# wwPDB X-ray Structure Validation Summary Report (i)

Jan 8, 2024 – 03:35 pm GMT

| | | |
|---|---|---|
| PDB ID | : | 5TBW |
| Title | : | Crystal structure of chlorolissoclimide bound to the yeast 80S ribosome |
| Authors | : | Konst, Z.A.; Szklarski, A.R.; Pellegrino, S.; Michalak, S.E.; Meyer, M.; Zanette, C.; Cencic, R.; Nam, S.; Horne, D.A.; Pelletier, J.; Mobley, D.L.; Yusupova, G.; Yusupov, M.; Vanderwal, C.D. |
| Deposited on | : | 2016-09-13 |
| 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

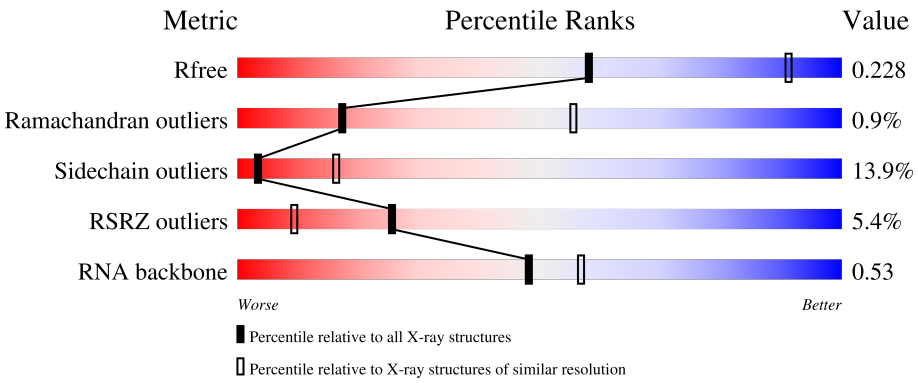
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.36 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36 |

# 1 Overall quality at a glance (i)

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 (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 2092 (3.00-3.00) |
| Ramachandran outliers | 138981 | 2333 (3.00-3.00) |
| Sidechain outliers | 138945 | 2336 (3.00-3.00) |
| RSRZ outliers | 127900 | 1990 (3.00-3.00) |
| RNA backbone | 3102 | 1173 (3.30-2.70) |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | 1 | 3149 | 2%, 81%, 18%, • |
| 1 | AR | 3149 | 3%, 81%, 18%, • |
| 2 | 3 | 121 | 88%, 12% |
| 2 | AS | 121 | 88%, 12% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 3 | 4 | 158 | .% 79% 21% |
| 3 | AT | 158 | .% 81% 18% • |
| 4 | CD | 252 | .% 89% 11% |
| 4 | j | 252 | 88% 11% |
| 5 | CE | 386 | .% 87% 13% |
| 5 | k | 386 | 86% 14% |
| 6 | CF | 361 | 89% 11% |
| 6 | l | 361 | 87% 12% • |
| 7 | CG | 296 | .% 86% 14% |
| 7 | m | 296 | 2% 88% 12% |
| 8 | CH | 175 | 2% 81% 8% • 11% |
| 8 | n | 175 | 79% 10% • 11% |
| 9 | CI | 222 | .% 92% 8% |
| 9 | o | 222 | .% 90% 9% • |
| 10 | CJ | 233 | 9% 91% 8% |
| 10 | p | 233 | 2% 85% 15% |
| 11 | CK | 191 | 2% 87% 13% |
| 11 | q | 191 | .% 86% 14% |
| 12 | CL | 220 | 3% 86% 10% • |
| 12 | r | 220 | 84% 12% • |
| 13 | CM | 169 | .% 85% 14% • |
| 13 | s | 169 | .% 85% 15% |
| 14 | CN | 193 | 3% 89% 11% |
| 14 | t | 193 | .% 86% 14% |
| 15 | CO | 136 | .% 90% 10% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 15 | u | 136 | 88% 11% |
| 16 | CP | 203 | 89% 11% |
| 16 | v | 203 | 89% 11% |
| 17 | CQ | 197 | 2% 89% 11% |
| 17 | w | 197 | 90% 9% |
| 18 | CR | 183 | 16% 86% 14% |
| 18 | x | 183 | 8% 90% 10% |
| 19 | CS | 185 | 85% 15% |
| 19 | y | 185 | 86% 14% |
| 20 | CT | 188 | 6% 85% 15% |
| 20 | z | 188 | 7% 91% 9% |
| 21 | 0 | 172 | % 85% 15% |
| 21 | CU | 172 | % 85% 15% |
| 22 | 2 | 159 | % 82% 18% |
| 22 | CV | 159 | 84% 14% |
| 23 | 5 | 100 | 11% 89% 11% |
| 23 | CW | 100 | 19% 88% 12% |
| 24 | 6 | 136 | % 88% 12% |
| 24 | CX | 136 | 2% 90% 10% |
| 25 | 7 | 98 | 33% 93% 7% |
| 25 | CY | 98 | 17% 91% 9% |
| 26 | 8 | 121 | 86% 14% |
| 26 | CZ | 121 | 2% 85% 14% |
| 27 | 9 | 126 | % 84% 15% |
| 27 | DA | 126 | 2% 87% 13% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 28 | AA | 135 | 4% 87% 13% |
| 28 | DB | 135 | 7% 90% 10% |
| 29 | AB | 148 | 85% 14% |
| 29 | DC | 148 | 87% 13% |
| 30 | AC | 58 | 86% 14% |
| 30 | DD | 58 | 2% 86% 14% |
| 31 | AD | 97 | 3% 88% 12% |
| 31 | DE | 97 | 5% 93% 7% |
| 32 | AE | 109 | 3% 85% 15% |
| 32 | DF | 109 | 5% 82% 17% |
| 33 | AF | 127 | 2% 88% 12% |
| 33 | DG | 127 | 2% 91% 9% |
| 34 | AG | 106 | 94% 6% |
| 34 | DH | 106 | 91% 9% |
| 35 | AH | 112 | 4% 86% 14% |
| 35 | DI | 112 | 2% 91% 9% |
| 36 | AI | 119 | % 87% 13% |
| 36 | DJ | 119 | 2% 80% 19% |
| 37 | AJ | 99 | 6% 84% 16% |
| 37 | DK | 99 | 6% 83% 17% |
| 38 | AK | 87 | 2% 90% 10% |
| 38 | DL | 87 | 2% 87% 13% |
| 39 | AL | 77 | % 84% 16% |
| 39 | DM | 77 | 26% 83% 17% |
| 40 | AM | 50 | 2% 86% 14% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 40 | DN | 50 | 90% 10% |
| 41 | AN | 52 | 2% 83% 17% |
| 41 | DO | 52 | 87% 13% |
| 42 | AO | 25 | 84% 16% |
| 42 | DP | 25 | 84% 16% |
| 43 | AP | 105 | 2% 90% 10% |
| 43 | DQ | 105 | % 84% 16% |
| 44 | AQ | 91 | 85% 15% |
| 44 | DR | 91 | 90% 10% |
| 45 | i | 168 | 15% 83% 11% • 5% |
| 46 | p0 | 219 | 17% 57% 9% 35% |
| 47 | sM | 104 | 12% 93% 6% • |
| 48 | A | 1800 | 5% 75% 23% •• |
| 48 | sR | 1800 | 5% 77% 21% •• |
| 49 | B | 206 | 12% 92% 8% |
| 49 | s0 | 206 | 7% 86% 14% |
| 50 | C | 216 | 20% 84% 15% • |
| 50 | s1 | 216 | 6% 87% 12% |
| 51 | D | 217 | 2% 83% 16% • |
| 51 | s2 | 217 | 3% 84% 16% |
| 52 | E | 223 | 6% 88% 11% • |
| 52 | s3 | 223 | 4% 90% 10% |
| 53 | F | 260 | 3% 88% 12% |
| 53 | s4 | 260 | 2% 88% 12% |
| 54 | G | 206 | 15% 91% 9% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 54 | s5 | 206 | 13% 88% 12% |
| 55 | H | 226 | 8% 86% 13% |
| 55 | s6 | 226 | 6% 85% 11% • |
| 56 | I | 186 | 13% 84% 14% •• |
| 56 | s7 | 186 | 13% 90% 10% • |
| 57 | J | 199 | 3% 86% 7% • 6% |
| 57 | s8 | 199 | 5% 86% 8% • 6% |
| 58 | K | 185 | 11% 84% 16% |
| 58 | s9 | 185 | 5% 89% 11% |
| 59 | L | 105 | % 84% 7% • 9% |
| 59 | c0 | 105 | 23% 79% 10% • 9% |
| 60 | M | 155 | 12% 85% 15% |
| 60 | c1 | 155 | 6% 81% 12% • 6% |
| 61 | N | 143 | 35% 71% 15% • 13% |
| 61 | c2 | 143 | 54% 69% 17% • 13% |
| 62 | O | 150 | 3% 85% 15% |
| 62 | c3 | 150 | 87% 12% • |
| 63 | P | 128 | 24% 88% 12% • |
| 63 | c4 | 128 | 9% 87% 13% |
| 64 | Q | 135 | 4% 79% 13% • 8% |
| 64 | c5 | 135 | 12% 88% 11% • |
| 65 | R | 142 | 13% 84% 14% •• |
| 65 | c6 | 142 | 9% 87% 13% |
| 66 | S | 125 | 9% 78% 16% •• • |
| 67 | T | 145 | 10% 81% 17% • |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 67 | c8 | 145 | 9% 86% 14% |
| 68 | U | 143 | 7% 85% 15% |
| 68 | c9 | 143 | 8% 92% 6% |
| 69 | V | 110 | 22% 82% 15% |
| 69 | d0 | 110 | 25% 87% 12% |
| 70 | W | 87 | 8% 84% 16% |
| 70 | d1 | 87 | 6% 86% 14% |
| 71 | X | 129 | % 84% 15% |
| 71 | d2 | 129 | 91% 8% |
| 72 | Y | 144 | 86% 14% |
| 72 | d3 | 144 | % 91% 9% |
| 73 | Z | 134 | 5% 89% 10% |
| 73 | d4 | 134 | 4% 91% 8% |
| 74 | a | 70 | 33% 71% 27% |
| 74 | d5 | 70 | 31% 91% 7% |
| 75 | b | 97 | 15% 86% 14% |
| 75 | d6 | 97 | 2% 92% 8% |
| 76 | c | 81 | 12% 90% 10% |
| 76 | d7 | 81 | 15% 89% 11% |
| 77 | d | 63 | 17% 89% 11% |
| 77 | d8 | 63 | 32% 90% 10% |
| 78 | d9 | 53 | 4% 81% 17% |
| 78 | e | 53 | 2% 85% 15% |
| 79 | e0 | 62 | 10% 84% 16% |
| 79 | f | 62 | 13% 82% 15% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 80 | g | 71 | 21% 79% 21% |
| 81 | Rb | 318 | 25% 95% 5% |
| 81 | h | 318 | 14% 94% 6% |
| 82 | c7 | 121 | 5% 88% 8% |
| 83 | e1 | 51 | 29% 78% 22% |

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 |
|---|---|---|---|---|---|---|---|
| 84 | OHX | 1 | 3673 | - | - | - | X |
| 84 | OHX | 1 | 3718 | - | - | - | X |
| 84 | OHX | A | 2039 | - | - | - | X |
| 84 | OHX | AR | 3740 | - | - | - | X |
| 84 | OHX | sR | 2040 | - | - | - | X |
| 85 | MG | 1 | 3772 | - | - | - | X |
| 85 | MG | 1 | 3787 | - | - | - | X |
| 85 | MG | 1 | 3790 | - | - | - | X |
| 85 | MG | 1 | 3802 | - | - | - | X |
| 85 | MG | 1 | 3822 | - | - | - | X |
| 85 | MG | 1 | 3834 | - | - | - | X |
| 85 | MG | 1 | 3866 | - | - | - | X |
| 85 | MG | 1 | 3878 | - | - | - | X |
| 85 | MG | 1 | 3913 | - | - | - | X |
| 85 | MG | 1 | 3985 | - | - | - | X |
| 85 | MG | 1 | 3988 | - | - | - | X |
| 85 | MG | 1 | 3994 | - | - | - | X |
| 85 | MG | 1 | 4001 | - | - | - | X |
| 85 | MG | 1 | 4003 | - | - | - | X |
| 85 | MG | 1 | 4032 | - | - | - | X |
| 85 | MG | 1 | 4104 | - | - | - | X |
| 85 | MG | 1 | 4108 | - | - | - | X |
| 85 | MG | 1 | 4116 | - | - | - | X |
| 85 | MG | 1 | 4155 | - | - | - | X |
| 85 | MG | 1 | 4162 | - | - | - | X |
| 85 | MG | 1 | 4194 | - | - | - | X |
| 85 | MG | 3 | 210 | - | - | - | X |
| 85 | MG | 3 | 216 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 85 | MG | A | 2068 | - | - | - | X |
| 85 | MG | A | 2102 | - | - | - | X |
| 85 | MG | A | 2104 | - | - | - | X |
| 85 | MG | A | 2113 | - | - | - | X |
| 85 | MG | A | 2119 | - | - | - | X |
| 85 | MG | A | 2134 | - | - | - | X |
| 85 | MG | AR | 3803 | - | - | - | X |
| 85 | MG | AR | 3834 | - | - | - | X |
| 85 | MG | AR | 3966 | - | - | - | X |
| 85 | MG | AR | 3972 | - | - | - | X |
| 85 | MG | AR | 3974 | - | - | - | X |
| 85 | MG | AR | 3989 | - | - | - | X |
| 85 | MG | AR | 4038 | - | - | - | X |
| 85 | MG | AR | 4055 | - | - | - | X |
| 85 | MG | AR | 4085 | - | - | - | X |
| 85 | MG | AR | 4091 | - | - | - | X |
| 85 | MG | AR | 4102 | - | - | - | X |
| 85 | MG | AR | 4113 | - | - | - | X |
| 85 | MG | AR | 4126 | - | - | - | X |
| 85 | MG | AR | 4138 | - | - | - | X |
| 85 | MG | AR | 4156 | - | - | - | X |
| 85 | MG | AR | 4157 | - | - | - | X |
| 85 | MG | AR | 4169 | - | - | - | X |
| 85 | MG | AR | 4171 | - | - | - | X |
| 85 | MG | AR | 4186 | - | - | - | X |
| 85 | MG | AR | 4227 | - | - | - | X |
| 85 | MG | AR | 4233 | - | - | - | X |
| 85 | MG | AR | 4236 | - | - | - | X |
| 85 | MG | AT | 221 | - | - | - | X |
| 85 | MG | AT | 225 | - | - | - | X |
| 85 | MG | l | 403 | - | - | - | X |
| 85 | MG | l | 404 | - | - | - | X |
| 85 | MG | l | 406 | - | - | - | X |
| 85 | MG | sR | 2066 | - | - | - | X |
| 85 | MG | sR | 2082 | - | - | - | X |
| 85 | MG | sR | 2157 | - | - | - | X |
| 85 | MG | sR | 2159 | - | - | - | X |
| 85 | MG | sR | 2185 | - | - | - | X |
| 85 | MG | sR | 2187 | - | - | - | X |
| 85 | MG | sR | 2188 | - | - | - | X |
| 85 | MG | x | 206 | - | - | - | X |

# 2 Entry composition (i)

There are 87 unique types of molecules in this entry. The entry contains 409612 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 25S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | | |
| 1 | 1 | 3149 | 67355 | 30086 | 12142 | 21978 | 3149 | 0 | 0 | 0 |
| 1 | AR | 3149 | 67355 | 30086 | 12142 | 21978 | 3149 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | | |
| 2 | 3 | 121 | 2579 | 1152 | 461 | 845 | 121 | 0 | 0 | 0 |
| 2 | AS | 121 | 2579 | 1152 | 461 | 845 | 121 | 0 | 0 | 0 |

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | | |
| 3 | 4 | 158 | 3353 | 1500 | 586 | 1109 | 158 | 0 | 0 | 0 |
| 3 | AT | 158 | 3353 | 1500 | 586 | 1109 | 158 | 0 | 0 | 0 |

- Molecule 4 is a protein called 60S ribosomal protein L2-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 4 | j | 252 | 1914 | 1191 | 388 | 334 | 1 | 0 | 0 | 0 |
| 4 | CD | 252 | 1914 | 1191 | 388 | 334 | 1 | 0 | 0 | 0 |

- Molecule 5 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 5 | k | 386 | 3075 | 1950 | 584 | 533 | 8 | 0 | 0 | 0 |
| 5 | CE | 386 | 3075 | 1950 | 584 | 533 | 8 | 0 | 0 | 0 |

- Molecule 6 is a protein called 60S ribosomal protein L4-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 6 | l | 361 | 2748 | 1729 | 522 | 494 | 3 | 0 | 0 | 0 |
| 6 | CF | 361 | 2748 | 1729 | 522 | 494 | 3 | 0 | 0 | 0 |

- Molecule 7 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 7 | m | 296 | 2375 | 1501 | 414 | 458 | 2 | 0 | 0 | 0 |
| 7 | CG | 296 | 2375 | 1501 | 414 | 458 | 2 | 0 | 0 | 0 |

- Molecule 8 is a protein called 60S ribosomal protein L6-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 8 | n | 156 | 1239 | 800 | 222 | 216 | 1 | 0 | 0 | 0 |
| 8 | CH | 156 | 1239 | 800 | 222 | 216 | 1 | 0 | 0 | 0 |

