0.08 | 145,145,145,145             | 0     |
| 86  | OHX  | 5     | 4016 | 7/7   | 0.97 | 0.22 | 95,95,95,95                 | 0     |
| 86  | OHX  | 1     | 3897 | 7/7   | 0.97 | 0.13 | 76,76,76,76                 | 0     |
| 86  | OHX  | 5     | 4018 | 7/7   | 0.97 | 0.09 | 103,103,103,103             | 0     |
| 86  | OHX  | 6     | 2111 | 7/7   | 0.97 | 0.09 | 115,115,115,115             | 0     |
| 86  | OHX  | 5     | 4020 | 7/7   | 0.97 | 0.08 | 118,118,118,118             | 0     |
| 86  | OHX  | 5     | 4021 | 7/7   | 0.97 | 0.21 | 99,99,99,99                 | 0     |
| 86  | OHX  | 5     | 4022 | 7/7   | 0.97 | 0.24 | 96,96,96,96                 | 0     |
| 86  | OHX  | 5     | 4023 | 7/7   | 0.97 | 0.09 | 110,110,110,110             | 0     |
| 85  | MG   | 1     | 3540 | 1/1   | 0.97 | 0.18 | 37,37,37,37                 | 0     |
| 86  | OHX  | 5     | 4025 | 7/7   | 0.97 | 0.21 | 101,101,101,101             | 0     |
| 85  | MG   | n0    | 201  | 1/1   | 0.97 | 0.07 | 42,42,42,42                 | 0     |
| 86  | OHX  | 1     | 3912 | 7/7   | 0.97 | 0.11 | 94,94,94,94                 | 0     |
| 86  | OHX  | 6     | 2115 | 7/7   | 0.97 | 0.23 | 97,97,97,97                 | 0     |
| 85  | MG   | 1     | 3615 | 1/1   | 0.97 | 0.23 | 36,36,36,36                 | 0     |
| 86  | OHX  | 5     | 4032 | 7/7   | 0.97 | 0.13 | 110,110,110,110             | 0     |
| 86  | OHX  | 1     | 3922 | 7/7   | 0.97 | 0.14 | 91,91,91,91                 | 0     |
| 86  | OHX  | 1     | 3927 | 7/7   | 0.97 | 0.12 | 109,109,109,109             | 0     |
| 86  | OHX  | 5     | 4035 | 7/7   | 0.97 | 0.20 | 100,100,100,100             | 0     |
| 86  | OHX  | 1     | 4059 | 7/7   | 0.97 | 0.09 | 144,144,144,144             | 0     |
| 85  | MG   | L7    | 301  | 1/1   | 0.97 | 0.20 | 37,37,37,37                 | 0     |
| 86  | OHX  | 1     | 3933 | 7/7   | 0.97 | 0.10 | 101,101,101,101             | 0     |
| 86  | OHX  | 5     | 4201 | 7/7   | 0.97 | 0.24 | 87,87,87,87                 | 0     |
| 85  | MG   | 1     | 3855 | 1/1   | 0.97 | 0.18 | 21,21,21,21                 | 0     |
| 86  | OHX  | 5     | 4041 | 7/7   | 0.97 | 0.26 | 86,86,86,86                 | 0     |
| 85  | MG   | 5     | 3474 | 1/1   | 0.97 | 0.36 | 67,67,67,67                 | 0     |
| 86  | OHX  | 1     | 3939 | 7/7   | 0.97 | 0.13 | 91,91,91,91                 | 0     |
| 85  | MG   | 5     | 3577 | 1/1   | 0.97 | 0.17 | 34,34,34,34                 | 0     |
| 85  | MG   | 1     | 3541 | 1/1   | 0.97 | 0.28 | 23,23,23,23                 | 0     |
| 85  | MG   | 5     | 3430 | 1/1   | 0.97 | 0.13 | 29,29,29,29                 | 0     |
| 86  | OHX  | 1     | 4068 | 7/7   | 0.97 | 0.24 | 99,99,99,99                 | 0     |
| 86  | OHX  | 5     | 4048 | 7/7   | 0.97 | 0.20 | 101,101,101,101             | 0     |
| 86  | OHX  | 1     | 4176 | 7/7   | 0.97 | 0.21 | 100,100,100,100             | 0     |
| 86  | OHX  | 1     | 3949 | 7/7   | 0.97 | 0.09 | 111,111,111,111             | 0     |
| 86  | OHX  | 1     | 3950 | 7/7   | 0.97 | 0.11 | 103,103,103,103             | 0     |
| 85  | MG   | 1     | 3412 | 1/1   | 0.97 | 0.15 | 31,31,31,31                 | 0     |
| 85  | MG   | O7    | 103  | 1/1   | 0.97 | 0.16 | 34,34,34,34                 | 0     |
| 85  | MG   | 5     | 3479 | 1/1   | 0.97 | 0.23 | 58,58,58,58                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 5     | 4055 | 7/7   | 0.97 | 0.20 | 93,93,93,93                 | 0     |
| 86  | OHX  | 5     | 4056 | 7/7   | 0.97 | 0.17 | 90,90,90,90                 | 0     |
| 85  | MG   | 5     | 3763 | 1/1   | 0.97 | 0.09 | 36,36,36,36                 | 0     |
| 86  | OHX  | 1     | 3957 | 7/7   | 0.97 | 0.19 | 99,99,99,99                 | 0     |
| 85  | MG   | 5     | 3529 | 1/1   | 0.97 | 0.21 | 28,28,28,28                 | 0     |
| 86  | OHX  | 5     | 4061 | 7/7   | 0.97 | 0.10 | 105,105,105,105             | 0     |
| 86  | OHX  | 5     | 4062 | 7/7   | 0.97 | 0.09 | 134,134,134,134             | 0     |
| 86  | OHX  | 1     | 3962 | 7/7   | 0.97 | 0.08 | 110,110,110,110             | 0     |
| 85  | MG   | 5     | 3530 | 1/1   | 0.97 | 0.32 | 26,26,26,26                 | 0     |
| 85  | MG   | 5     | 3701 | 1/1   | 0.97 | 0.11 | 36,36,36,36                 | 0     |
| 86  | OHX  | 1     | 3967 | 7/7   | 0.97 | 0.17 | 98,98,98,98                 | 0     |
| 85  | MG   | 5     | 3834 | 1/1   | 0.97 | 0.05 | 40,40,40,40                 | 0     |
| 86  | OHX  | 5     | 4068 | 7/7   | 0.97 | 0.09 | 112,112,112,112             | 0     |
| 86  | OHX  | 1     | 3969 | 7/7   | 0.97 | 0.19 | 97,97,97,97                 | 0     |
| 86  | OHX  | 1     | 3970 | 7/7   | 0.97 | 0.09 | 125,125,125,125             | 0     |