- Molecule 9 is a protein called 60S ribosomal protein L7-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 9 | o | 222 | 1784 | 1151 | 324 | 308 | 1 | 0 | 0 | 0 |
| 9 | CI | 222 | 1784 | 1151 | 324 | 308 | 1 | 0 | 0 | 0 |

- Molecule 10 is a protein called 60S ribosomal protein L8-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 10 | p | 233 | 1804 | 1151 | 323 | 327 | 3 | 0 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 10 | CJ | 233 | 1804 | 1151 | 323 | 327 | 3 | 0 | 0 | 0 |

- Molecule 11 is a protein called 60S ribosomal protein L9-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 11 | q | 191 | 1518 | 963 | 274 | 277 | 4 | 0 | 0 | 0 |
| 11 | CK | 191 | 1518 | 963 | 274 | 277 | 4 | 0 | 0 | 0 |

- Molecule 12 is a protein called 60S ribosomal protein L10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 12 | r | 211 | 1705 | 1083 | 322 | 294 | 6 | 0 | 0 | 0 |
| 12 | CL | 211 | 1705 | 1083 | 322 | 294 | 6 | 0 | 0 | 0 |

- Molecule 13 is a protein called 60S ribosomal protein L11-B.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 13 | s | 169 | 1353 | 847 | 253 | 249 | 4 | 0 | 0 | 0 |
| 13 | CM | 169 | 1353 | 847 | 253 | 249 | 4 | 0 | 0 | 0 |

- Molecule 14 is a protein called 60S ribosomal protein L13-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 14 | t | 193 | 1543 | 962 | 315 | 266 | 0 | 0 | 0 |
| 14 | CN | 193 | 1543 | 962 | 315 | 266 | 0 | 0 | 0 |

- Molecule 15 is a protein called 60S ribosomal protein L14-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 15 | u | 136 | 1053 | 675 | 199 | 177 | 2 | 0 | 0 | 0 |
| 15 | CO | 136 | 1053 | 675 | 199 | 177 | 2 | 0 | 0 | 0 |

- Molecule 16 is a protein called 60S ribosomal protein L15-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 16 | v | 203 | 1720 | 1077 | 361 | 281 | 1 | 0 | 0 | 0 |
| 16 | CP | 203 | 1720 | 1077 | 361 | 281 | 1 | 0 | 0 | 0 |

- Molecule 17 is a protein called 60S ribosomal protein L16-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 17 | w | 197 | 1555 | 1003 | 289 | 262 | 1 | 0 | 0 | 0 |
| 17 | CQ | 197 | 1555 | 1003 | 289 | 262 | 1 | 0 | 0 | 0 |

- Molecule 18 is a protein called 60S ribosomal protein L17-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 18 | x | 183 | 1420 | 882 | 281 | 257 | 0 | 0 | 0 |
| 18 | CR | 183 | 1420 | 882 | 281 | 257 | 0 | 0 | 0 |

- Molecule 19 is a protein called 60S ribosomal protein L18-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 19 | y | 185 | 1441 | 908 | 290 | 241 | 2 | 0 | 0 | 0 |
| 19 | CS | 185 | 1441 | 908 | 290 | 241 | 2 | 0 | 0 | 0 |

- Molecule 20 is a protein called 60S ribosomal protein L19-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 20 | z | 188 | 1521 | 935 | 326 | 260 | 0 | 0 | 0 |
| 20 | CT | 188 | 1521 | 935 | 326 | 260 | 0 | 0 | 0 |

- Molecule 21 is a protein called 60S ribosomal protein L20-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 21 | 0 | 172 | 1445 | 930 | 267 | 244 | 4 | 0 | 0 | 0 |
| 21 | CU | 172 | 1445 | 930 | 267 | 244 | 4 | 0 | 0 | 0 |

- Molecule 22 is a protein called 60S ribosomal protein L21-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 22 | 2 | 159 | 1276 | 805 | 246 | 221 | 4 | 0 | 0 | 0 |
| 22 | CV | 159 | 1276 | 805 | 246 | 221 | 4 | 0 | 0 | 0 |

- Molecule 23 is a protein called 60S ribosomal protein L22-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 23 | 5 | 100 | 796 | 516 | 131 | 149 | 0 | 0 | 0 |
| 23 | CW | 100 | 796 | 516 | 131 | 149 | 0 | 0 | 0 |

- Molecule 24 is a protein called 60S ribosomal protein L23-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 24 | 6 | 136 | 1003 | 628 | 189 | 179 | 7 | 0 | 0 | 0 |
| 24 | CX | 136 | 1003 | 628 | 189 | 179 | 7 | 0 | 0 | 0 |

- Molecule 25 is a protein called 60S ribosomal protein L24-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 25 | 7 | 98 | 699 | 443 | 137 | 118 | 1 | 0 | 0 | 0 |
| 25 | CY | 98 | 699 | 443 | 137 | 118 | 1 | 0 | 0 | 0 |

- Molecule 26 is a protein called 60S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 26 | 8 | 121 | 964 | 620 | 169 | 173 | 2 | 0 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 26 | CZ | 121 | 964 | 620 | 169 | 173 | 2 | 0 | 0 | 0 |

- Molecule 27 is a protein called 60S ribosomal protein L26-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 27 | 9 | 126 | 993 | 625 | 192 | 176 | 0 | 0 | 0 |
| 27 | DA | 126 | 993 | 625 | 192 | 176 | 0 | 0 | 0 |

- Molecule 28 is a protein called 60S ribosomal protein L27-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 28 | AA | 135 | 1092 | 710 | 202 | 180 | 0 | 0 | 0 |
| 28 | DB | 135 | 1092 | 710 | 202 | 180 | 0 | 0 | 0 |

- Molecule 29 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 29 | AB | 148 | 1173 | 749 | 231 | 190 | 3 | 0 | 0 | 0 |
| 29 | DC | 148 | 1173 | 749 | 231 | 190 | 3 | 0 | 0 | 0 |

- Molecule 30 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 30 | AC | 58 | 462 | 289 | 100 | 73 | 0 | 0 | 0 |
| 30 | DD | 58 | 462 | 289 | 100 | 73 | 0 | 0 | 0 |

- Molecule 31 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 31 | AD | 97 | 743 | 479 | 124 | 139 | 1 | 0 | 0 | 0 |
| 31 | DE | 97 | 743 | 479 | 124 | 139 | 1 | 0 | 0 | 0 |

- Molecule 32 is a protein called 60S ribosomal protein L31-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 32 | AE | 109 | 876 | 556 | 167 | 152 | 1 | 0 | 0 | 0 |
| 32 | DF | 109 | 876 | 556 | 167 | 152 | 1 | 0 | 0 | 0 |

- Molecule 33 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 33 | AF | 127 | 1020 | 647 | 205 | 167 | 1 | 0 | 0 | 0 |
| 33 | DG | 127 | 1020 | 647 | 205 | 167 | 1 | 0 | 0 | 0 |

- Molecule 34 is a protein called 60S ribosomal protein L33-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 34 | AG | 106 | 850 | 540 | 165 | 144 | 1 | 0 | 0 | 0 |
| 34 | DH | 106 | 850 | 540 | 165 | 144 | 1 | 0 | 0 | 0 |

- Molecule 35 is a protein called 60S ribosomal protein L34-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 35 | AH | 112 | 880 | 545 | 179 | 152 | 4 | 0 | 0 | 0 |
| 35 | DI | 112 | 880 | 545 | 179 | 152 | 4 | 0 | 0 | 0 |

- Molecule 36 is a protein called 60S ribosomal protein L35-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 36 | AI | 119 | 969 | 615 | 186 | 167 | 1 | 0 | 0 | 0 |
| 36 | DJ | 119 | 969 | 615 | 186 | 167 | 1 | 0 | 0 | 0 |

- Molecule 37 is a protein called 60S ribosomal protein L36-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 37 | AJ | 99 | 771 | 481 | 156 | 132 | 2 | 0 | 0 | 0 |
| 37 | DK | 99 | 771 | 481 | 156 | 132 | 2 | 0 | 0 | 0 |

- Molecule 38 is a protein called 60S ribosomal protein L37-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 38 | AK | 87 | 681 | 414 | 148 | 114 | 5 | 0 | 0 | 0 |
| 38 | DL | 87 | 681 | 414 | 148 | 114 | 5 | 0 | 0 | 0 |

- Molecule 39 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 39 | AL | 77 | 612 | 391 | 115 | 106 | 0 | 0 | 0 |
| 39 | DM | 77 | 612 | 391 | 115 | 106 | 0 | 0 | 0 |

- Molecule 40 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 40 | AM | 50 | 436 | 272 | 97 | 65 | 2 | 0 | 0 | 0 |
| 40 | DN | 50 | 436 | 272 | 97 | 65 | 2 | 0 | 0 | 0 |

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 41 | AN | 52 | 417 | 259 | 86 | 67 | 5 | 0 | 0 | 0 |
| 41 | DO | 52 | 417 | 259 | 86 | 67 | 5 | 0 | 0 | 0 |

- Molecule 42 is a protein called 60S ribosomal protein L41-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 42 | AO | 25 | 233 | 142 | 63 | 27 | 1 | 0 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 42 | DP | 25 | 233 | 142 | 63 | 27 | 1 | 0 | 0 | 0 |

- Molecule 43 is a protein called 60S ribosomal protein L42-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 43 | AP | 105 | 847 | 534 | 170 | 138 | 5 | 0 | 0 | 0 |
| 43 | DQ | 105 | 847 | 534 | 170 | 138 | 5 | 0 | 0 | 0 |

- Molecule 44 is a protein called 60S ribosomal protein L43-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 44 | AQ | 91 | 694 | 429 | 138 | 121 | 6 | 0 | 0 | 0 |
| 44 | DR | 91 | 694 | 429 | 138 | 121 | 6 | 0 | 0 | 0 |

- Molecule 45 is a protein called Suppressor protein STM1.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 45 | i | 159 | 1104 | 654 | 221 | 229 | 0 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| i | 134 | LEU | ASP | conflict | UNP P39015 |

- Molecule 46 is a protein called 60S acidic ribosomal protein P0.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 46 | p0 | 143 | 1077 | 687 | 192 | 195 | 3 | 0 | 0 | 0 |

- Molecule 47 is a protein called Suppressor protein STM1.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 47 | sM | 104 | 681 | 404 | 140 | 137 | 0 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| sM | 59 | ALA | GLY | conflict | UNP P39015 |

- Molecule 48 is a RNA chain called 18S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | | |
| 48 | A | 1781 | 37948 | 16965 | 6715 | 12487 | 1781 | 0 | 0 | 0 |
| 48 | sR | 1783 | 37990 | 16984 | 6723 | 12500 | 1783 | 0 | 0 | 0 |

- Molecule 49 is a protein called 40S ribosomal protein S0-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 49 | B | 206 | 1577 | 1014 | 278 | 283 | 2 | 0 | 0 | 0 |
| 49 | s0 | 206 | 1583 | 1017 | 281 | 283 | 2 | 0 | 0 | 0 |

- Molecule 50 is a protein called 40S ribosomal protein S1-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 50 | C | 214 | 1709 | 1084 | 310 | 311 | 4 | 0 | 0 | 0 |
| 50 | s1 | 216 | 1722 | 1091 | 312 | 315 | 4 | 0 | 0 | 0 |

- Molecule 51 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 51 | D | 217 | 1635 | 1047 | 289 | 297 | 2 | 0 | 0 | 0 |
| 51 | s2 | 217 | 1635 | 1047 | 289 | 297 | 2 | 0 | 0 | 0 |

- Molecule 52 is a protein called 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 52 | E | 223 | 1734 | 1101 | 313 | 314 | 6 | 0 | 0 | 0 |
| 52 | s3 | 223 | 1734 | 1101 | 313 | 314 | 6 | 0 | 0 | 0 |

- Molecule 53 is a protein called 40S ribosomal protein S4-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 53 | F | 260 | 2068 | 1316 | 389 | 360 | 3 | 0 | 0 | 0 |
| 53 | s4 | 260 | 2068 | 1316 | 389 | 360 | 3 | 0 | 0 | 0 |

- Molecule 54 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 54 | G | 206 | 1609 | 1007 | 300 | 299 | 3 | 0 | 0 | 0 |
| 54 | s5 | 206 | 1609 | 1007 | 300 | 299 | 3 | 0 | 0 | 0 |

- Molecule 55 is a protein called 40S ribosomal protein S6-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 55 | H | 226 | 1799 | 1129 | 346 | 321 | 3 | 0 | 0 | 0 |
| 55 | s6 | 218 | 1755 | 1102 | 337 | 313 | 3 | 0 | 0 | 0 |

- Molecule 56 is a protein called 40S ribosomal protein S7-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 56 | I | 184 | 1481 | 951 | 265 | 265 | 0 | 0 | 0 |
| 56 | s7 | 186 | 1491 | 957 | 267 | 267 | 0 | 0 | 0 |

- Molecule 57 is a protein called 40S ribosomal protein S8-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 57 | J | 188 | 1489 | 925 | 298 | 264 | 2 | 0 | 0 | 0 |
| 57 | s8 | 188 | 1489 | 925 | 298 | 264 | 2 | 0 | 0 | 0 |

- Molecule 58 is a protein called 40S ribosomal protein S9-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 58 | K | 185 | 1494 | 943 | 289 | 261 | 1 | 0 | 0 | 0 |
| 58 | s9 | 185 | 1494 | 943 | 289 | 261 | 1 | 0 | 0 | 0 |

- Molecule 59 is a protein called 40S ribosomal protein S10-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 59 | L | 96 | 772 | 499 | 126 | 145 | 2 | 0 | 0 | 0 |
| 59 | c0 | 96 | 760 | 489 | 125 | 144 | 2 | 0 | 0 | 0 |

- Molecule 60 is a protein called 40S ribosomal protein S11-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 60 | M | 155 | 1213 | 774 | 230 | 206 | 3 | 0 | 0 | 0 |
| 60 | c1 | 146 | 1168 | 747 | 221 | 197 | 3 | 0 | 0 | 0 |

- Molecule 61 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 61 | N | 124 | 890 | 560 | 156 | 172 | 2 | 0 | 0 | 0 |
| 61 | c2 | 124 | 890 | 560 | 156 | 172 | 2 | 0 | 0 | 0 |

- Molecule 62 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 62 | O | 150 | 1192 | 759 | 224 | 207 | 2 | 0 | 0 | 0 |
| 62 | c3 | 150 | 1192 | 759 | 224 | 207 | 2 | 0 | 0 | 0 |

- Molecule 63 is a protein called 40S ribosomal protein S14-B.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 63 | P | 127 | 891 | 545 | 182 | 163 | 1 | 0 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 63 | c4 | 128 | 949 | 582 | 188 | 176 | 3 | 0 | 0 | 0 |

- Molecule 64 is a protein called 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 64 | Q | 124 | 977 | 622 | 182 | 166 | 7 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 64 | c5 | 135 | 1039 | 658 | 196 | 178 | 7 | 0 | 0 | 0 |

- Molecule 65 is a protein called 40S ribosomal protein S16-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 65 | R | 141 | 1105 | 708 | 203 | 194 | 0 | 0 | 0 |
| | | | Total | C | N | O | | | |
| 65 | c6 | 142 | 1111 | 711 | 204 | 196 | 0 | 0 | 0 |

- Molecule 66 is a protein called 40S ribosomal protein S17-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 66 | S | 120 | 926 | 577 | 177 | 170 | 2 | 0 | 0 | 0 |

- Molecule 67 is a protein called 40S ribosomal protein S18-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 67 | T | 145 | 1192 | 743 | 237 | 210 | 2 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 67 | c8 | 145 | 1192 | 743 | 237 | 210 | 2 | 0 | 0 | 0 |

- Molecule 68 is a protein called 40S ribosomal protein S19-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 68 | U | 143 | 1112 | 694 | 208 | 208 | 2 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 68 | c9 | 143 | 1112 | 694 | 208 | 208 | 2 | 0 | 0 | 0 |

- Molecule 69 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 69 | V | 107 | 855 | 539 | 156 | 159 | 1 | 0 | 0 | 0 |
| 69 | d0 | 110 | 882 | 554 | 161 | 166 | 1 | 0 | 0 | 0 |

- Molecule 70 is a protein called 40S ribosomal protein S21-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 70 | W | 87 | 684 | 420 | 125 | 137 | 2 | 0 | 0 | 0 |
| 70 | d1 | 87 | 684 | 420 | 125 | 137 | 2 | 0 | 0 | 0 |

- Molecule 71 is a protein called 40S ribosomal protein S22-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 71 | X | 129 | 1021 | 650 | 188 | 180 | 3 | 0 | 0 | 0 |
| 71 | d2 | 129 | 1021 | 650 | 188 | 180 | 3 | 0 | 0 | 0 |

- Molecule 72 is a protein called 40S ribosomal protein S23-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 72 | Y | 144 | 1121 | 708 | 220 | 191 | 2 | 0 | 0 | 0 |
| 72 | d3 | 144 | 1121 | 708 | 220 | 191 | 2 | 0 | 0 | 0 |

- Molecule 73 is a protein called 40S ribosomal protein S24-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 73 | Z | 134 | 1073 | 676 | 208 | 189 | 0 | 0 | 0 |
| 73 | d4 | 134 | 1073 | 676 | 208 | 189 | 0 | 0 | 0 |

- Molecule 74 is a protein called 40S ribosomal protein S25-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 74 | a | 70 | 563 | 360 | 104 | 99 | 0 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 74 | d5 | 69 | 558 | 357 | 103 | 98 | 0 | 0 | 0 |

- Molecule 75 is a protein called 40S ribosomal protein S26-B.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 75 | b | 97 | 769 | 475 | 160 | 129 | 5 | 0 | 0 | 0 |
| 75 | d6 | 97 | 769 | 475 | 160 | 129 | 5 | 0 | 0 | 0 |

- Molecule 76 is a protein called 40S ribosomal protein S27-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 76 | c | 81 | 610 | 382 | 110 | 113 | 5 | 0 | 0 | 0 |
| 76 | d7 | 81 | 610 | 382 | 110 | 113 | 5 | 0 | 0 | 0 |

- Molecule 77 is a protein called 40S ribosomal protein S28-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 77 | d | 63 | 497 | 306 | 99 | 91 | 1 | 0 | 0 | 0 |
| 77 | d8 | 63 | 497 | 306 | 99 | 91 | 1 | 0 | 0 | 0 |

- Molecule 78 is a protein called 40S ribosomal protein S29-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 78 | e | 53 | 442 | 274 | 92 | 72 | 4 | 0 | 0 | 0 |
| 78 | d9 | 53 | 442 | 274 | 92 | 72 | 4 | 0 | 0 | 0 |

- Molecule 79 is a protein called 40S ribosomal protein S30-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 79 | f | 60 | 475 | 299 | 98 | 77 | 1 | 0 | 0 | 0 |
| 79 | e0 | 62 | 491 | 309 | 101 | 80 | 1 | 0 | 0 | 0 |

- Molecule 80 is a protein called Ubiquitin-40S ribosomal protein S31.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 80 | g | 71 | 566 | 362 | 106 | 94 | 4 | 0 | 0 | 0 |

- Molecule 81 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 81 | h | 318 | 2437 | 1541 | 418 | 470 | 8 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 81 | Rb | 318 | 2442 | 1544 | 418 | 472 | 8 | 0 | 0 | 0 |

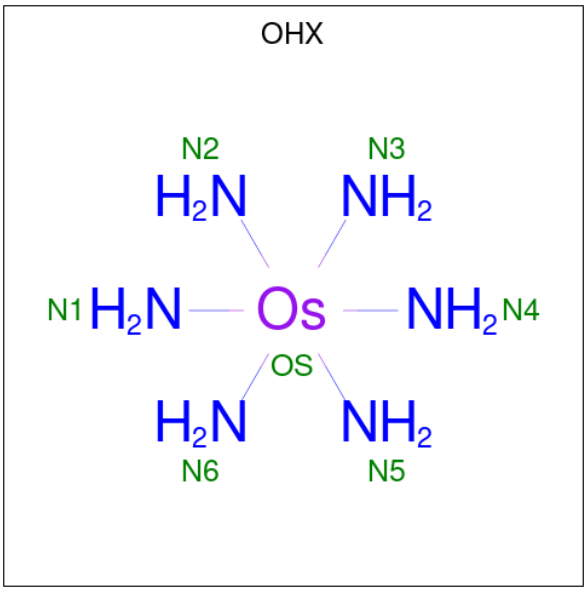
- Molecule 82 is a protein called 40S ribosomal protein S17-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 82 | c7 | 117 | 906 | 563 | 174 | 167 | 2 | 0 | 0 | 0 |

- Molecule 83 is a protein called Ubiquitin-40S ribosomal protein S31.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 83 | e1 | 51 | 397 | 249 | 73 | 71 | 4 | 0 | 0 | 0 |

- Molecule 84 is osmium (III) hexammine (three-letter code: OHX) (formula: $H_{12}N_6Os$).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | N | Os | | |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
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| | | | Total | N | Os | | |
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| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | 1 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | 3 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | 3 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | 3 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | 3 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | 3 | 1 | 7 | 6 | 1 | 0 | 0 |
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| | | | Total | N | Os | | |
| 84 | 3 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | 3 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | 4 | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | k | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | l | 1 | 7 | 6 | 1 | 0 | 0 |
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| | | | Total | N | Os | | |
| 84 | v | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | x | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | x | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | y | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | z | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AC | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AG | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AK | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AK | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AP | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
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| | | | Total | N | Os | | |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
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| | | | Total | N | Os | | |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | AS | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
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| | | | Total | N | Os | | |
| 84 | AS | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | AS | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | AS | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | AS | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | AS | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | AS | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | AS | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | AS | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | AS | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | AS | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | AT | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | AT | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | AT | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | AT | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | AT | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | AT | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | AT | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | AT | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | AT | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | AT | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
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| 84 | AT | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 84 | AT | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 84 | AT | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 84 | AT | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 84 | AT | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 84 | AT | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 84 | CE | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 84 | CE | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 84 | CF | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 84 | CF | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 84 | CG | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 84 | CG | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 84 | CG | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 84 | CK | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 84 | CL | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 84 | CL | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 84 | CM | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 84 | CO | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 84 | CP | 1 | Total N Os<br>7 6 1 | 0 | 0 |
| 84 | CS | 1 | Total Os<br>1 1 | 0 | 0 |
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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
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| | | | Total | N | Os | | |
| 84 | CX | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | CX | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | DD | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | DH | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | DL | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | DQ | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
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| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | N | Os | | |
| 84 | A | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | H | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | J | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | M | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | O | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | Q | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | T | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | e | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | h | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | sR | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | Rb | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | s1 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | s4 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | s8 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | c3 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | c5 | 1 | 7 | 6 | 1 | 0 | 0 |
| | | | Total | N | Os | | |
| 84 | c8 | 1 | 7 | 6 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | N | Os | | |
| 84 | d4 | 1 | 7 | 6 | 1 | 0 | 0 |
| 84 | d9 | 1 | 7 | 6 | 1 | 0 | 0 |

- Molecule 85 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Mg | | |
| 85 | 1 | 485 | 485 | 485 | 0 | 0 |
| 85 | 3 | 12 | 12 | 12 | 0 | 0 |
| 85 | 4 | 19 | 19 | 19 | 0 | 0 |
| 85 | j | 1 | 1 | 1 | 0 | 0 |
| 85 | k | 2 | 2 | 2 | 0 | 0 |
| 85 | l | 5 | 5 | 5 | 0 | 0 |
| 85 | n | 1 | 1 | 1 | 0 | 0 |
| 85 | o | 1 | 1 | 1 | 0 | 0 |
| 85 | r | 2 | 2 | 2 | 0 | 0 |
| 85 | s | 1 | 1 | 1 | 0 | 0 |
| 85 | t | 3 | 3 | 3 | 0 | 0 |
| 85 | u | 1 | 1 | 1 | 0 | 0 |
| 85 | v | 2 | 2 | 2 | 0 | 0 |
| 85 | w | 1 | 1 | 1 | 0 | 0 |
| 85 | x | 5 | 5 | 5 | 0 | 0 |
| 85 | z | 1 | 1 | 1 | 0 | 0 |
| 85 | 6 | 2 | 2 | 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Mg | | |
| 85 | AB | 4 | 4 | 4 | 0 | 0 |
| 85 | AH | 1 | 1 | 1 | 0 | 0 |
| 85 | AK | 1 | 1 | 1 | 0 | 0 |
| 85 | AP | 1 | 1 | 1 | 0 | 0 |
| 85 | AR | 504 | 504 | 504 | 0 | 0 |
| 85 | AS | 17 | 17 | 17 | 0 | 0 |
| 85 | AT | 13 | 13 | 13 | 0 | 0 |
| 85 | CD | 2 | 2 | 2 | 0 | 0 |
| 85 | CE | 2 | 2 | 2 | 0 | 0 |
| 85 | CF | 1 | 1 | 1 | 0 | 0 |
| 85 | CG | 1 | 1 | 1 | 0 | 0 |
| 85 | CJ | 1 | 1 | 1 | 0 | 0 |
| 85 | CM | 2 | 2 | 2 | 0 | 0 |
| 85 | CN | 1 | 1 | 1 | 0 | 0 |
| 85 | CP | 4 | 4 | 4 | 0 | 0 |
| 85 | CQ | 3 | 3 | 3 | 0 | 0 |
| 85 | CR | 6 | 6 | 6 | 0 | 0 |
| 85 | CU | 1 | 1 | 1 | 0 | 0 |
| 85 | CX | 3 | 3 | 3 | 0 | 0 |
| 85 | DA | 1 | 1 | 1 | 0 | 0 |
| 85 | DC | 6 | 6 | 6 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Mg | | |
| 85 | DD | 1 | 1 | 1 | 0 | 0 |
| 85 | DH | 2 | 2 | 2 | 0 | 0 |
| 85 | DO | 1 | 1 | 1 | 0 | 0 |
| 85 | DP | 1 | 1 | 1 | 0 | 0 |
| 85 | DR | 2 | 2 | 2 | 0 | 0 |
| 85 | sM | 1 | 1 | 1 | 0 | 0 |
| 85 | A | 109 | 109 | 109 | 0 | 0 |
| 85 | D | 1 | 1 | 1 | 0 | 0 |
| 85 | J | 1 | 1 | 1 | 0 | 0 |
| 85 | O | 1 | 1 | 1 | 0 | 0 |
| 85 | Y | 1 | 1 | 1 | 0 | 0 |
| 85 | b | 1 | 1 | 1 | 0 | 0 |
| 85 | e | 1 | 1 | 1 | 0 | 0 |
| 85 | sR | 139 | 139 | 139 | 0 | 0 |
| 85 | s1 | 1 | 1 | 1 | 0 | 0 |
| 85 | s8 | 1 | 1 | 1 | 0 | 0 |
| 85 | c1 | 1 | 1 | 1 | 0 | 0 |
| 85 | c6 | 1 | 1 | 1 | 0 | 0 |
| 85 | c7 | 1 | 1 | 1 | 0 | 0 |
| 85 | c8 | 1 | 1 | 1 | 0 | 0 |
| 85 | d3 | 2 | 2 | 2 | 0 | 0 |

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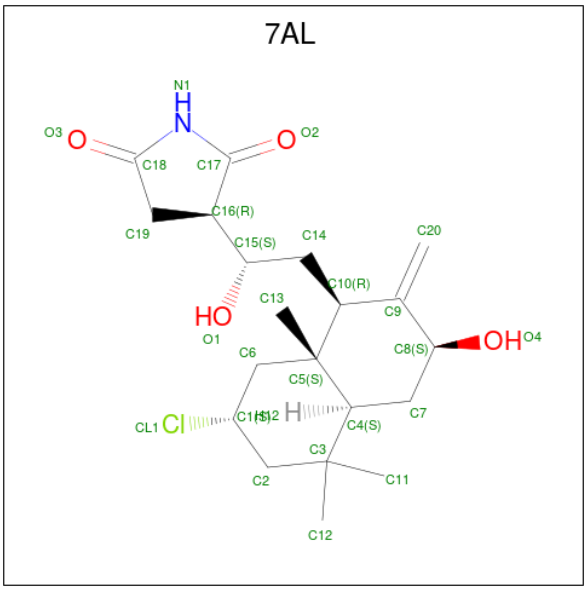
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 85 | d4 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 85 | d5 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 85 | d6 | 2 | Total Mg<br>2 2 | 0 | 0 |
| 85 | d9 | 1 | Total Mg<br>1 1 | 0 | 0 |

- Molecule 86 is Chlorolissoclimide (three-letter code: 7AL) (formula: $C_{20}H_{30}ClNO_4$).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 86 | 1 | 1 | Total C Cl N O<br>26 20 1 1 4 | 0 | 0 |
| 86 | AR | 1 | Total C Cl N O<br>26 20 1 1 4 | 0 | 0 |

- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 87 | AK | 1 | Total Zn<br>1 1 | 0 | 0 |
| 87 | AN | 1 | Total Zn<br>1 1 | 0 | 0 |
| 87 | AP | 1 | Total Zn<br>1 1 | 0 | 0 |

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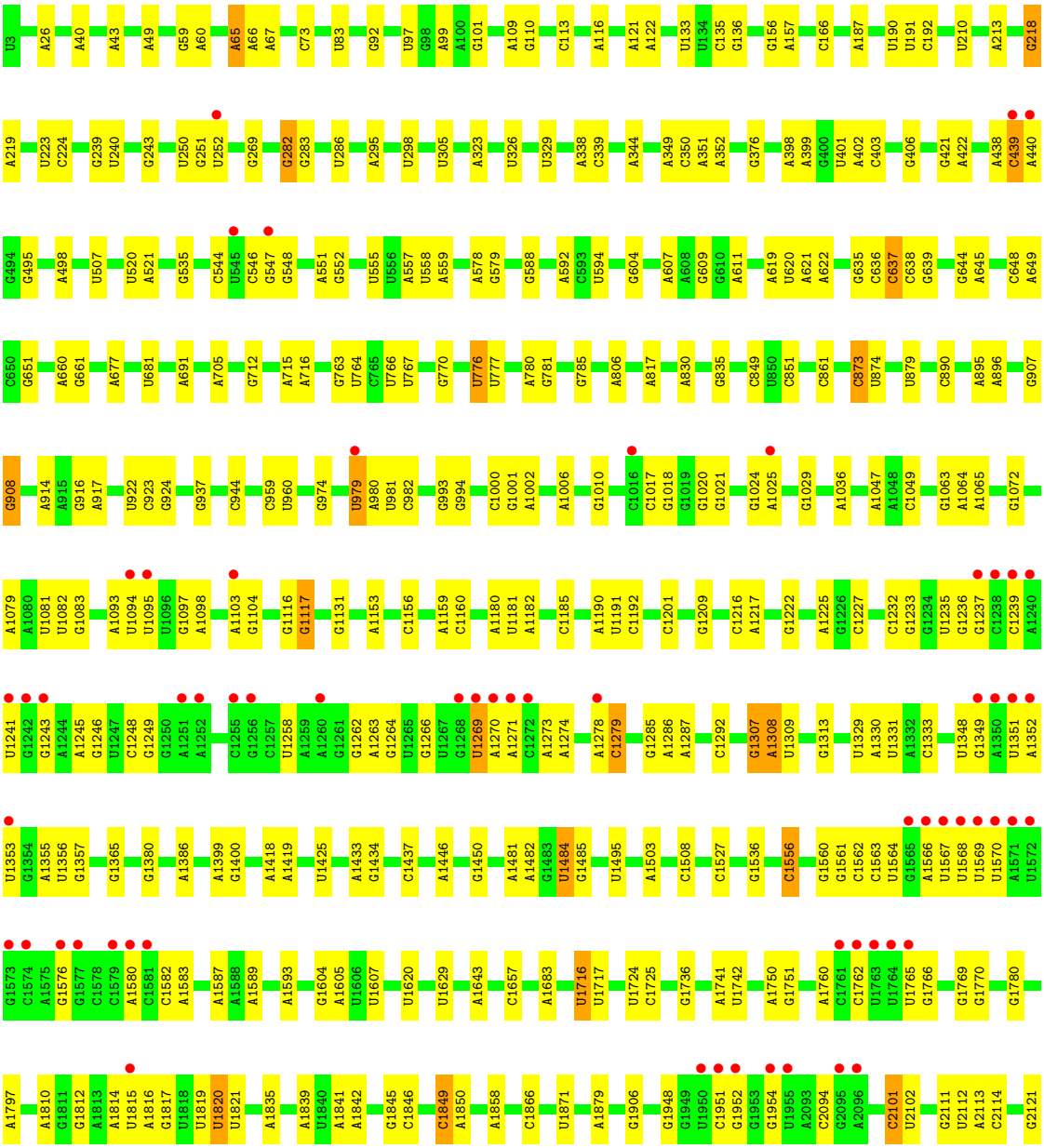
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Zn | | |
| 87 | AQ | 1 | 1 | 1 | 0 | 0 |
| 87 | DL | 1 | 1 | 1 | 0 | 0 |
| 87 | DO | 1 | 1 | 1 | 0 | 0 |
| 87 | DQ | 1 | 1 | 1 | 0 | 0 |
| 87 | DR | 1 | 1 | 1 | 0 | 0 |
| 87 | b | 1 | 1 | 1 | 0 | 0 |
| 87 | c | 1 | 1 | 1 | 0 | 0 |
| 87 | e | 1 | 1 | 1 | 0 | 0 |
| 87 | g | 1 | 1 | 1 | 0 | 0 |
| 87 | d6 | 1 | 1 | 1 | 0 | 0 |
| 87 | d7 | 1 | 1 | 1 | 0 | 0 |
| 87 | d9 | 1 | 1 | 1 | 0 | 0 |
| 87 | e1 | 1 | 1 | 1 | 0 | 0 |