| 85  | MG   | 5     | 3531 | 1/1   | 0.97 | 0.28 | 48,48,48,48                 | 0     |
| 85  | MG   | q0    | 202  | 1/1   | 0.97 | 0.08 | 39,39,39,39                 | 0     |
| 86  | OHX  | 1     | 3974 | 7/7   | 0.97 | 0.24 | 97,97,97,97                 | 0     |
| 85  | MG   | 6     | 2010 | 1/1   | 0.97 | 0.09 | 48,48,48,48                 | 0     |
| 86  | OHX  | 2     | 2032 | 7/7   | 0.97 | 0.12 | 111,111,111,111             | 0     |
| 86  | OHX  | 1     | 3979 | 7/7   | 0.97 | 0.18 | 91,91,91,91                 | 0     |
| 85  | MG   | 1     | 3497 | 1/1   | 0.97 | 0.22 | 30,30,30,30                 | 0     |
| 86  | OHX  | 2     | 2037 | 7/7   | 0.97 | 0.10 | 100,100,100,100             | 0     |
| 85  | MG   | 1     | 3658 | 1/1   | 0.97 | 0.30 | 45,45,45,45                 | 0     |
| 85  | MG   | 5     | 3436 | 1/1   | 0.97 | 0.19 | 33,33,33,33                 | 0     |
| 86  | OHX  | 1     | 3986 | 7/7   | 0.97 | 0.17 | 95,95,95,95                 | 0     |
| 86  | OHX  | 2     | 2045 | 7/7   | 0.97 | 0.10 | 119,119,119,119             | 0     |
| 85  | MG   | 1     | 3742 | 1/1   | 0.97 | 0.18 | 52,52,52,52                 | 0     |
| 86  | OHX  | 1     | 3989 | 7/7   | 0.97 | 0.12 | 109,109,109,109             | 0     |
| 85  | MG   | 1     | 3763 | 1/1   | 0.97 | 0.13 | 33,33,33,33                 | 0     |
| 86  | OHX  | 1     | 3991 | 7/7   | 0.97 | 0.17 | 101,101,101,101             | 0     |
| 86  | OHX  | 1     | 3992 | 7/7   | 0.97 | 0.13 | 105,105,105,105             | 0     |
| 86  | OHX  | 2     | 2050 | 7/7   | 0.97 | 0.10 | 104,104,104,104             | 0     |
| 86  | OHX  | 2     | 2051 | 7/7   | 0.97 | 0.10 | 110,110,110,110             | 0     |
| 85  | MG   | 5     | 3649 | 1/1   | 0.97 | 0.19 | 42,42,42,42                 | 0     |
| 86  | OHX  | 1     | 3996 | 7/7   | 0.97 | 0.09 | 123,123,123,123             | 0     |
| 85  | MG   | 5     | 3538 | 1/1   | 0.97 | 0.36 | 33,33,33,33                 | 0     |
| 86  | OHX  | 1     | 3999 | 7/7   | 0.97 | 0.17 | 94,94,94,94                 | 0     |
| 86  | OHX  | 7     | 218  | 7/7   | 0.97 | 0.13 | 90,90,90,90                 | 0     |
| 85  | MG   | 4     | 209  | 1/1   | 0.97 | 0.23 | 40,40,40,40                 | 0     |
| 86  | OHX  | 1     | 4001 | 7/7   | 0.97 | 0.08 | 144,144,144,144             | 0     |
| 85  | MG   | 4     | 210  | 1/1   | 0.97 | 0.27 | 47,47,47,47                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 1     | 3571 | 1/1   | 0.97 | 0.26 | 26,26,26,26                 | 0     |
| 86  | OHX  | 2     | 2057 | 7/7   | 0.97 | 0.11 | 108,108,108,108             | 0     |
| 86  | OHX  | 2     | 2060 | 7/7   | 0.97 | 0.08 | 130,130,130,130             | 0     |
| 86  | OHX  | 8     | 218  | 7/7   | 0.97 | 0.08 | 110,110,110,110             | 0     |
| 85  | MG   | 6     | 1942 | 1/1   | 0.97 | 0.22 | 32,32,32,32                 | 0     |
| 85  | MG   | d3    | 202  | 1/1   | 0.97 | 0.11 | 53,53,53,53                 | 0     |
| 85  | MG   | 1     | 3462 | 1/1   | 0.97 | 0.30 | 27,27,27,27                 | 0     |
| 86  | OHX  | 2     | 2065 | 7/7   | 0.97 | 0.10 | 131,131,131,131             | 0     |
| 85  | MG   | 1     | 3745 | 1/1   | 0.97 | 0.07 | 38,38,38,38                 | 0     |
| 85  | MG   | 1     | 3813 | 1/1   | 0.97 | 0.08 | 51,51,51,51                 | 0     |
| 86  | OHX  | 4     | 227  | 7/7   | 0.97 | 0.16 | 98,98,98,98                 | 0     |
| 86  | OHX  | 4     | 228  | 7/7   | 0.97 | 0.09 | 114,114,114,114             | 0     |
| 85  | MG   | 4     | 215  | 1/1   | 0.97 | 0.22 | 56,56,56,56                 | 0     |
| 86  | OHX  | 2     | 2069 | 7/7   | 0.97 | 0.08 | 130,130,130,130             | 0     |
| 85  | MG   | 5     | 3495 | 1/1   | 0.97 | 0.09 | 39,39,39,39                 | 0     |
| 85  | MG   | 6     | 1984 | 1/1   | 0.97 | 0.07 | 53,53,53,53                 | 0     |
| 86  | OHX  | 2     | 2072 | 7/7   | 0.97 | 0.07 | 142,142,142,142             | 0     |
| 85  | MG   | M6    | 201  | 1/1   | 0.97 | 0.12 | 44,44,44,44                 | 0     |
| 85  | MG   | 6     | 1948 | 1/1   | 0.97 | 0.34 | 42,42,42,42                 | 0     |
| 85  | MG   | 5     | 3664 | 1/1   | 0.97 | 0.31 | 55,55,55,55                 | 0     |
| 85  | MG   | 1     | 3492 | 1/1   | 0.97 | 0.22 | 27,27,27,27                 | 0     |
| 85  | MG   | 1     | 3575 | 1/1   | 0.97 | 0.32 | 31,31,31,31                 | 0     |
| 85  | MG   | 5     | 3862 | 1/1   | 0.97 | 0.10 | 57,57,57,57                 | 0     |
| 85  | MG   | 1     | 3649 | 1/1   | 0.97 | 0.20 | 38,38,38,38                 | 0     |
| 85  | MG   | 5     | 3610 | 1/1   | 0.97 | 0.27 | 32,32,32,32                 | 0     |
| 85  | MG   | 1     | 3791 | 1/1   | 0.97 | 0.21 | 25,25,25,25                 | 0     |
| 85  | MG   | 1     | 3749 | 1/1   | 0.97 | 0.08 | 38,38,38,38                 | 0     |
| 85  | MG   | 5     | 3613 | 1/1   | 0.97 | 0.12 | 33,33,33,33                 | 0     |
| 85  | MG   | 1     | 3713 | 1/1   | 0.97 | 0.12 | 37,37,37,37                 | 0     |
| 85  | MG   | 1     | 3794 | 1/1   | 0.97 | 0.06 | 58,58,58,58                 | 0     |
| 85  | MG   | 6     | 1956 | 1/1   | 0.97 | 0.42 | 50,50,50,50                 | 0     |
| 85  | MG   | 1     | 3821 | 1/1   | 0.97 | 0.19 | 55,55,55,55                 | 0     |
| 86  | OHX  | o7    | 503  | 7/7   | 0.97 | 0.16 | 99,99,99,99                 | 0     |
| 86  | OHX  | 2     | 2089 | 7/7   | 0.97 | 0.12 | 122,122,122,122             | 0     |
| 86  | OHX  | O7    | 104  | 7/7   | 0.97 | 0.14 | 94,94,94,94                 | 0     |
| 86  | OHX  | O7    | 105  | 7/7   | 0.97 | 0.18 | 94,94,94,94                 | 0     |
| 85  | MG   | 5     | 3508 | 1/1   | 0.97 | 0.29 | 26,26,26,26                 | 0     |
| 85  | MG   | 14    | 401  | 1/1   | 0.97 | 0.06 | 31,31,31,31                 | 0     |
| 86  | OHX  | 6     | 2068 | 7/7   | 0.97 | 0.13 | 115,115,115,115             | 0     |
| 86  | OHX  | 6     | 2073 | 7/7   | 0.97 | 0.09 | 104,104,104,104             | 0     |
| 85  | MG   | 1     | 3678 | 1/1   | 0.97 | 0.07 | 67,67,67,67                 | 0     |
| 86  | OHX  | 2     | 2034 | 7/7   | 0.98 | 0.13 | 100,100,100,100             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 5     | 3818 | 1/1   | 0.98 | 0.11 | 37,37,37,37                 | 0     |
| 85  | MG   | 1     | 3522 | 1/1   | 0.98 | 0.06 | 33,33,33,33                 | 0     |
| 86  | OHX  | 2     | 2038 | 7/7   | 0.98 | 0.10 | 96,96,96,96                 | 0     |
| 86  | OHX  | 2     | 2082 | 7/7   | 0.98 | 0.07 | 130,130,130,130             | 0     |
| 86  | OHX  | 1     | 4036 | 7/7   | 0.98 | 0.17 | 94,94,94,94                 | 0     |
| 86  | OHX  | 1     | 3956 | 7/7   | 0.98 | 0.15 | 98,98,98,98                 | 0     |
| 85  | MG   | 5     | 3820 | 1/1   | 0.98 | 0.17 | 61,61,61,61                 | 0     |
| 86  | OHX  | 1     | 3958 | 7/7   | 0.98 | 0.11 | 99,99,99,99                 | 0     |
| 85  | MG   | 1     | 3683 | 1/1   | 0.98 | 0.14 | 66,66,66,66                 | 0     |
| 86  | OHX  | 1     | 3960 | 7/7   | 0.98 | 0.20 | 78,78,78,78                 | 0     |
| 86  | OHX  | 1     | 3961 | 7/7   | 0.98 | 0.07 | 106,106,106,106             | 0     |
| 86  | OHX  | 6     | 2106 | 7/7   | 0.98 | 0.08 | 118,118,118,118             | 0     |
| 86  | OHX  | 2     | 2044 | 7/7   | 0.98 | 0.08 | 101,101,101,101             | 0     |
| 86  | OHX  | 1     | 3963 | 7/7   | 0.98 | 0.13 | 92,92,92,92                 | 0     |
| 85  | MG   | 5     | 3616 | 1/1   | 0.98 | 0.14 | 38,38,38,38                 | 0     |
| 86  | OHX  | 2     | 2046 | 7/7   | 0.98 | 0.06 | 129,129,129,129             | 0     |
| 86  | OHX  | 2     | 2047 | 7/7   | 0.98 | 0.07 | 115,115,115,115             | 0     |
| 85  | MG   | 5     | 3425 | 1/1   | 0.98 | 0.18 | 37,37,37,37                 | 0     |
| 85  | MG   | 1     | 3833 | 1/1   | 0.98 | 0.21 | 20,20,20,20                 | 0     |
| 85  | MG   | 5     | 3584 | 1/1   | 0.98 | 0.37 | 33,33,33,33                 | 0     |
| 85  | MG   | 1     | 3531 | 1/1   | 0.98 | 0.36 | 33,33,33,33                 | 0     |
| 86  | OHX  | 1     | 3972 | 7/7   | 0.98 | 0.07 | 107,107,107,107             | 0     |
| 85  | MG   | 5     | 3523 | 1/1   | 0.98 | 0.34 | 44,44,44,44                 | 0     |
| 85  | MG   | 5     | 3428 | 1/1   | 0.98 | 0.40 | 44,44,44,44                 | 0     |
| 85  | MG   | 1     | 3604 | 1/1   | 0.98 | 0.16 | 32,32,32,32                 | 0     |
| 85  | MG   | 1     | 3629 | 1/1   | 0.98 | 0.21 | 35,35,35,35                 | 0     |
| 86  | OHX  | 1     | 3977 | 7/7   | 0.98 | 0.12 | 101,101,101,101             | 0     |
| 86  | OHX  | 1     | 3978 | 7/7   | 0.98 | 0.13 | 97,97,97,97                 | 0     |
| 86  | OHX  | 5     | 4080 | 7/7   | 0.98 | 0.20 | 91,91,91,91                 | 0     |
| 85  | MG   | 5     | 3557 | 1/1   | 0.98 | 0.27 | 24,24,24,24                 | 0     |
| 86  | OHX  | 3     | 214  | 7/7   | 0.98 | 0.07 | 95,95,95,95                 | 0     |
| 86  | OHX  | 5     | 3934 | 7/7   | 0.98 | 0.10 | 73,73,73,73                 | 0     |
| 86  | OHX  | 5     | 3935 | 7/7   | 0.98 | 0.13 | 89,89,89,89                 | 0     |
| 85  | MG   | 5     | 3698 | 1/1   | 0.98 | 0.23 | 41,41,41,41                 | 0     |
| 86  | OHX  | 5     | 3946 | 7/7   | 0.98 | 0.10 | 79,79,79,79                 | 0     |
| 86  | OHX  | 5     | 3947 | 7/7   | 0.98 | 0.09 | 84,84,84,84                 | 0     |
| 86  | OHX  | 5     | 3949 | 7/7   | 0.98 | 0.09 | 73,73,73,73                 | 0     |