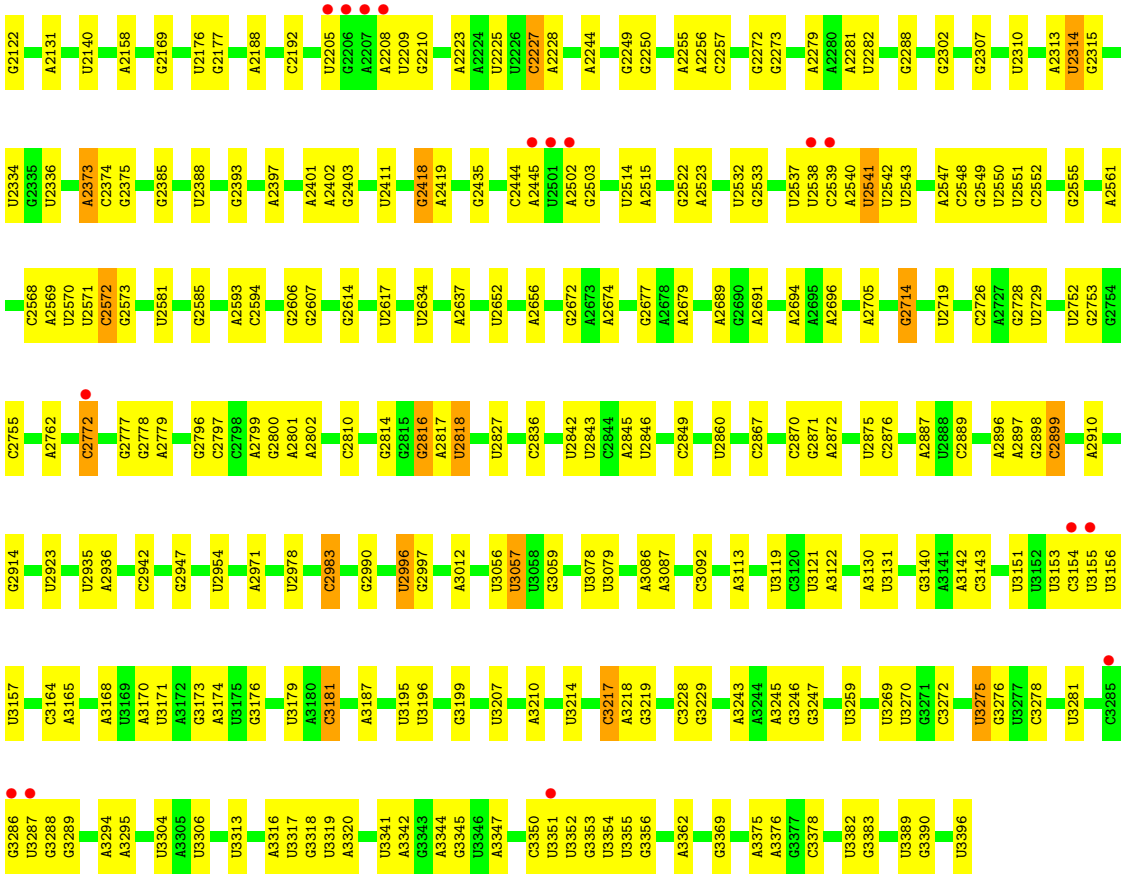
# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 25S ribosomal RNA

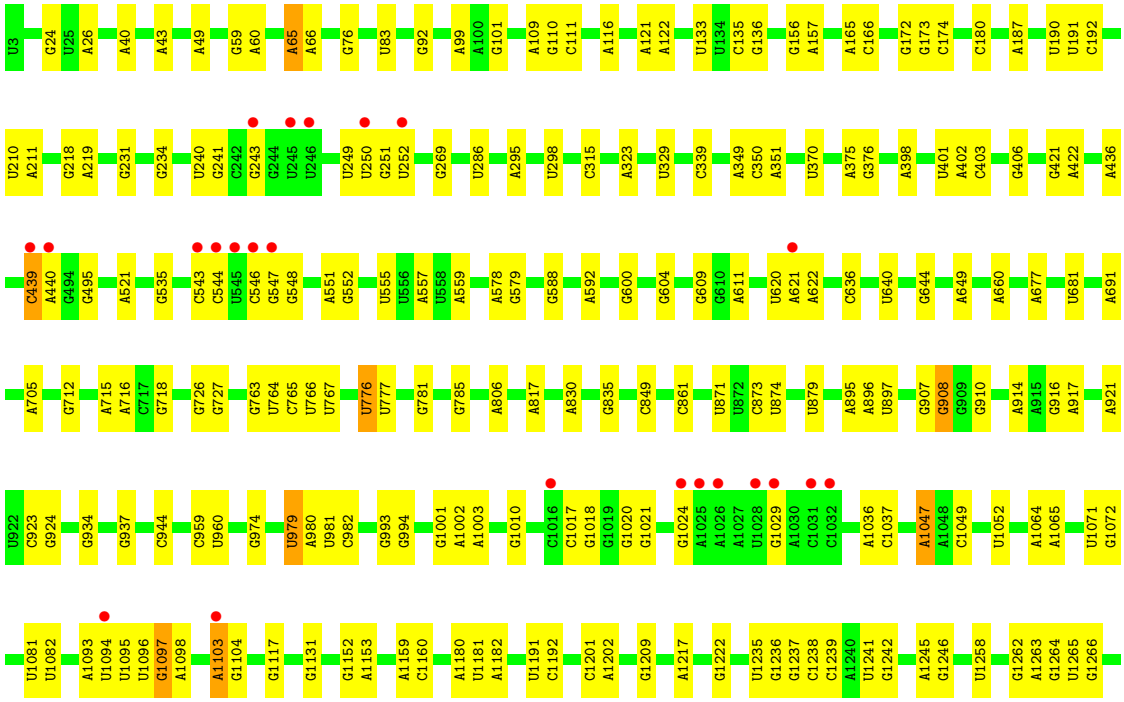
Chain 1:

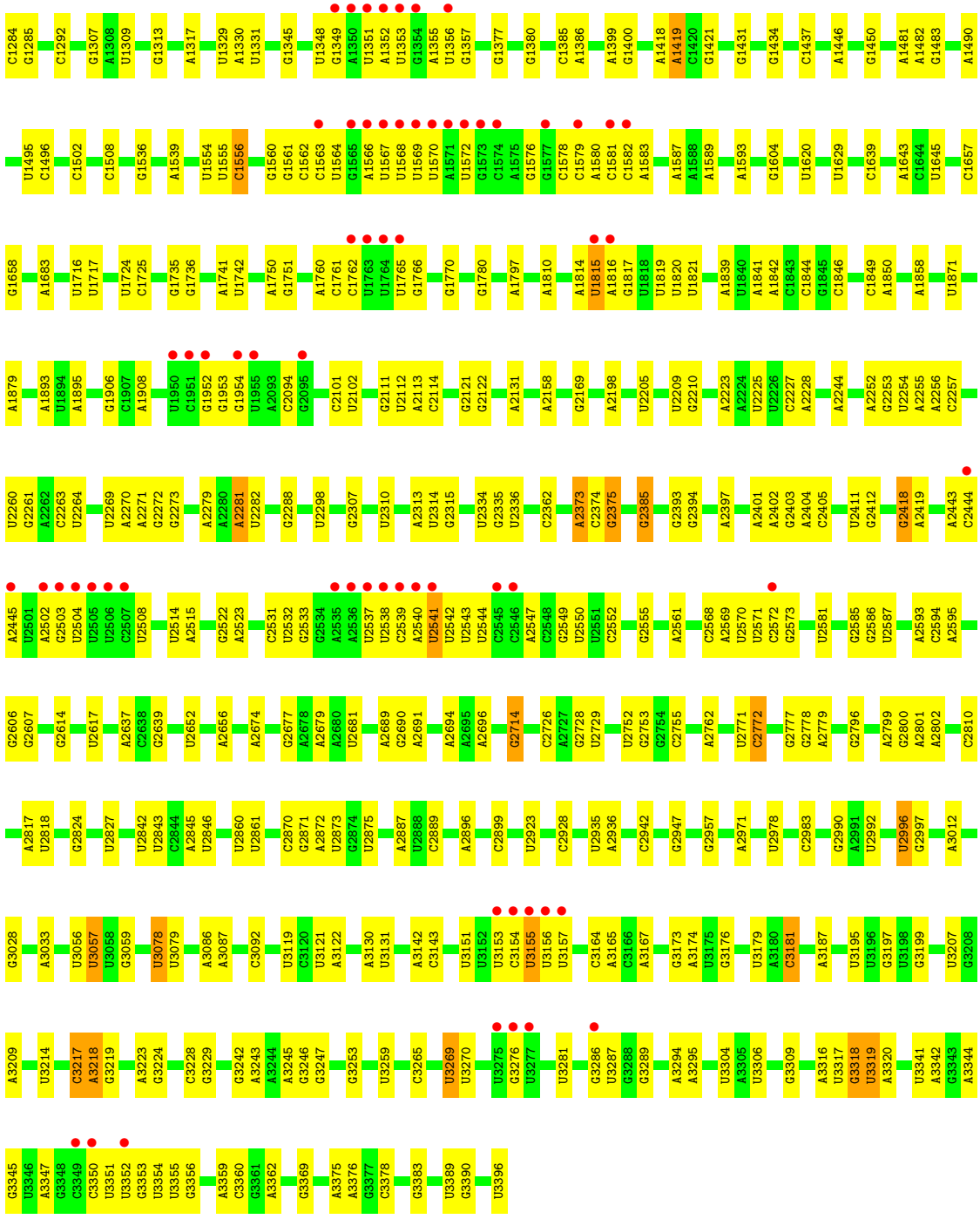





• Molecule 1: 25S ribosomal RNA

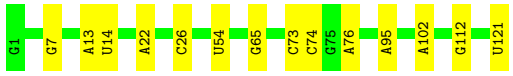
Chain AR:





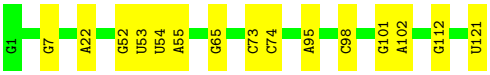

- Molecule 2: 5S ribosomal RNA

Chain 3:



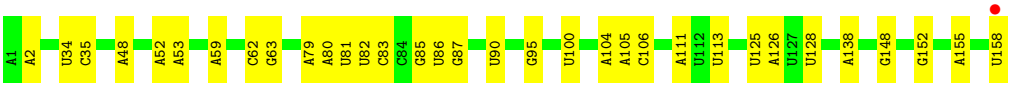

- Molecule 2: 5S ribosomal RNA

Chain AS:



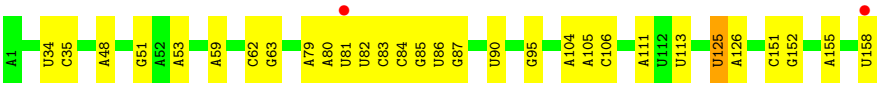

• Molecule 3: 5.8S ribosomal RNA

Chain 4:



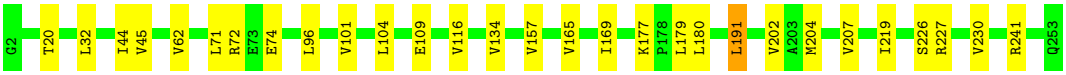

• Molecule 3: 5.8S ribosomal RNA

Chain AT:




• Molecule 4: 60S ribosomal protein L2-A

Chain j:

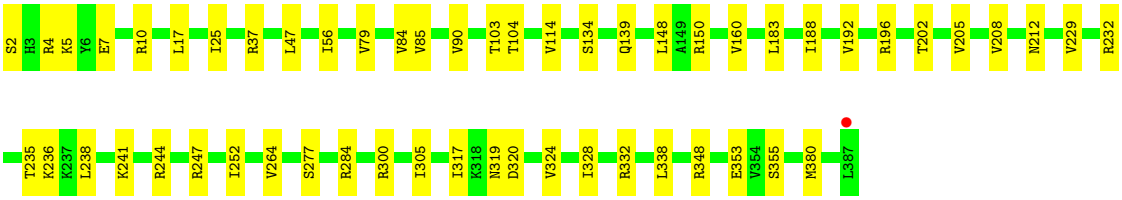



• Molecule 4: 60S ribosomal protein L2-A

Chain CD:

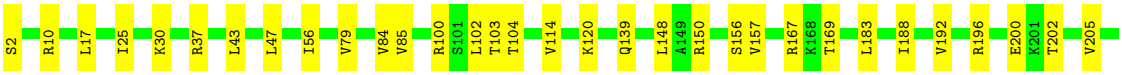
• Molecule 5: 60S ribosomal protein L3

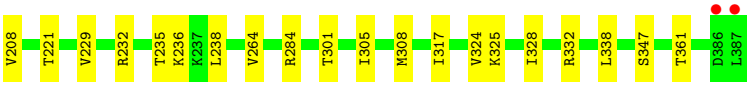
Chain k:




• Molecule 5: 60S ribosomal protein L3

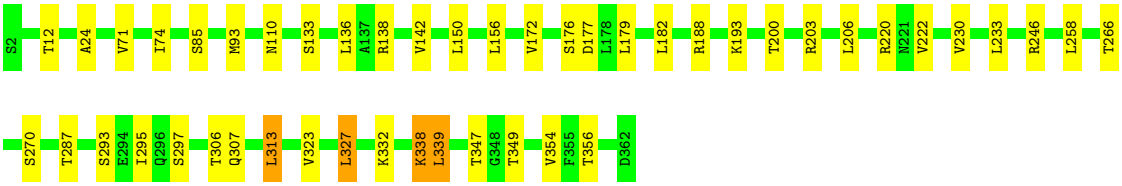
Chain CE:





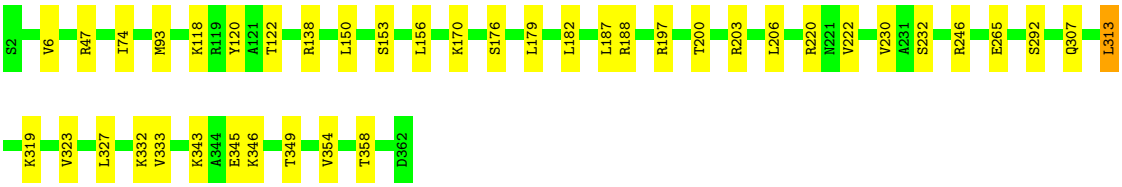

• Molecule 6: 60S ribosomal protein L4-A

Chain l:



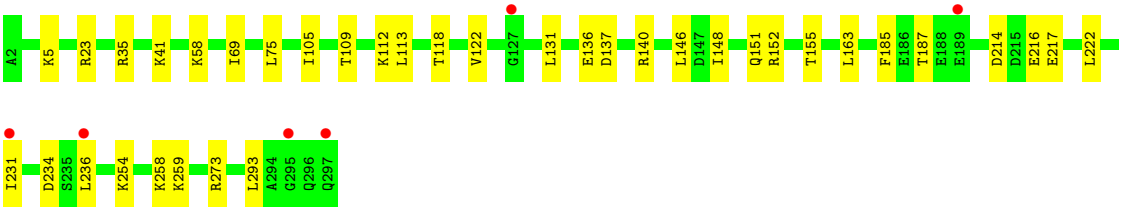

• Molecule 6: 60S ribosomal protein L4-A

Chain CF:



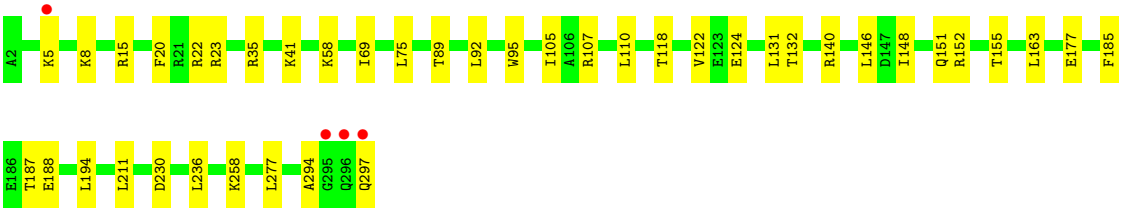

• Molecule 7: 60S ribosomal protein L5

Chain m:




• Molecule 7: 60S ribosomal protein L5

Chain CG:

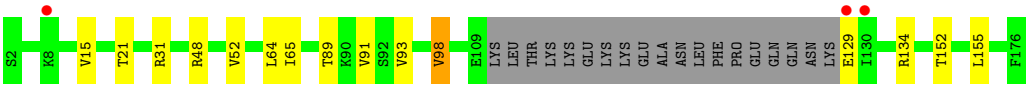



• Molecule 8: 60S ribosomal protein L6-A

Chain n:

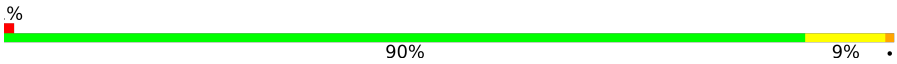
• Molecule 8: 60S ribosomal protein L6-A

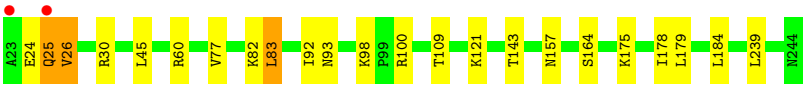
Chain CH:




• Molecule 9: 60S ribosomal protein L7-A

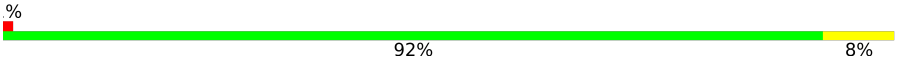
Chain o:



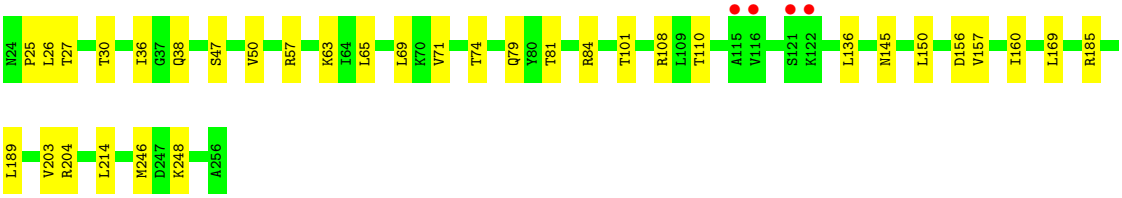

• Molecule 9: 60S ribosomal protein L7-A

Chain CI:



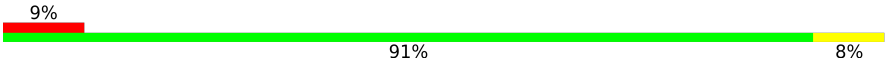
• Molecule 10: 60S ribosomal protein L8-A