| 86  | OHX  | 5     | 3950 | 7/7   | 0.98 | 0.09 | 87,87,87,87                 | 0     |
| 86  | OHX  | 2     | 2058 | 7/7   | 0.98 | 0.08 | 121,121,121,121             | 0     |
| 86  | OHX  | 5     | 3953 | 7/7   | 0.98 | 0.08 | 78,78,78,78                 | 0     |
| 86  | OHX  | 2     | 2059 | 7/7   | 0.98 | 0.11 | 101,101,101,101             | 0     |
| 85  | MG   | 5     | 3443 | 1/1   | 0.98 | 0.12 | 31,31,31,31                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 5     | 3956 | 7/7   | 0.98 | 0.14 | 79,79,79,79                 | 0     |
| 86  | OHX  | 5     | 3958 | 7/7   | 0.98 | 0.10 | 91,91,91,91                 | 0     |
| 86  | OHX  | 5     | 3959 | 7/7   | 0.98 | 0.11 | 84,84,84,84                 | 0     |
| 85  | MG   | 5     | 3457 | 1/1   | 0.98 | 0.23 | 24,24,24,24                 | 0     |
| 86  | OHX  | 1     | 3871 | 7/7   | 0.98 | 0.15 | 59,59,59,59                 | 0     |
| 86  | OHX  | 1     | 3891 | 7/7   | 0.98 | 0.13 | 79,79,79,79                 | 0     |
| 86  | OHX  | 5     | 3968 | 7/7   | 0.98 | 0.12 | 96,96,96,96                 | 0     |
| 85  | MG   | 1     | 3410 | 1/1   | 0.98 | 0.23 | 26,26,26,26                 | 0     |
| 86  | OHX  | 5     | 3970 | 7/7   | 0.98 | 0.14 | 93,93,93,93                 | 0     |
| 86  | OHX  | 2     | 2063 | 7/7   | 0.98 | 0.10 | 110,110,110,110             | 0     |
| 86  | OHX  | 5     | 3973 | 7/7   | 0.98 | 0.08 | 96,96,96,96                 | 0     |
| 86  | OHX  | 5     | 3974 | 7/7   | 0.98 | 0.15 | 91,91,91,91                 | 0     |
| 86  | OHX  | 5     | 3975 | 7/7   | 0.98 | 0.11 | 78,78,78,78                 | 0     |
| 86  | OHX  | 1     | 3898 | 7/7   | 0.98 | 0.10 | 81,81,81,81                 | 0     |
| 86  | OHX  | 1     | 3900 | 7/7   | 0.98 | 0.12 | 89,89,89,89                 | 0     |
| 86  | OHX  | 1     | 3901 | 7/7   | 0.98 | 0.10 | 81,81,81,81                 | 0     |
| 86  | OHX  | 5     | 3979 | 7/7   | 0.98 | 0.08 | 96,96,96,96                 | 0     |
| 86  | OHX  | 1     | 3904 | 7/7   | 0.98 | 0.08 | 85,85,85,85                 | 0     |
| 85  | MG   | 5     | 3787 | 1/1   | 0.98 | 0.06 | 40,40,40,40                 | 0     |
| 86  | OHX  | 1     | 3906 | 7/7   | 0.98 | 0.10 | 84,84,84,84                 | 0     |
| 86  | OHX  | 5     | 3984 | 7/7   | 0.98 | 0.12 | 81,81,81,81                 | 0     |
| 86  | OHX  | 5     | 3986 | 7/7   | 0.98 | 0.17 | 94,94,94,94                 | 0     |
| 86  | OHX  | 1     | 3997 | 7/7   | 0.98 | 0.18 | 96,96,96,96                 | 0     |
| 86  | OHX  | 5     | 3989 | 7/7   | 0.98 | 0.14 | 92,92,92,92                 | 0     |
| 86  | OHX  | 5     | 3990 | 7/7   | 0.98 | 0.12 | 95,95,95,95                 | 0     |
| 86  | OHX  | 1     | 3907 | 7/7   | 0.98 | 0.08 | 91,91,91,91                 | 0     |
| 86  | OHX  | 5     | 3993 | 7/7   | 0.98 | 0.12 | 99,99,99,99                 | 0     |
| 85  | MG   | 1     | 3631 | 1/1   | 0.98 | 0.13 | 61,61,61,61                 | 0     |
| 85  | MG   | 1     | 3600 | 1/1   | 0.98 | 0.37 | 22,22,22,22                 | 0     |
| 86  | OHX  | 1     | 3915 | 7/7   | 0.98 | 0.07 | 85,85,85,85                 | 0     |
| 86  | OHX  | 1     | 3916 | 7/7   | 0.98 | 0.09 | 99,99,99,99                 | 0     |
| 86  | OHX  | 1     | 4159 | 7/7   | 0.98 | 0.14 | 97,97,97,97                 | 0     |
| 86  | OHX  | 5     | 3999 | 7/7   | 0.98 | 0.08 | 111,111,111,111             | 0     |
| 86  | OHX  | 5     | 4000 | 7/7   | 0.98 | 0.08 | 104,104,104,104             | 0     |
| 86  | OHX  | 1     | 3917 | 7/7   | 0.98 | 0.11 | 88,88,88,88                 | 0     |
| 86  | OHX  | 1     | 3918 | 7/7   | 0.98 | 0.09 | 94,94,94,94                 | 0     |
| 86  | OHX  | 7     | 217  | 7/7   | 0.98 | 0.10 | 85,85,85,85                 | 0     |
| 86  | OHX  | 1     | 3919 | 7/7   | 0.98 | 0.08 | 97,97,97,97                 | 0     |
| 86  | OHX  | 7     | 219  | 7/7   | 0.98 | 0.10 | 98,98,98,98                 | 0     |
| 86  | OHX  | 7     | 220  | 7/7   | 0.98 | 0.17 | 89,89,89,89                 | 0     |
| 86  | OHX  | 7     | 221  | 7/7   | 0.98 | 0.17 | 95,95,95,95                 | 0     |
| 86  | OHX  | 7     | 222  | 7/7   | 0.98 | 0.10 | 101,101,101,101             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | MG   | 1     | 3572 | 1/1   | 0.98 | 0.19 | 23,23,23,23                 | 0     |
| 86  | OHX  | 2     | 2109 | 7/7   | 0.98 | 0.06 | 124,124,124,124             | 0     |
| 86  | OHX  | 1     | 3923 | 7/7   | 0.98 | 0.08 | 95,95,95,95                 | 0     |
| 86  | OHX  | 5     | 4007 | 7/7   | 0.98 | 0.16 | 99,99,99,99                 | 0     |
| 86  | OHX  | 1     | 3924 | 7/7   | 0.98 | 0.09 | 85,85,85,85                 | 0     |
| 86  | OHX  | 5     | 4009 | 7/7   | 0.98 | 0.07 | 118,118,118,118             | 0     |
| 86  | OHX  | 5     | 4012 | 7/7   | 0.98 | 0.09 | 100,100,100,100             | 0     |
| 86  | OHX  | 1     | 3925 | 7/7   | 0.98 | 0.09 | 85,85,85,85                 | 0     |
| 85  | MG   | 5     | 3768 | 1/1   | 0.98 | 0.05 | 47,47,47,47                 | 0     |
| 85  | MG   | 5     | 3724 | 1/1   | 0.98 | 0.05 | 55,55,55,55                 | 0     |
| 86  | OHX  | 1     | 3930 | 7/7   | 0.98 | 0.09 | 103,103,103,103             | 0     |
| 86  | OHX  | 1     | 4092 | 7/7   | 0.98 | 0.19 | 82,82,82,82                 | 0     |
| 86  | OHX  | 1     | 3931 | 7/7   | 0.98 | 0.08 | 84,84,84,84                 | 0     |
| 86  | OHX  | 2     | 2024 | 7/7   | 0.98 | 0.14 | 90,90,90,90                 | 0     |
| 86  | OHX  | 6     | 2052 | 7/7   | 0.98 | 0.11 | 74,74,74,74                 | 0     |
| 86  | OHX  | 6     | 2055 | 7/7   | 0.98 | 0.12 | 77,77,77,77                 | 0     |
| 86  | OHX  | 6     | 2056 | 7/7   | 0.98 | 0.12 | 85,85,85,85                 | 0     |
| 86  | OHX  | 6     | 2061 | 7/7   | 0.98 | 0.10 | 96,96,96,96                 | 0     |
| 86  | OHX  | 1     | 3934 | 7/7   | 0.98 | 0.10 | 99,99,99,99                 | 0     |
| 86  | OHX  | l3    | 404  | 7/7   | 0.98 | 0.12 | 95,95,95,95                 | 0     |
| 86  | OHX  | 6     | 2067 | 7/7   | 0.98 | 0.08 | 103,103,103,103             | 0     |
| 86  | OHX  | 5     | 4026 | 7/7   | 0.98 | 0.07 | 113,113,113,113             | 0     |
| 86  | OHX  | 2     | 2027 | 7/7   | 0.98 | 0.10 | 99,99,99,99                 | 0     |
| 86  | OHX  | 6     | 2070 | 7/7   | 0.98 | 0.18 | 92,92,92,92                 | 0     |
| 86  | OHX  | 6     | 2071 | 7/7   | 0.98 | 0.09 | 98,98,98,98                 | 0     |
| 86  | OHX  | 5     | 4030 | 7/7   | 0.98 | 0.13 | 84,84,84,84                 | 0     |
| 86  | OHX  | 6     | 2072 | 7/7   | 0.98 | 0.14 | 87,87,87,87                 | 0     |
| 86  | OHX  | 1     | 3937 | 7/7   | 0.98 | 0.08 | 93,93,93,93                 | 0     |
| 86  | OHX  | 6     | 2074 | 7/7   | 0.98 | 0.21 | 89,89,89,89                 | 0     |
| 86  | OHX  | 2     | 2028 | 7/7   | 0.98 | 0.09 | 106,106,106,106             | 0     |
| 86  | OHX  | 2     | 2029 | 7/7   | 0.98 | 0.12 | 98,98,98,98                 | 0     |
| 86  | OHX  | 5     | 4036 | 7/7   | 0.98 | 0.10 | 104,104,104,104             | 0     |
| 86  | OHX  | 6     | 2078 | 7/7   | 0.98 | 0.08 | 104,104,104,104             | 0     |
| 86  | OHX  | m6    | 203  | 7/7   | 0.98 | 0.11 | 93,93,93,93                 | 0     |
| 86  | OHX  | 1     | 3940 | 7/7   | 0.98 | 0.07 | 113,113,113,113             | 0     |
| 86  | OHX  | 6     | 2080 | 7/7   | 0.98 | 0.13 | 88,88,88,88                 | 0     |
| 86  | OHX  | 6     | 2081 | 7/7   | 0.98 | 0.10 | 102,102,102,102             | 0     |
| 86  | OHX  | o2    | 201  | 7/7   | 0.98 | 0.18 | 95,95,95,95                 | 0     |
| 86  | OHX  | o3    | 203  | 7/7   | 0.98 | 0.15 | 98,98,98,98                 | 0     |
| 86  | OHX  | 6     | 2082 | 7/7   | 0.98 | 0.10 | 99,99,99,99                 | 0     |
| 86  | OHX  | 2     | 2030 | 7/7   | 0.98 | 0.08 | 114,114,114,114             | 0     |
| 86  | OHX  | q2    | 502  | 7/7   | 0.98 | 0.10 | 79,79,79,79                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 1     | 3942 | 7/7   | 0.98 | 0.08 | 96,96,96,96                 | 0     |
| 87  | ZN   | E1    | 501  | 1/1   | 0.98 | 0.03 | 122,122,122,122             | 0     |
| 86  | OHX  | 1     | 3943 | 7/7   | 0.98 | 0.19 | 96,96,96,96                 | 0     |
| 86  | OHX  | 1     | 3945 | 7/7   | 0.98 | 0.09 | 102,102,102,102             | 0     |
| 86  | OHX  | 1     | 3946 | 7/7   | 0.98 | 0.12 | 89,89,89,89                 | 0     |
| 86  | OHX  | 2     | 2031 | 7/7   | 0.98 | 0.08 | 102,102,102,102             | 0     |
| 85  | MG   | 5     | 3725 | 1/1   | 0.98 | 0.20 | 37,37,37,37                 | 0     |
| 86  | OHX  | 2     | 2033 | 7/7   | 0.98 | 0.10 | 104,104,104,104             | 0     |
| 86  | OHX  | 1     | 3966 | 7/7   | 0.99 | 0.12 | 69,69,69,69                 | 0     |
| 86  | OHX  | 5     | 3933 | 7/7   | 0.99 | 0.07 | 62,62,62,62                 | 0     |
| 86  | OHX  | 6     | 2057 | 7/7   | 0.99 | 0.09 | 72,72,72,72                 | 0     |
| 86  | OHX  | 6     | 2058 | 7/7   | 0.99 | 0.10 | 83,83,83,83                 | 0     |
| 86  | OHX  | 5     | 3937 | 7/7   | 0.99 | 0.07 | 78,78,78,78                 | 0     |
| 86  | OHX  | 5     | 3938 | 7/7   | 0.99 | 0.06 | 77,77,77,77                 | 0     |
| 86  | OHX  | 5     | 3939 | 7/7   | 0.99 | 0.05 | 68,68,68,68                 | 0     |
| 86  | OHX  | 5     | 3940 | 7/7   | 0.99 | 0.10 | 78,78,78,78                 | 0     |
| 86  | OHX  | 5     | 3941 | 7/7   | 0.99 | 0.10 | 81,81,81,81                 | 0     |