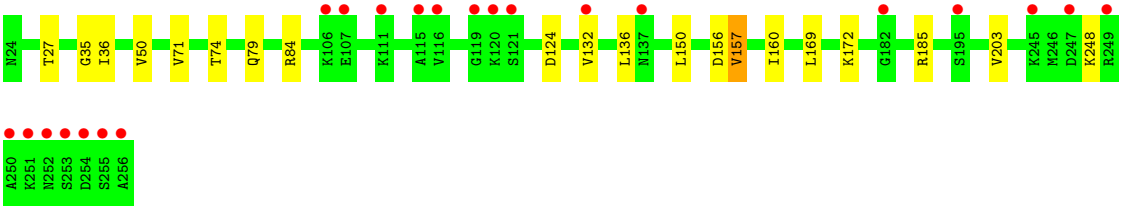
Chain p:




• Molecule 10: 60S ribosomal protein L8-A

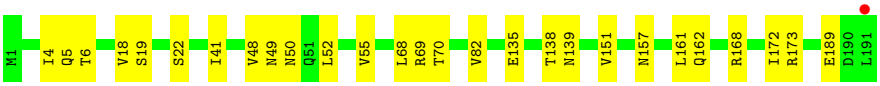
Chain CJ:



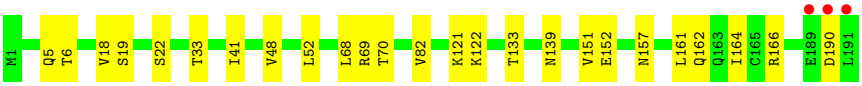

• Molecule 11: 60S ribosomal protein L9-A

Chain q:



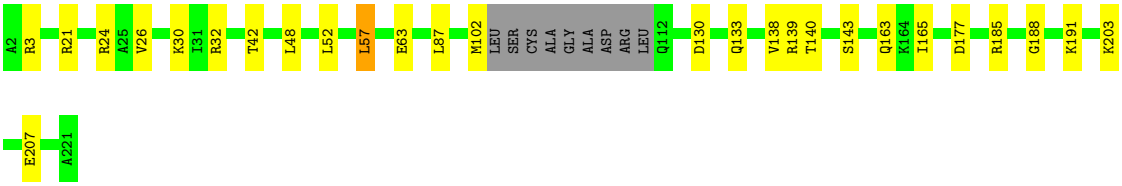

• Molecule 11: 60S ribosomal protein L9-A

Chain CK:



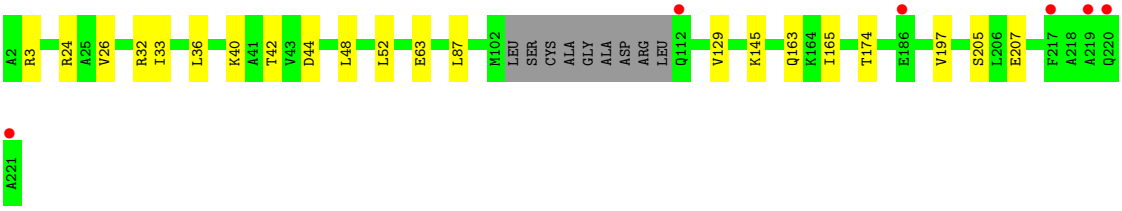

• Molecule 12: 60S ribosomal protein L10

Chain r:



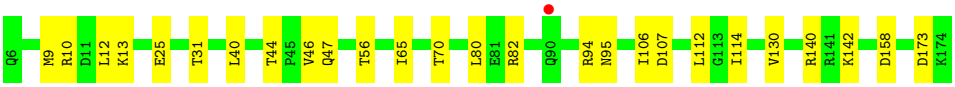

• Molecule 12: 60S ribosomal protein L10

Chain CL:



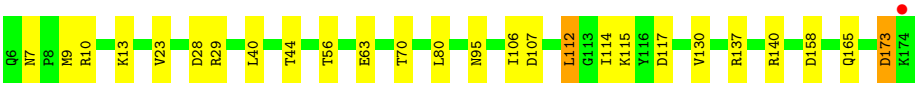

• Molecule 13: 60S ribosomal protein L11-B

Chain s:



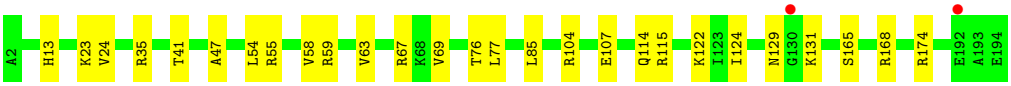

• Molecule 13: 60S ribosomal protein L11-B

Chain CM:



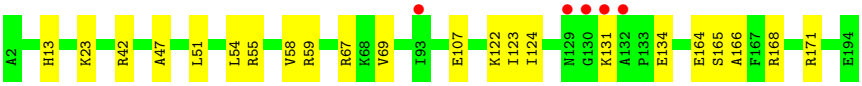

• Molecule 14: 60S ribosomal protein L13-A

Chain t:




• Molecule 14: 60S ribosomal protein L13-A

Chain CN:

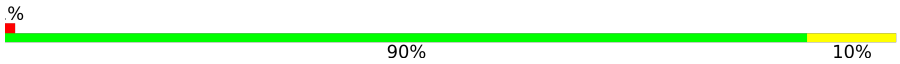


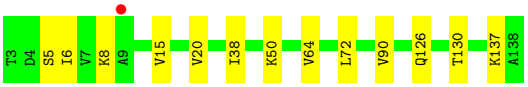

• Molecule 15: 60S ribosomal protein L14-A

Chain u:

• Molecule 15: 60S ribosomal protein L14-A

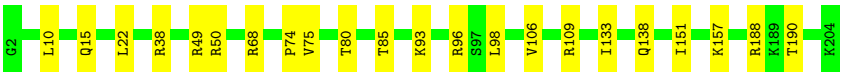
Chain CO:




• Molecule 16: 60S ribosomal protein L15-A

Chain v:

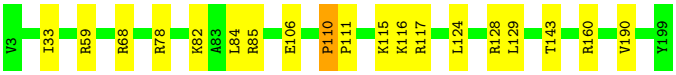



• Molecule 16: 60S ribosomal protein L15-A

Chain CP:

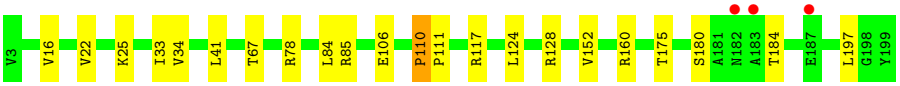
• Molecule 17: 60S ribosomal protein L16-A

Chain w:



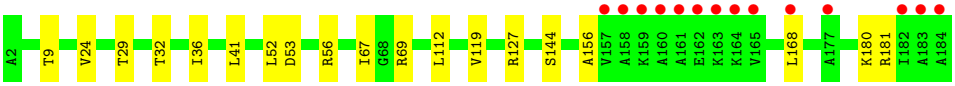

• Molecule 17: 60S ribosomal protein L16-A

Chain CQ:



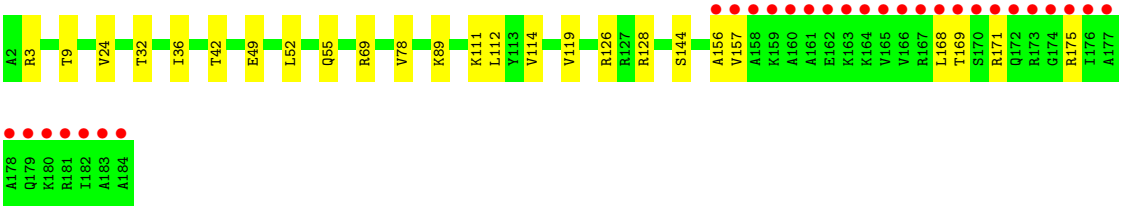

• Molecule 18: 60S ribosomal protein L17-A

Chain x:




• Molecule 18: 60S ribosomal protein L17-A

Chain CR:

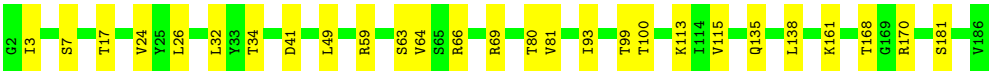



• Molecule 19: 60S ribosomal protein L18-A

Chain y:

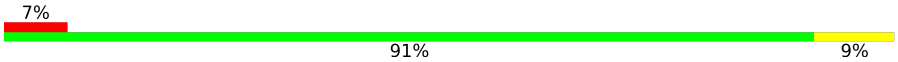
• Molecule 19: 60S ribosomal protein L18-A

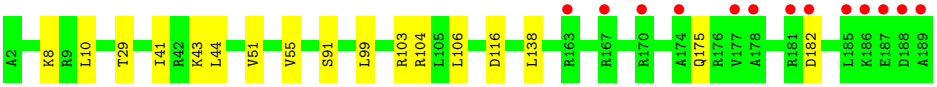
Chain CS:




• Molecule 20: 60S ribosomal protein L19-A

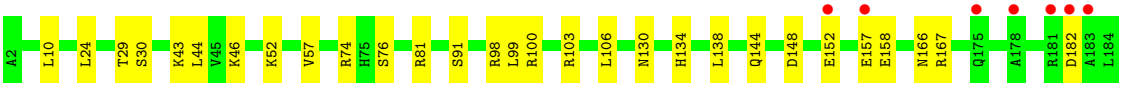
Chain z:




• Molecule 20: 60S ribosomal protein L19-A

Chain CT:

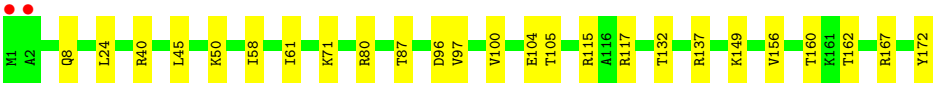


• Molecule 21: 60S ribosomal protein L20-A

Chain 0:

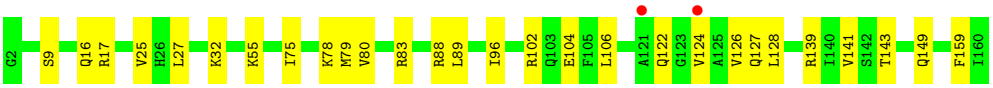
• Molecule 21: 60S ribosomal protein L20-A

Chain CU:




• Molecule 22: 60S ribosomal protein L21-A

Chain 2:




• Molecule 22: 60S ribosomal protein L21-A

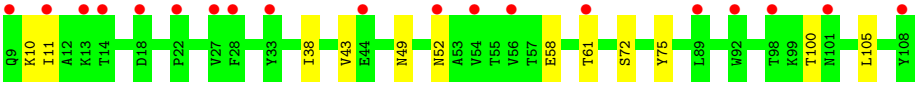
Chain CV:

• Molecule 23: 60S ribosomal protein L22-A

Chain 5:

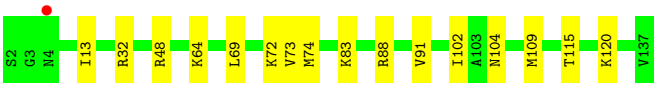
• Molecule 23: 60S ribosomal protein L22-A

Chain CW:

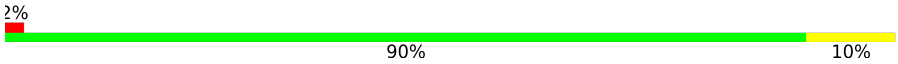



• Molecule 24: 60S ribosomal protein L23-A

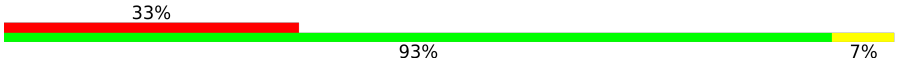
Chain 6:

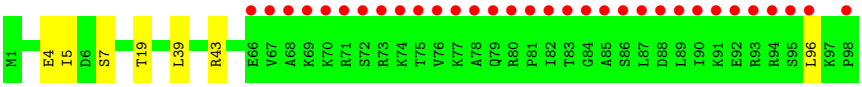




• Molecule 24: 60S ribosomal protein L23-A

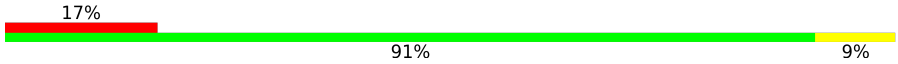
Chain CX: 

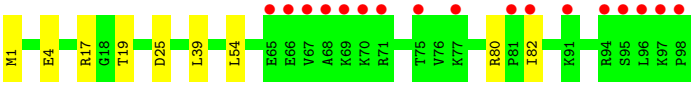
• Molecule 25: 60S ribosomal protein L24-A

Chain 7: 

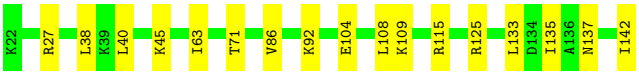

• Molecule 25: 60S ribosomal protein L24-A

Chain CY: 

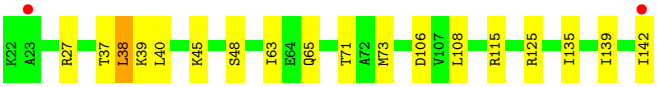

• Molecule 26: 60S ribosomal protein L25

Chain 8:

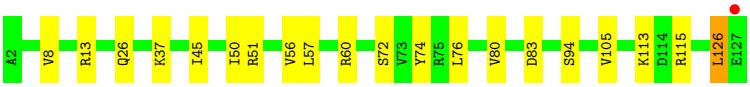

• Molecule 26: 60S ribosomal protein L25

Chain CZ:


• Molecule 27: 60S ribosomal protein L26-A

Chain 9:

• Molecule 27: 60S ribosomal protein L26-A

Chain DA: 2% 87% 13%

A2 V8 R13 K17 K37 I45 I50 V56 L57 V58 V59 S71 Y74 R75 L76 D83 V105 D112 K125 L126 E127

• Molecule 28: 60S ribosomal protein L27-A

Chain AA: 4% 87% 13%

A2 K3 F4 L5 V24 D30 I46 K52 T66 V75 L81 P82 T83 T86 V89 F92 V95 F101 E102 Q103 R107 E108 E109 L134 R135 F136

• Molecule 28: 60S ribosomal protein L27-A

Chain DB: 7% 90% 10%

A2 K3 F4 L5 K6 A7 V14 K21 V24 I25 V26 D30 K56 V75 L81 P82 T83 T86 F92 E99 E102 Q103 E120 L134 R135 F136

• Molecule 29: 60S ribosomal protein L28

Chain AB: 85% 14%

P2 S3 R4 F5 T6 K7 T8 R9 K10 R32 R42 D46 V56 Y60 D76 K77 L78 W79 T80 D88 L91 K92 T98 K115 N120 V130 S131 K132 L133 A149

• Molecule 29: 60S ribosomal protein L28

Chain DC: 87% 13%

P2 S3 R4 F5 T6 K7 T8 R9 K10 H25 R26 R42 K47 Y48 V56 Y60 L78 D85 L91 T98 K115 L133 A149

• Molecule 30: 60S ribosomal protein L29

Chain AC: 86% 14%

A2 N19 G20 K23 P24 K25 K28 S31 T50 K59

• Molecule 30: 60S ribosomal protein L29

Chain DD: 2% 86% 14%

A2 N19 G20 I21 K22 K23 T26 S31 T50 K58 K59

• Molecule 31: 60S ribosomal protein L30

Chain AD: 3% 88% 12%

S9 Q12 L16 V17 I18 L34 K40 L41 S54 M61 N74 M75 E76 K83 V87 I100 L104 A105

• Molecule 31: 60S ribosomal protein L30

Chain DE: 5% 93% 7%

S9 Q12 K22 L34 L41 Y59 A60 M61 V67 K83 V87 I100 L101 T102 A105

• Molecule 32: 60S ribosomal protein L31-A

Chain AE: 3% 85% 15%

L4 K5 D6 V7 V8 T13 L16 K26 R31 D47 V64 E68 R79 E82 E83 D84 T106 E110 E111 D112

• Molecule 32: 60S ribosomal protein L31-A

Chain DF: 5% 82% 17%

L4 V7 V8 T13 L16 H17 K18 K26 K27 R28 R31 T46 V64 R79 E82 E83 K86 S91 V98 L104 Q105 T106 E110 E111 D112

• Molecule 33: 60S ribosomal protein L32

Chain AF: 2% 88% 12%

A2 R19 N31 W32 R33 K34 Q35 S51 K54 K61 K62 T73 F74 L75 H88 V106 R111 R125 L126 A127 L128

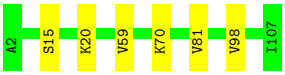
• Molecule 33: 60S ribosomal protein L32

Chain DG: 2% 91% 9%

A2 K8 R19 R33 K34 V41 T73 F74 L75 L82 L109 A110 R111 R125 L126 A127 L128

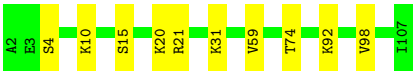
• Molecule 34: 60S ribosomal protein L33-A

Chain AG: 94% 6%




• Molecule 34: 60S ribosomal protein L33-A

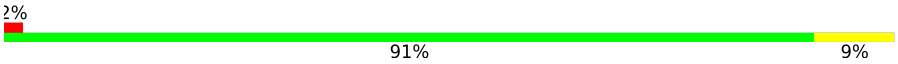
Chain DH:

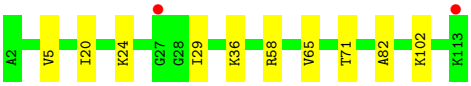




• Molecule 35: 60S ribosomal protein L34-A

Chain AH:


• Molecule 35: 60S ribosomal protein L34-A

Chain DI: 


• Molecule 36: 60S ribosomal protein L35-A

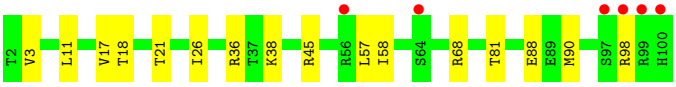
Chain AI:


• Molecule 36: 60S ribosomal protein L35-A

Chain DJ:

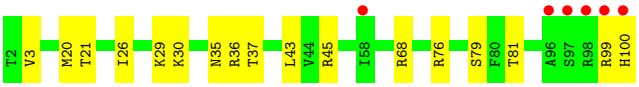

• Molecule 37: 60S ribosomal protein L36-A

Chain AJ:

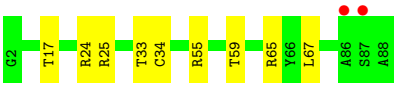

• Molecule 37: 60S ribosomal protein L36-A

Chain DK: 6% 83% 17%




• Molecule 38: 60S ribosomal protein L37-A

Chain AK: 2% 90% 10%

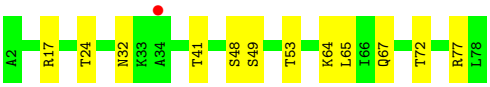



• Molecule 38: 60S ribosomal protein L37-A

Chain DL: 2% 87% 13%

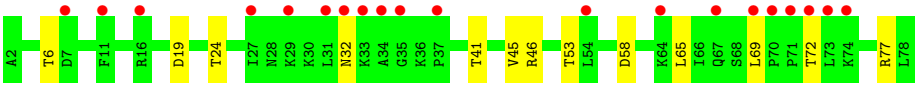
• Molecule 39: 60S ribosomal protein L38

Chain AL: % 84% 16%



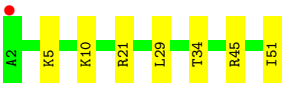

• Molecule 39: 60S ribosomal protein L38

Chain DM: 26% 83% 17%




• Molecule 40: 60S ribosomal protein L39

Chain AM: 2% 86% 14%




• Molecule 40: 60S ribosomal protein L39

Chain DN: 90% 10%

• Molecule 41: Ubiquitin-60S ribosomal protein L40

Chain AN: 2% 83% 17%

I77 I78 L85 D92 K93 S94 K112 R113 K114 K126 L127 K128

• Molecule 41: Ubiquitin-60S ribosomal protein L40

Chain DO: 87% 13%

I77 L85 S94 K112 R113 K114 L127 K128

• Molecule 42: 60S ribosomal protein L41-A

Chain AO: 84% 16%

M1 W5 R9 T10 R11 R21 K25

• Molecule 42: 60S ribosomal protein L41-A

Chain DP: 84% 16%

M1 R6 R9 L13 K14 R15 K25

• Molecule 43: 60S ribosomal protein L42-A

Chain AP: 2% 90% 10%

V2 M3 V4 K13 L35 Q47 K60 K78 L83 T84 L85 L93 Q99 L104 Q105 F106

• Molecule 43: 60S ribosomal protein L42-A

Chain DQ: % 84% 16%

V2 K6 T7 R8 Q22 L35 R45 S48 K60 K61 K78 T79 L83 T84 L93 K100 L104 Q105 F106

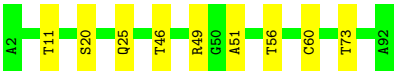
• Molecule 44: 60S ribosomal protein L43-A

Chain AQ: 85% 15%

A2 K7 T11 V16 R24 K45 T46 R49 G50 T56 C60 T78 T82 I83 R84 E91 A92

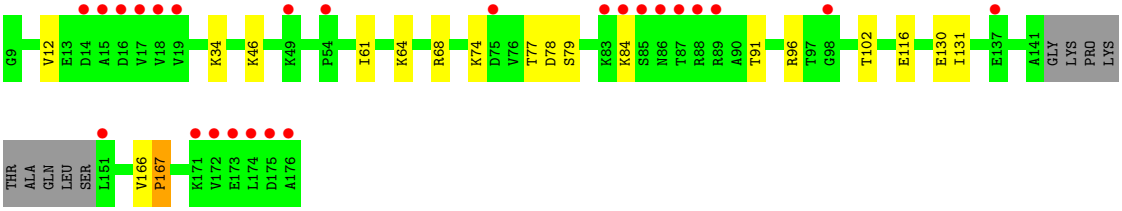
- Molecule 44: 60S ribosomal protein L43-A

Chain DR:



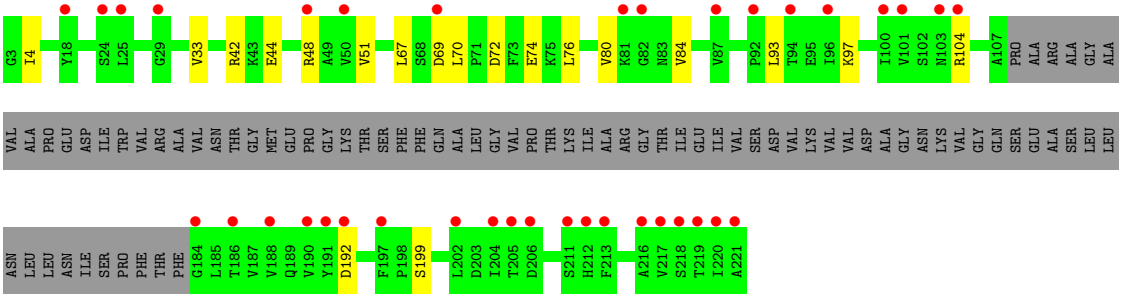

- Molecule 45: Suppressor protein STM1

Chain i:



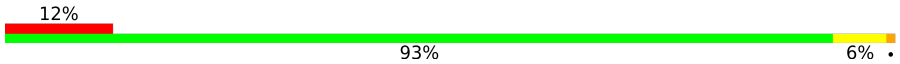

- Molecule 46: 60S acidic ribosomal protein P0

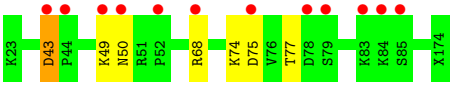
Chain p0:




- Molecule 47: Suppressor protein STM1

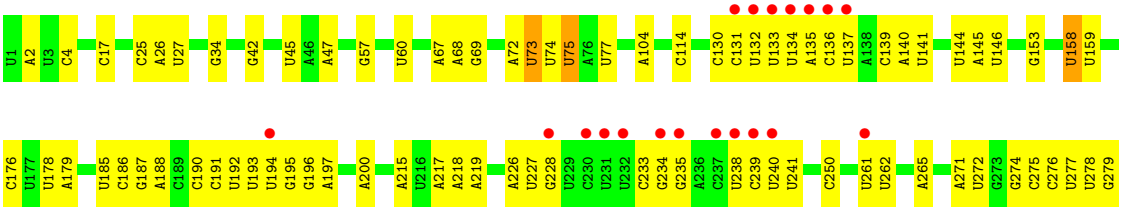
Chain sM:

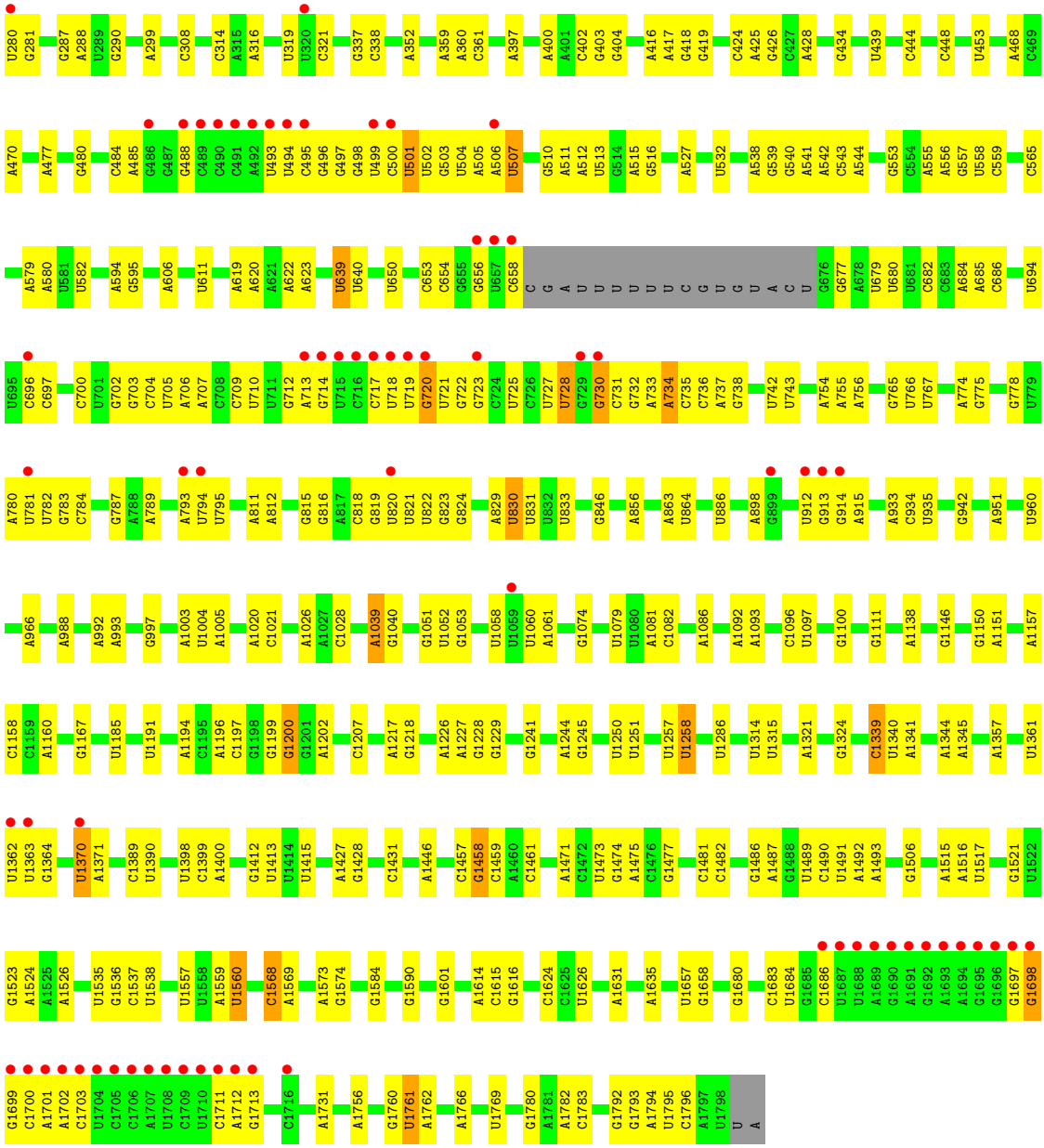



- Molecule 48: 18S ribosomal RNA

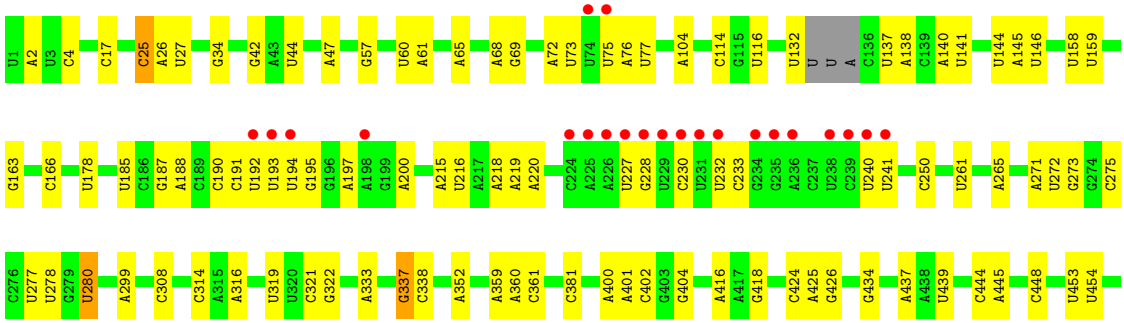
Chain A:

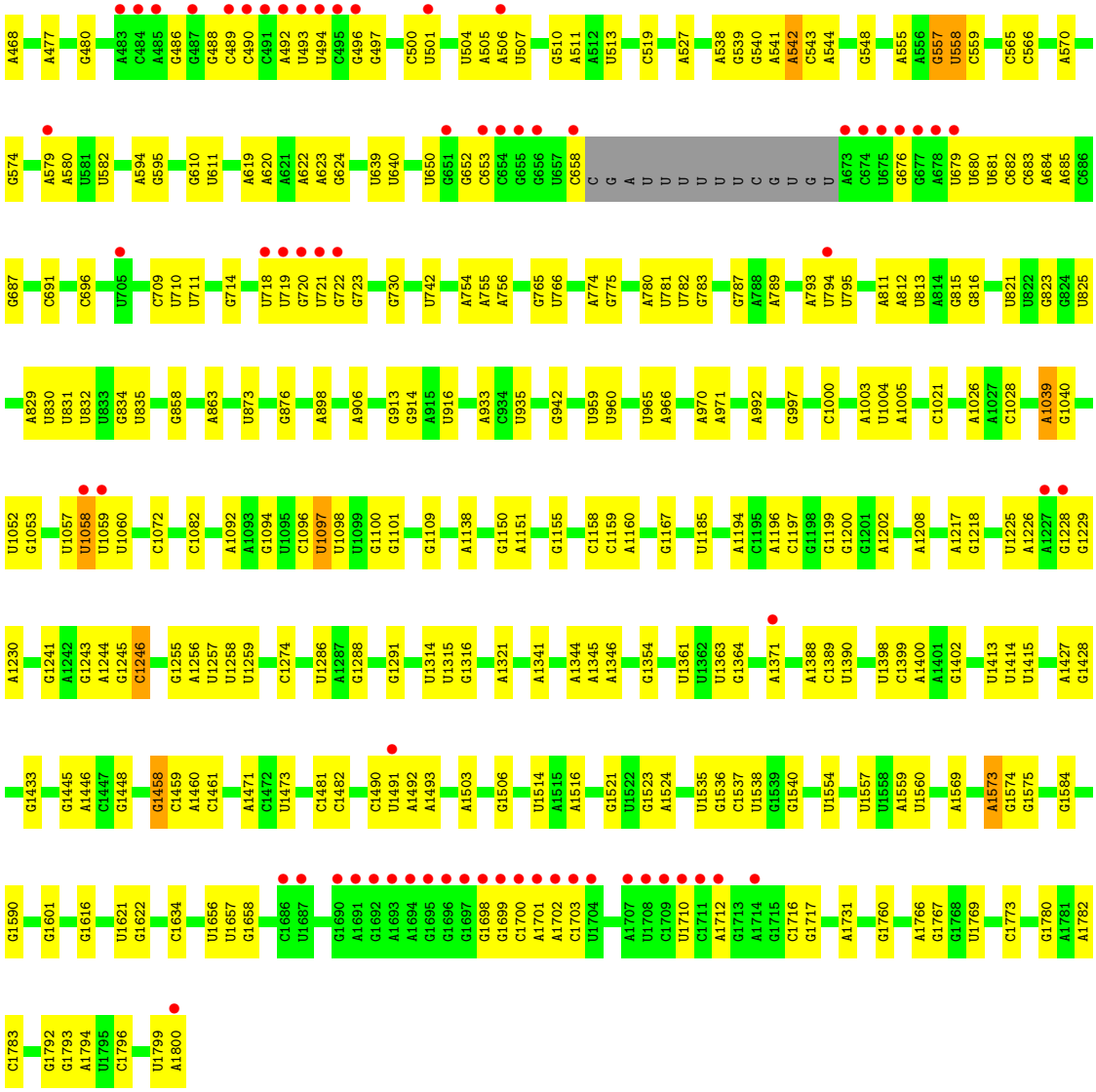




• Molecule 48: 18S ribosomal RNA

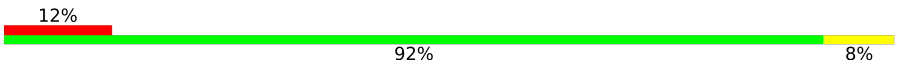
Chain sR:

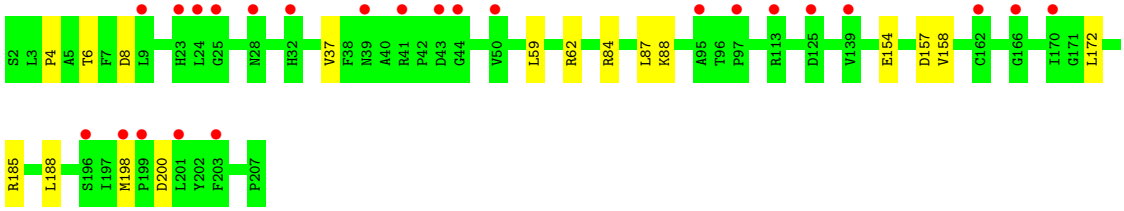





- Molecule 49: 40S ribosomal protein S0-A

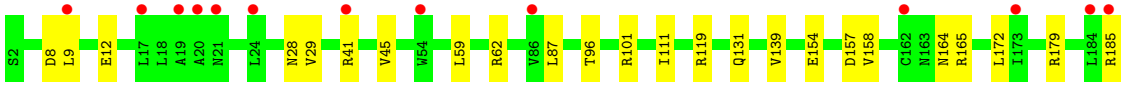
Chain B:

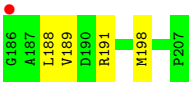



- Molecule 49: 40S ribosomal protein S0-A

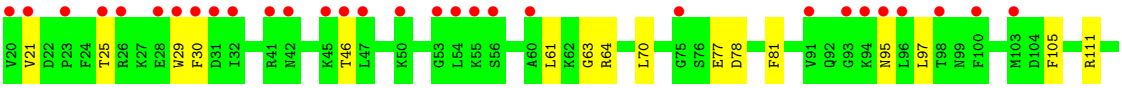
Chain s0:

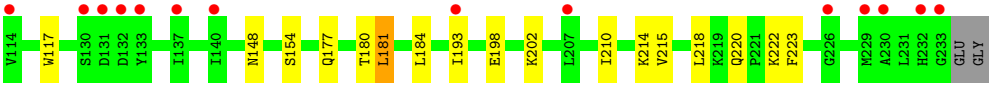





• Molecule 50: 40S ribosomal protein S1-A

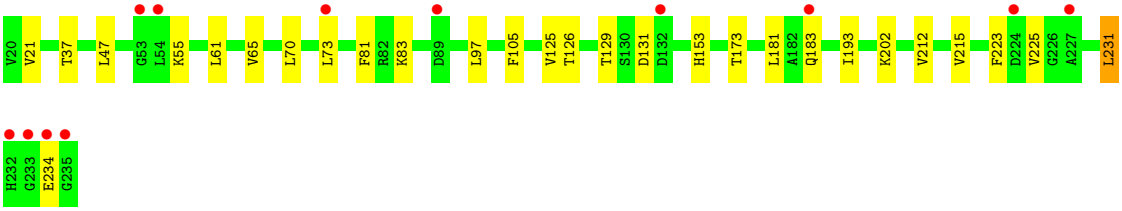
Chain C:




• Molecule 50: 40S ribosomal protein S1-A

Chain s1:

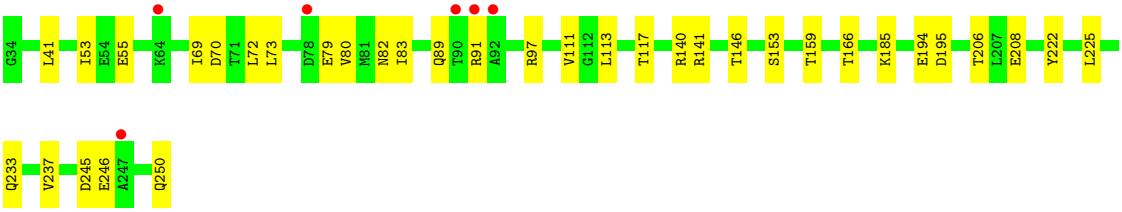



• Molecule 51: 40S ribosomal protein S2

Chain D:

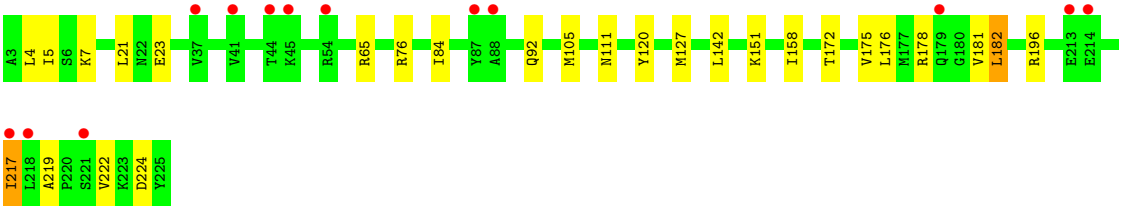
• Molecule 51: 40S ribosomal protein S2

Chain s2:



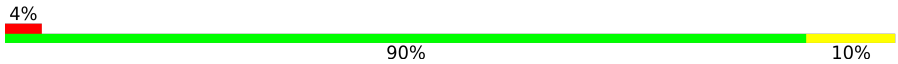

• Molecule 52: 40S ribosomal protein S3

Chain E:



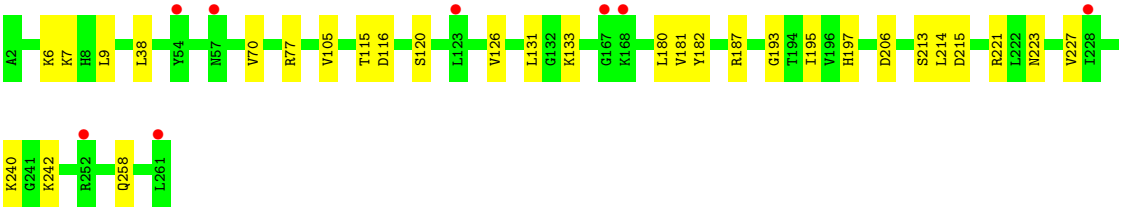

• Molecule 52: 40S ribosomal protein S3

Chain s3:



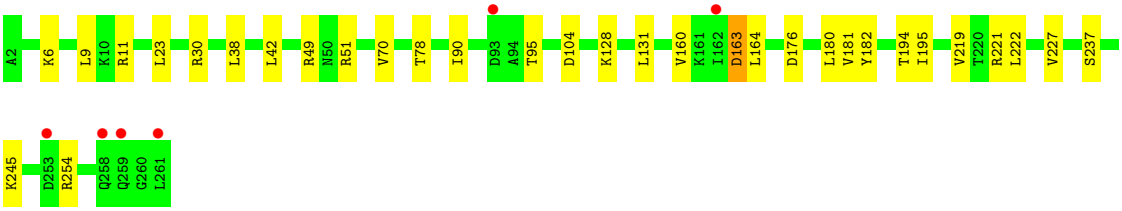
• Molecule 53: 40S ribosomal protein S4-A

Chain F:



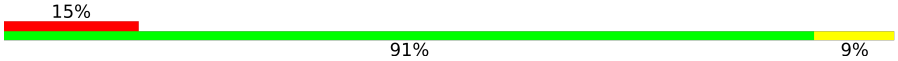

• Molecule 53: 40S ribosomal protein S4-A

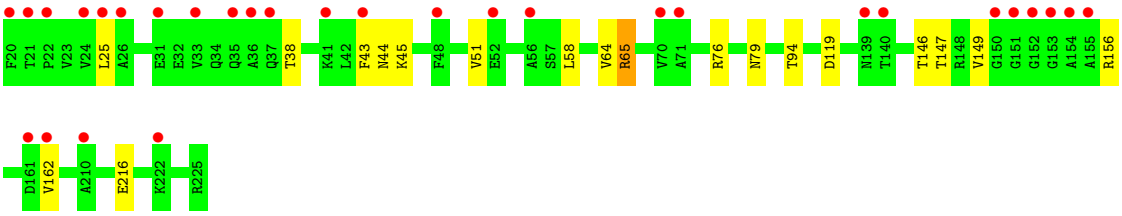
Chain s4:




• Molecule 54: 40S ribosomal protein S5

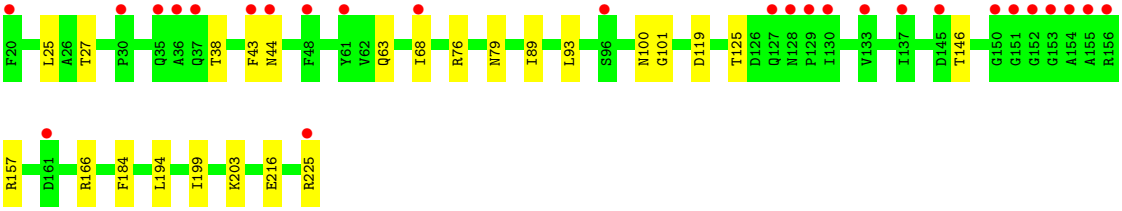
Chain G:



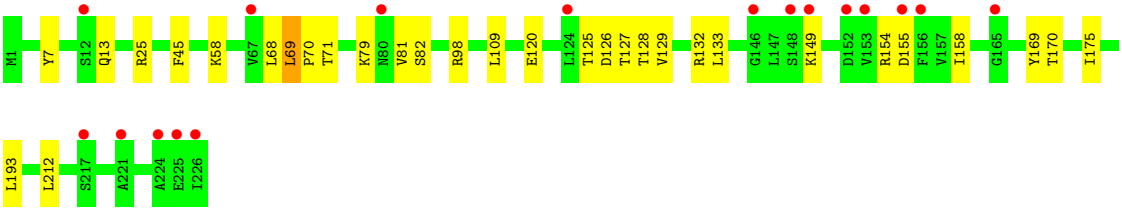

• Molecule 54: 40S ribosomal protein S5

Chain s5:



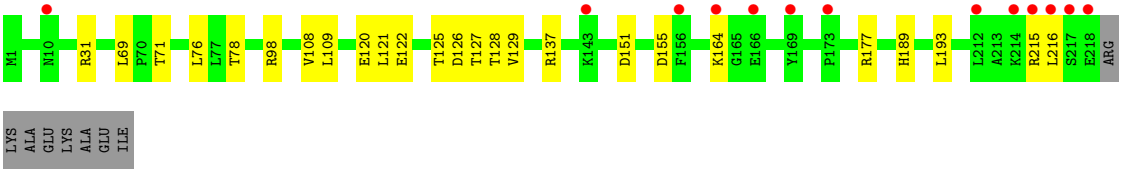

• Molecule 55: 40S ribosomal protein S6-A

Chain H:



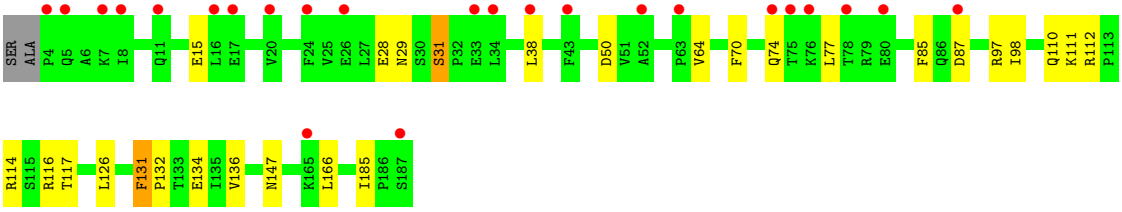

• Molecule 55: 40S ribosomal protein S6-A

Chain s6:



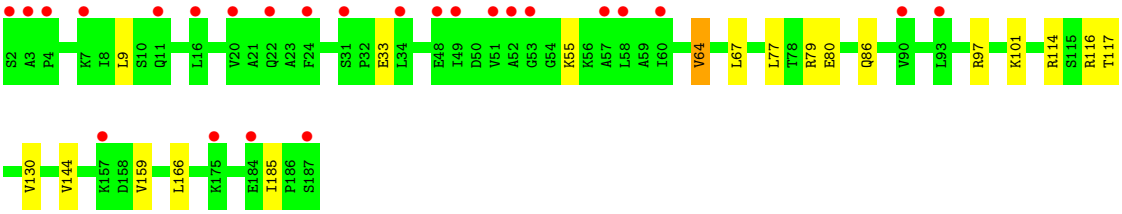

• Molecule 56: 40S ribosomal protein S7-A

Chain I:



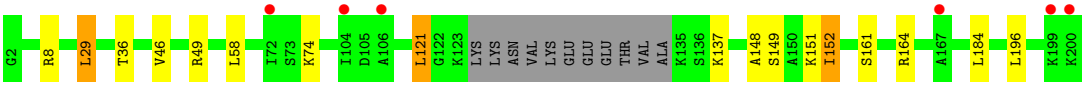

• Molecule 56: 40S ribosomal protein S7-A

Chain s7:



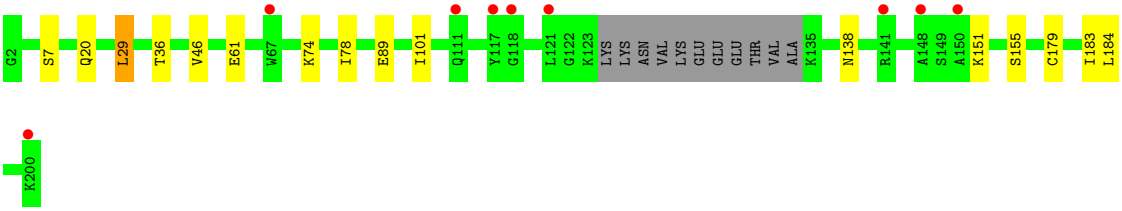
• Molecule 57: 40S ribosomal protein S8-A

Chain J:



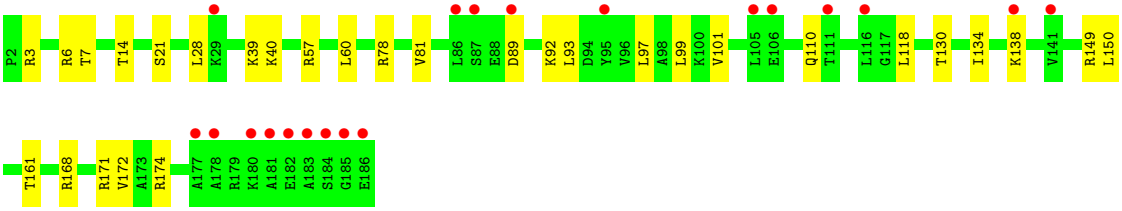

• Molecule 57: 40S ribosomal protein S8-A

Chain s8:



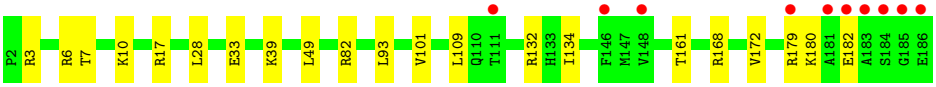

• Molecule 58: 40S ribosomal protein S9-A

Chain K:



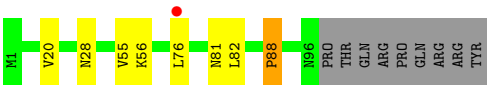

• Molecule 58: 40S ribosomal protein S9-A

Chain s9:



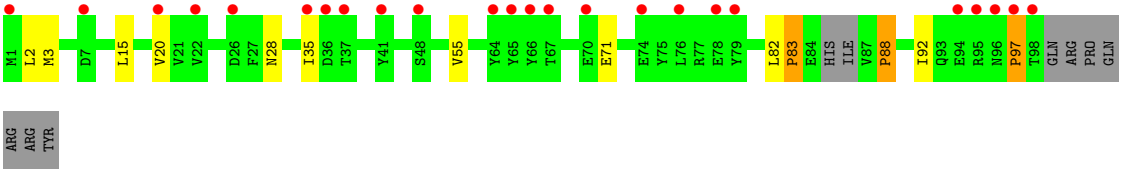

• Molecule 59: 40S ribosomal protein S10-A

Chain L:



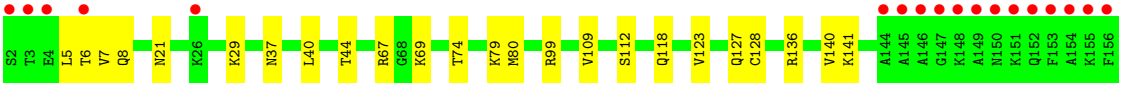

• Molecule 59: 40S ribosomal protein S10-A

Chain c0:




• Molecule 60: 40S ribosomal protein S11-A

Chain M:

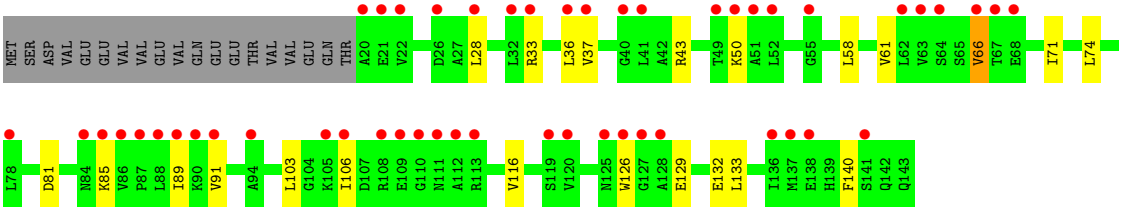



• Molecule 60: 40S ribosomal protein S11-A

Chain c1:

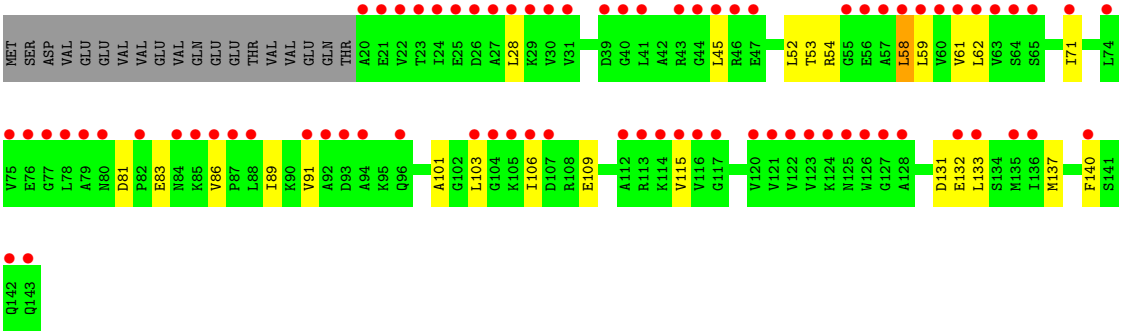
• Molecule 61: 40S ribosomal protein S12