| 86  | OHX  | 5     | 3942 | 7/7   | 0.99 | 0.07 | 86,86,86,86                 | 0     |
| 86  | OHX  | 6     | 2059 | 7/7   | 0.99 | 0.08 | 78,78,78,78                 | 0     |
| 86  | OHX  | 5     | 3944 | 7/7   | 0.99 | 0.07 | 80,80,80,80                 | 0     |
| 86  | OHX  | 5     | 3945 | 7/7   | 0.99 | 0.12 | 89,89,89,89                 | 0     |
| 86  | OHX  | 6     | 2060 | 7/7   | 0.99 | 0.07 | 89,89,89,89                 | 0     |
| 85  | MG   | 6     | 2028 | 1/1   | 0.99 | 0.03 | 86,86,86,86                 | 0     |
| 86  | OHX  | 5     | 3948 | 7/7   | 0.99 | 0.06 | 74,74,74,74                 | 0     |
| 86  | OHX  | 6     | 2062 | 7/7   | 0.99 | 0.05 | 82,82,82,82                 | 0     |
| 86  | OHX  | 6     | 2063 | 7/7   | 0.99 | 0.07 | 83,83,83,83                 | 0     |
| 86  | OHX  | 5     | 3951 | 7/7   | 0.99 | 0.09 | 92,92,92,92                 | 0     |
| 86  | OHX  | 6     | 2064 | 7/7   | 0.99 | 0.08 | 86,86,86,86                 | 0     |
| 86  | OHX  | 6     | 2065 | 7/7   | 0.99 | 0.06 | 87,87,87,87                 | 0     |
| 86  | OHX  | 1     | 3913 | 7/7   | 0.99 | 0.06 | 84,84,84,84                 | 0     |
| 86  | OHX  | 1     | 3914 | 7/7   | 0.99 | 0.07 | 81,81,81,81                 | 0     |
| 85  | MG   | 1     | 3686 | 1/1   | 0.99 | 0.18 | 43,43,43,43                 | 0     |
| 86  | OHX  | 5     | 3957 | 7/7   | 0.99 | 0.07 | 89,89,89,89                 | 0     |
| 86  | OHX  | 6     | 2069 | 7/7   | 0.99 | 0.16 | 89,89,89,89                 | 0     |
| 85  | MG   | m6    | 202  | 1/1   | 0.99 | 0.04 | 31,31,31,31                 | 0     |
| 86  | OHX  | 5     | 3960 | 7/7   | 0.99 | 0.09 | 80,80,80,80                 | 0     |
| 85  | MG   | 1     | 3694 | 1/1   | 0.99 | 0.24 | 39,39,39,39                 | 0     |
| 86  | OHX  | 5     | 3962 | 7/7   | 0.99 | 0.07 | 70,70,70,70                 | 0     |
| 86  | OHX  | 2     | 2035 | 7/7   | 0.99 | 0.08 | 92,92,92,92                 | 0     |
| 86  | OHX  | 5     | 3964 | 7/7   | 0.99 | 0.11 | 90,90,90,90                 | 0     |
| 85  | MG   | N8    | 204  | 1/1   | 0.99 | 0.30 | 38,38,38,38                 | 0     |
| 86  | OHX  | 5     | 3967 | 7/7   | 0.99 | 0.10 | 76,76,76,76                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 1     | 3920 | 7/7   | 0.99 | 0.08 | 85,85,85,85                 | 0     |
| 85  | MG   | 5     | 3798 | 1/1   | 0.99 | 0.16 | 37,37,37,37                 | 0     |
| 85  | MG   | 5     | 3821 | 1/1   | 0.99 | 0.08 | 54,54,54,54                 | 0     |
| 86  | OHX  | 5     | 3971 | 7/7   | 0.99 | 0.07 | 88,88,88,88                 | 0     |
| 86  | OHX  | 6     | 2077 | 7/7   | 0.99 | 0.09 | 83,83,83,83                 | 0     |
| 85  | MG   | 5     | 3412 | 1/1   | 0.99 | 0.16 | 30,30,30,30                 | 0     |
| 86  | OHX  | 2     | 2040 | 7/7   | 0.99 | 0.07 | 96,96,96,96                 | 0     |
| 86  | OHX  | 2     | 2041 | 7/7   | 0.99 | 0.06 | 97,97,97,97                 | 0     |
| 86  | OHX  | 1     | 3926 | 7/7   | 0.99 | 0.09 | 77,77,77,77                 | 0     |
| 85  | MG   | 5     | 3759 | 1/1   | 0.99 | 0.10 | 41,41,41,41                 | 0     |
| 86  | OHX  | 6     | 2083 | 7/7   | 0.99 | 0.10 | 96,96,96,96                 | 0     |
| 86  | OHX  | 6     | 2084 | 7/7   | 0.99 | 0.06 | 101,101,101,101             | 0     |
| 86  | OHX  | 1     | 3983 | 7/7   | 0.99 | 0.14 | 78,78,78,78                 | 0     |
| 86  | OHX  | 5     | 3981 | 7/7   | 0.99 | 0.11 | 77,77,77,77                 | 0     |
| 86  | OHX  | 1     | 3984 | 7/7   | 0.99 | 0.07 | 113,113,113,113             | 0     |
| 86  | OHX  | 1     | 3928 | 7/7   | 0.99 | 0.09 | 83,83,83,83                 | 0     |
| 86  | OHX  | 2     | 2043 | 7/7   | 0.99 | 0.08 | 102,102,102,102             | 0     |
| 86  | OHX  | 5     | 3985 | 7/7   | 0.99 | 0.13 | 83,83,83,83                 | 0     |
| 86  | OHX  | 6     | 2089 | 7/7   | 0.99 | 0.07 | 106,106,106,106             | 0     |
| 86  | OHX  | 5     | 4112 | 7/7   | 0.99 | 0.15 | 83,83,83,83                 | 0     |
| 86  | OHX  | 1     | 3872 | 7/7   | 0.99 | 0.08 | 53,53,53,53                 | 0     |
| 86  | OHX  | 5     | 3988 | 7/7   | 0.99 | 0.14 | 80,80,80,80                 | 0     |
| 86  | OHX  | 1     | 3873 | 7/7   | 0.99 | 0.12 | 58,58,58,58                 | 0     |
| 86  | OHX  | 1     | 3932 | 7/7   | 0.99 | 0.07 | 87,87,87,87                 | 0     |
| 86  | OHX  | 1     | 3875 | 7/7   | 0.99 | 0.10 | 61,61,61,61                 | 0     |
| 86  | OHX  | 5     | 3992 | 7/7   | 0.99 | 0.09 | 80,80,80,80                 | 0     |
| 86  | OHX  | 1     | 3876 | 7/7   | 0.99 | 0.09 | 59,59,59,59                 | 0     |
| 86  | OHX  | 1     | 3935 | 7/7   | 0.99 | 0.09 | 79,79,79,79                 | 0     |
| 86  | OHX  | 1     | 3877 | 7/7   | 0.99 | 0.08 | 65,65,65,65                 | 0     |
| 86  | OHX  | 1     | 3880 | 7/7   | 0.99 | 0.07 | 65,65,65,65                 | 0     |
| 86  | OHX  | 1     | 3881 | 7/7   | 0.99 | 0.10 | 65,65,65,65                 | 0     |
| 86  | OHX  | 4     | 225  | 7/7   | 0.99 | 0.10 | 64,64,64,64                 | 0     |
| 86  | OHX  | 4     | 226  | 7/7   | 0.99 | 0.09 | 82,82,82,82                 | 0     |
| 86  | OHX  | 1     | 3882 | 7/7   | 0.99 | 0.06 | 64,64,64,64                 | 0     |
| 86  | OHX  | 1     | 3883 | 7/7   | 0.99 | 0.09 | 63,63,63,63                 | 0     |
| 86  | OHX  | 1     | 3884 | 7/7   | 0.99 | 0.11 | 67,67,67,67                 | 0     |
| 86  | OHX  | 1     | 3886 | 7/7   | 0.99 | 0.08 | 73,73,73,73                 | 0     |
| 86  | OHX  | 1     | 3887 | 7/7   | 0.99 | 0.08 | 70,70,70,70                 | 0     |
| 86  | OHX  | 1     | 3944 | 7/7   | 0.99 | 0.13 | 84,84,84,84                 | 0     |
| 85  | MG   | 5     | 3863 | 1/1   | 0.99 | 0.06 | 65,65,65,65                 | 0     |
| 86  | OHX  | 1     | 4003 | 7/7   | 0.99 | 0.16 | 88,88,88,88                 | 0     |
| 86  | OHX  | 1     | 3892 | 7/7   | 0.99 | 0.07 | 70,70,70,70                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 86  | OHX  | 1     | 3894 | 7/7   | 0.99 | 0.09 | 74,74,74,74                 | 0     |
| 86  | OHX  | 5     | 4010 | 7/7   | 0.99 | 0.08 | 69,69,69,69                 | 0     |
| 86  | OHX  | 5     | 4011 | 7/7   | 0.99 | 0.14 | 88,88,88,88                 | 0     |
| 86  | OHX  | 1     | 3895 | 7/7   | 0.99 | 0.09 | 74,74,74,74                 | 0     |
| 85  | MG   | 1     | 3688 | 1/1   | 0.99 | 0.11 | 38,38,38,38                 | 0     |
| 86  | OHX  | 2     | 2022 | 7/7   | 0.99 | 0.13 | 74,74,74,74                 | 0     |
| 86  | OHX  | 8     | 216  | 7/7   | 0.99 | 0.10 | 57,57,57,57                 | 0     |
| 86  | OHX  | 8     | 217  | 7/7   | 0.99 | 0.12 | 86,86,86,86                 | 0     |
| 86  | OHX  | 2     | 2023 | 7/7   | 0.99 | 0.12 | 83,83,83,83                 | 0     |
| 86  | OHX  | 1     | 3899 | 7/7   | 0.99 | 0.07 | 77,77,77,77                 | 0     |
| 86  | OHX  | 1     | 3953 | 7/7   | 0.99 | 0.06 | 94,94,94,94                 | 0     |
| 85  | MG   | 5     | 3837 | 1/1   | 0.99 | 0.03 | 64,64,64,64                 | 0     |
| 86  | OHX  | 2     | 2025 | 7/7   | 0.99 | 0.08 | 89,89,89,89                 | 0     |
| 86  | OHX  | 1     | 3902 | 7/7   | 0.99 | 0.07 | 70,70,70,70                 | 0     |
| 86  | OHX  | 1     | 3903 | 7/7   | 0.99 | 0.05 | 79,79,79,79                 | 0     |
| 86  | OHX  | 2     | 2026 | 7/7   | 0.99 | 0.08 | 78,78,78,78                 | 0     |
| 86  | OHX  | N9    | 101  | 7/7   | 0.99 | 0.09 | 63,63,63,63                 | 0     |
| 85  | MG   | 1     | 3812 | 1/1   | 0.99 | 0.04 | 35,35,35,35                 | 0     |
| 85  | MG   | 5     | 3852 | 1/1   | 0.99 | 0.08 | 46,46,46,46                 | 0     |
| 85  | MG   | 5     | 3743 | 1/1   | 0.99 | 0.09 | 29,29,29,29                 | 0     |
| 86  | OHX  | 1     | 3908 | 7/7   | 0.99 | 0.10 | 84,84,84,84                 | 0     |
| 86  | OHX  | 1     | 3909 | 7/7   | 0.99 | 0.09 | 90,90,90,90                 | 0     |
| 86  | OHX  | Q2    | 502  | 7/7   | 0.99 | 0.14 | 77,77,77,77                 | 0     |
| 86  | OHX  | 6     | 2048 | 7/7   | 0.99 | 0.12 | 56,56,56,56                 | 0     |
| 86  | OHX  | 6     | 2049 | 7/7   | 0.99 | 0.14 | 74,74,74,74                 | 0     |
| 86  | OHX  | 6     | 2050 | 7/7   | 0.99 | 0.10 | 66,66,66,66                 | 0     |
| 86  | OHX  | 6     | 2051 | 7/7   | 0.99 | 0.09 | 74,74,74,74                 | 0     |
| 86  | OHX  | 1     | 3910 | 7/7   | 0.99 | 0.08 | 74,74,74,74                 | 0     |
| 86  | OHX  | 6     | 2053 | 7/7   | 0.99 | 0.10 | 70,70,70,70                 | 0     |
| 86  | OHX  | 6     | 2054 | 7/7   | 0.99 | 0.11 | 75,75,75,75                 | 0     |
| 86  | OHX  | 5     | 3901 | 7/7   | 0.99 | 0.13 | 49,49,49,49                 | 0     |
| 86  | OHX  | 5     | 3905 | 7/7   | 0.99 | 0.11 | 54,54,54,54                 | 0     |
| 86  | OHX  | 5     | 3906 | 7/7   | 0.99 | 0.10 | 54,54,54,54                 | 0     |
| 86  | OHX  | 5     | 3908 | 7/7   | 0.99 | 0.11 | 56,56,56,56                 | 0     |
| 86  | OHX  | 5     | 3909 | 7/7   | 0.99 | 0.12 | 62,62,62,62                 | 0     |
| 86  | OHX  | 5     | 3910 | 7/7   | 0.99 | 0.10 | 58,58,58,58                 | 0     |
| 86  | OHX  | 5     | 3912 | 7/7   | 0.99 | 0.15 | 66,66,66,66                 | 0     |
| 86  | OHX  | 5     | 3913 | 7/7   | 0.99 | 0.08 | 55,55,55,55                 | 0     |
| 86  | OHX  | n3    | 203  | 7/7   | 0.99 | 0.08 | 90,90,90,90                 | 0     |
| 86  | OHX  | 5     | 3914 | 7/7   | 0.99 | 0.07 | 57,57,57,57                 | 0     |
| 86  | OHX  | n9    | 101  | 7/7   | 0.99 | 0.08 | 66,66,66,66                 | 0     |
| 86  | OHX  | 5     | 3916 | 7/7   | 0.99 | 0.09 | 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  | OHX  | 5     | 3917 | 7/7   | 0.99 | 0.10 | 61,61,61,61                 | 0     |
| 86  | OHX  | 5     | 3918 | 7/7   | 0.99 | 0.08 | 70,70,70,70                 | 0     |
| 86  | OHX  | 5     | 3919 | 7/7   | 0.99 | 0.05 | 59,59,59,59                 | 0     |
| 86  | OHX  | 5     | 3920 | 7/7   | 0.99 | 0.09 | 62,62,62,62                 | 0     |
| 86  | OHX  | 5     | 3921 | 7/7   | 0.99 | 0.07 | 71,71,71,71                 | 0     |
| 87  | ZN   | D9    | 101  | 1/1   | 0.99 | 0.04 | 84,84,84,84                 | 0     |
| 86  | OHX  | 5     | 3923 | 7/7   | 0.99 | 0.07 | 67,67,67,67                 | 0     |
| 86  | OHX  | 5     | 3925 | 7/7   | 0.99 | 0.07 | 67,67,67,67                 | 0     |
| 87  | ZN   | d6    | 101  | 1/1   | 0.99 | 0.03 | 60,60,60,60                 | 0     |
| 86  | OHX  | 5     | 3926 | 7/7   | 0.99 | 0.10 | 70,70,70,70                 | 0     |
| 87  | ZN   | d9    | 101  | 1/1   | 0.99 | 0.03 | 82,82,82,82                 | 0     |
| 86  | OHX  | 5     | 3927 | 7/7   | 0.99 | 0.05 | 66,66,66,66                 | 0     |
| 85  | MG   | 1     | 3804 | 1/1   | 0.99 | 0.09 | 58,58,58,58                 | 0     |
| 87  | ZN   | q3    | 501  | 1/1   | 0.99 | 0.02 | 63,63,63,63                 | 0     |
| 86  | OHX  | 5     | 4057 | 7/7   | 0.99 | 0.10 | 93,93,93,93                 | 0     |
| 86  | OHX  | 5     | 3931 | 7/7   | 0.99 | 0.06 | 77,77,77,77                 | 0     |
| 86  | OHX  | 5     | 3930 | 7/7   | 1.00 | 0.04 | 75,75,75,75                 | 0     |
| 86  | OHX  | 5     | 3907 | 7/7   | 1.00 | 0.06 | 56,56,56,56                 | 0     |
| 86  | OHX  | 1     | 3888 | 7/7   | 1.00 | 0.09 | 67,67,67,67                 | 0     |
| 86  | OHX  | 1     | 3889 | 7/7   | 1.00 | 0.09 | 78,78,78,78                 | 0     |
| 86  | OHX  | N1    | 201  | 7/7   | 1.00 | 0.06 | 65,65,65,65                 | 0     |
| 86  | OHX  | 5     | 3911 | 7/7   | 1.00 | 0.08 | 47,47,47,47                 | 0     |
| 86  | OHX  | 5     | 3936 | 7/7   | 1.00 | 0.05 | 70,70,70,70                 | 0     |
| 86  | OHX  | 1     | 3890 | 7/7   | 1.00 | 0.06 | 71,71,71,71                 | 0     |
| 86  | OHX  | 1     | 3869 | 7/7   | 1.00 | 0.10 | 46,46,46,46                 | 0     |
| 86  | OHX  | 4     | 224  | 7/7   | 1.00 | 0.09 | 55,55,55,55                 | 0     |
| 86  | OHX  | 5     | 3965 | 7/7   | 1.00 | 0.05 | 88,88,88,88                 | 0     |
| 86  | OHX  | 5     | 3915 | 7/7   | 1.00 | 0.08 | 62,62,62,62                 | 0     |
| 86  | OHX  | 1     | 3874 | 7/7   | 1.00 | 0.07 | 53,53,53,53                 | 0     |
| 86  | OHX  | 1     | 3893 | 7/7   | 1.00 | 0.04 | 67,67,67,67                 | 0     |
| 87  | ZN   | D6    | 500  | 1/1   | 1.00 | 0.02 | 85,85,85,85                 | 0     |
| 86  | OHX  | 1     | 3870 | 7/7   | 1.00 | 0.09 | 54,54,54,54                 | 0     |
| 86  | OHX  | 1     | 3867 | 7/7   | 1.00 | 0.11 | 44,44,44,44                 | 0     |
| 86  | OHX  | 1     | 3868 | 7/7   | 1.00 | 0.09 | 50,50,50,50                 | 0     |
| 87  | ZN   | O7    | 101  | 1/1   | 1.00 | 0.02 | 36,36,36,36                 | 0     |
| 87  | ZN   | Q0    | 500  | 1/1   | 1.00 | 0.02 | 47,47,47,47                 | 0     |
| 86  | OHX  | 1     | 3885 | 7/7   | 1.00 | 0.05 | 59,59,59,59                 | 0     |
| 87  | ZN   | Q3    | 501  | 1/1   | 1.00 | 0.01 | 60,60,60,60                 | 0     |
| 86  | OHX  | 5     | 3922 | 7/7   | 1.00 | 0.07 | 66,66,66,66                 | 0     |
| 86  | OHX  | 5     | 3902 | 7/7   | 1.00 | 0.11 | 43,43,43,43                 | 0     |
| 86  | OHX  | 5     | 3924 | 7/7   | 1.00 | 0.07 | 64,64,64,64                 | 0     |
| 86  | OHX  | 5     | 3903 | 7/7   | 1.00 | 0.12 | 43,43,43,43                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 87  | ZN   | o7    | 501  | 1/1   | 1.00 | 0.01 | 43,43,43,43                 | 0     |
| 87  | ZN   | q0    | 201  | 1/1   | 1.00 | 0.02 | 32,32,32,32                 | 0     |
| 86  | OHX  | 5     | 3904 | 7/7   | 1.00 | 0.07 | 46,46,46,46                 | 0     |
| 86  | OHX  | 1     | 3878 | 7/7   | 1.00 | 0.06 | 61,61,61,61                 | 0     |
| 86  | OHX  | 5     | 3928 | 7/7   | 1.00 | 0.05 | 61,61,61,61                 | 0     |
| 86  | OHX  | 1     | 3879 | 7/7   | 1.00 | 0.05 | 60,60,60,60                 | 0     |

## 5.5 Other polymers [i](#)

There are no such residues in this entry.