Chain N:



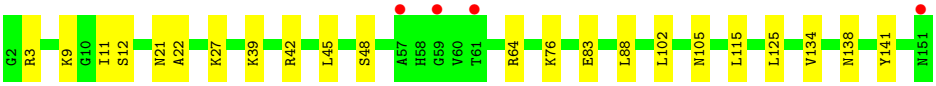

• Molecule 61: 40S ribosomal protein S12

Chain c2:



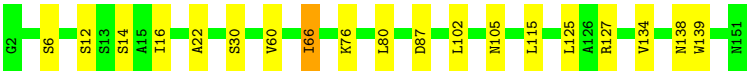

• Molecule 62: 40S ribosomal protein S13

Chain O:



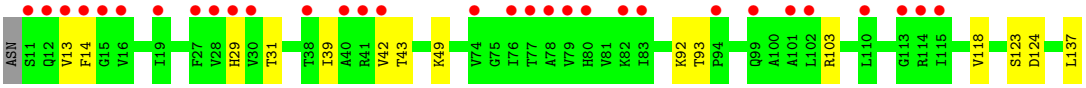

• Molecule 62: 40S ribosomal protein S13

Chain c3:



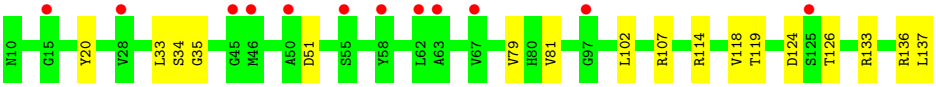

• Molecule 63: 40S ribosomal protein S14-B

Chain P:



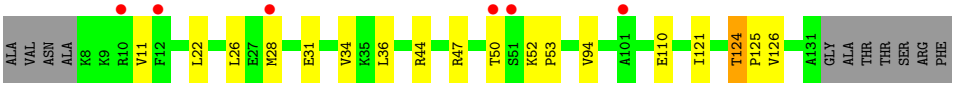

• Molecule 63: 40S ribosomal protein S14-B

Chain c4:




• Molecule 64: 40S ribosomal protein S15

Chain Q:

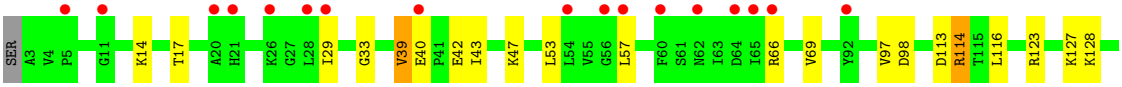



• Molecule 64: 40S ribosomal protein S15

Chain c5:

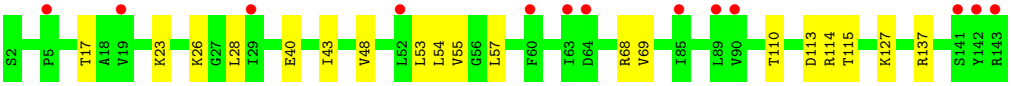
• Molecule 65: 40S ribosomal protein S16-A

Chain R:



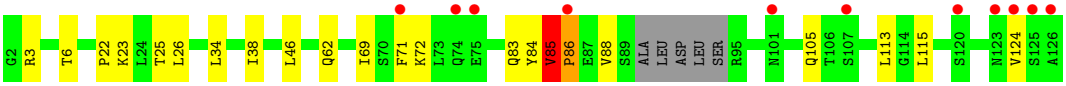
• Molecule 65: 40S ribosomal protein S16-A

Chain c6:



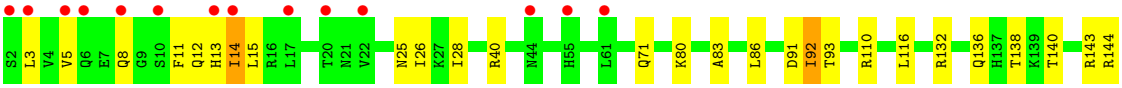

• Molecule 66: 40S ribosomal protein S17-A

Chain S:



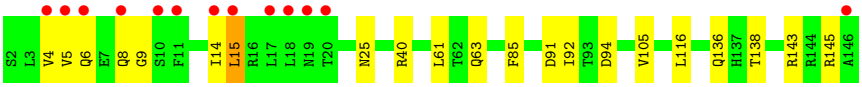

• Molecule 67: 40S ribosomal protein S18-A

Chain T:



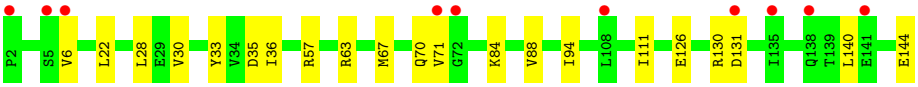
• Molecule 67: 40S ribosomal protein S18-A

Chain c8:



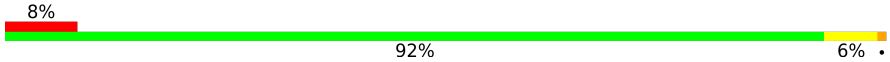

• Molecule 68: 40S ribosomal protein S19-A

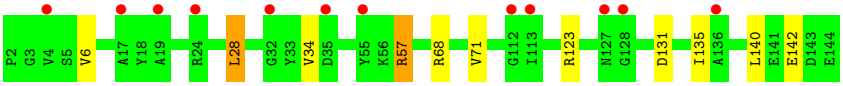
Chain U:




• Molecule 68: 40S ribosomal protein S19-A

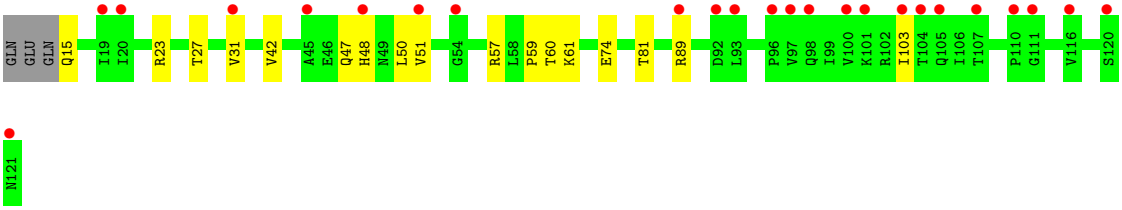
Chain c9:






• Molecule 69: 40S ribosomal protein S20

Chain V:




• Molecule 69: 40S ribosomal protein S20

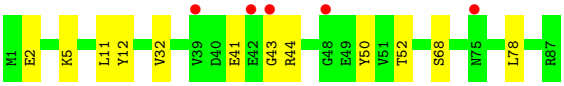
Chain d0:

• Molecule 70: 40S ribosomal protein S21-A

Chain W:

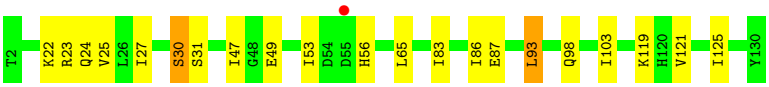
• Molecule 70: 40S ribosomal protein S21-A

Chain d1:



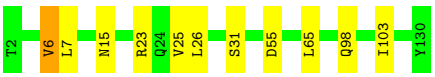

• Molecule 71: 40S ribosomal protein S22-A

Chain X:




• Molecule 71: 40S ribosomal protein S22-A

Chain d2:

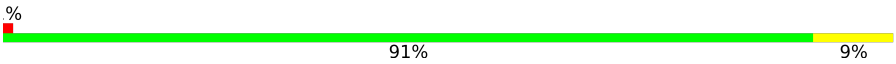


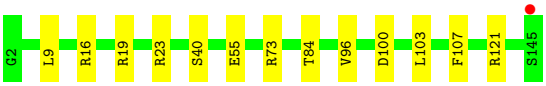
• Molecule 72: 40S ribosomal protein S23-A

Chain Y:

• Molecule 72: 40S ribosomal protein S23-A

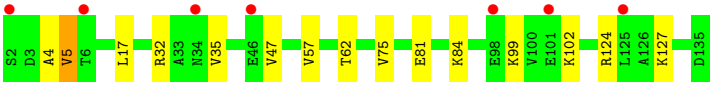
Chain d3:



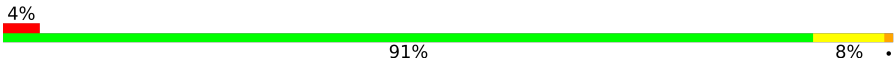

• Molecule 73: 40S ribosomal protein S24-A

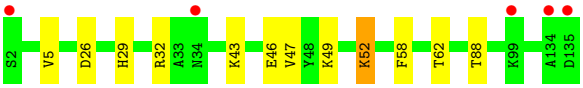
Chain Z:




• Molecule 73: 40S ribosomal protein S24-A

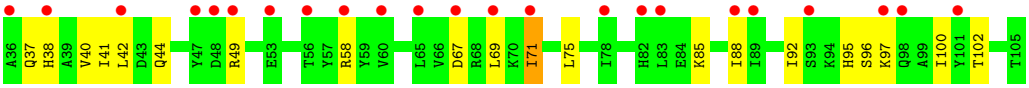
Chain d4:



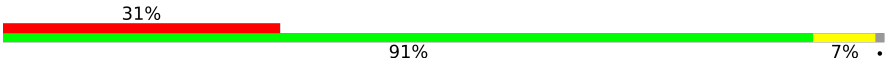

• Molecule 74: 40S ribosomal protein S25-A

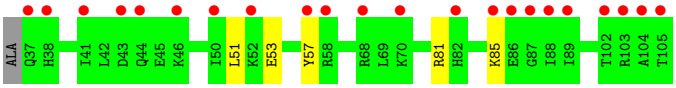
Chain a:




• Molecule 74: 40S ribosomal protein S25-A

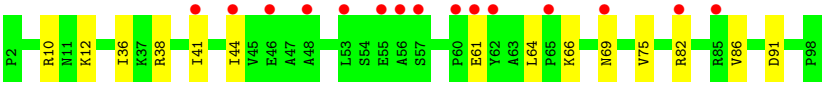
Chain d5:



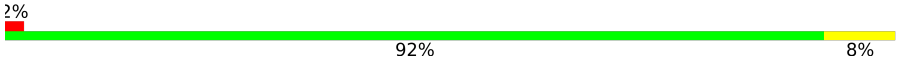

• Molecule 75: 40S ribosomal protein S26-B

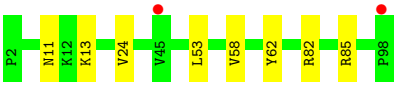
Chain b:




• Molecule 75: 40S ribosomal protein S26-B

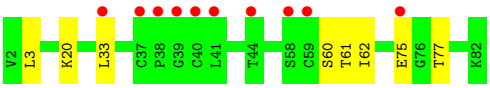
Chain d6:




• Molecule 76: 40S ribosomal protein S27-A

Chain c:

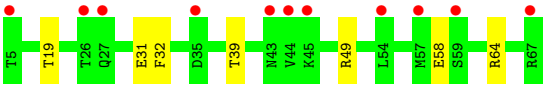



• Molecule 76: 40S ribosomal protein S27-A

Chain d7:

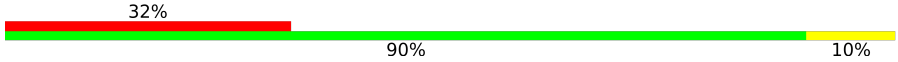
• Molecule 77: 40S ribosomal protein S28-A

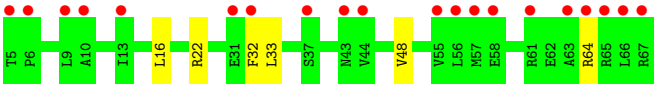
Chain d:




• Molecule 77: 40S ribosomal protein S28-A

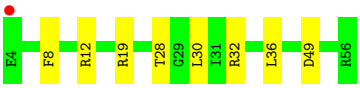
Chain d8:



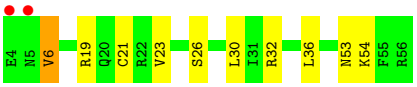

• Molecule 78: 40S ribosomal protein S29-A

Chain e:



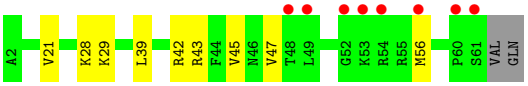

• Molecule 78: 40S ribosomal protein S29-A

Chain d9:



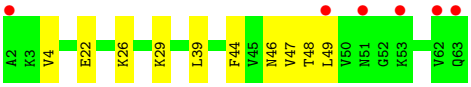

- Molecule 79: 40S ribosomal protein S30-A

Chain f:



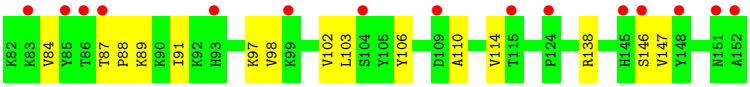

- Molecule 79: 40S ribosomal protein S30-A

Chain e0:



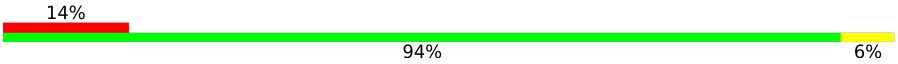

- Molecule 80: Ubiquitin-40S ribosomal protein S31

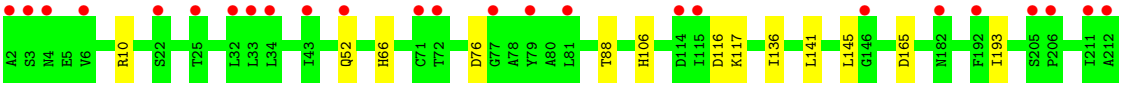
Chain g:

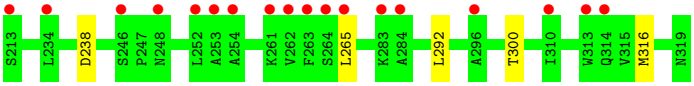



- Molecule 81: Guanine nucleotide-binding protein subunit beta-like protein

Chain h:

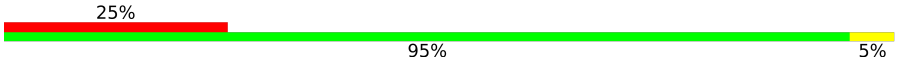


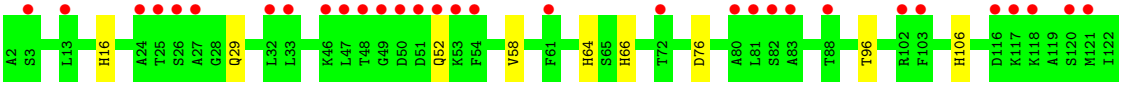



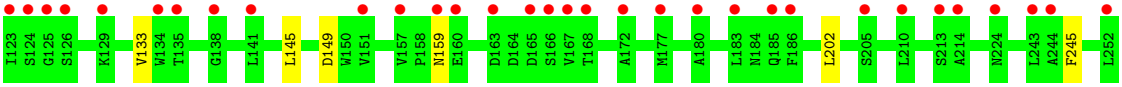



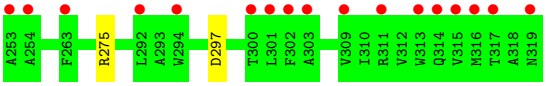

- Molecule 81: Guanine nucleotide-binding protein subunit beta-like protein

Chain Rb:



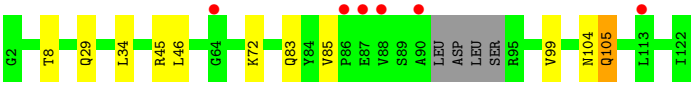





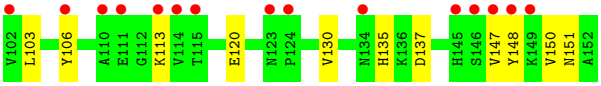

• Molecule 82: 40S ribosomal protein S17-A

Chain c7:




• Molecule 83: Ubiquitin-40S ribosomal protein S31

Chain e1:



# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 1 21 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 304.80Å 288.20Å 437.68Å<br>90.00° 98.71° 90.00° | Depositor |
| Resolution (Å) | 99.86 – 3.00<br>99.86 – 3.00 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 100.0 (99.86-3.00)<br>100.0 (99.86-3.00) | Depositor<br>EDS |
| $R_{merge}$ | 0.20 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.52 (at 3.01Å) | Xtriage |
| Refinement program | PHENIX | Depositor |
| R, $R_{free}$ | 0.194 , 0.227<br>0.196 , 0.228 | Depositor<br>DCC |
| $R_{free}$ test set | 29480 reflections (1.99%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 62.3 | Xtriage |
| Anisotropy | 0.296 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.30 , 63.7 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.49$, $< L^2 > = 0.32$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.93 | EDS |
| Total number of atoms | 409612 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 74.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 7AL, MG, ZN, OHX

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\|>5$ | RMSZ | $\#\|Z\|>5$ |
| 1 | 1 | 0.54 | 0/75394 | 1.00 | 128/117545 (0.1%) |
| 1 | AR | 0.54 | 0/75394 | 0.98 | 102/117545 (0.1%) |
| 2 | 3 | 0.47 | 0/2883 | 0.88 | 0/4491 |
| 2 | AS | 0.52 | 0/2883 | 0.94 | 1/4491 (0.0%) |
| 3 | 4 | 0.52 | 0/3746 | 0.96 | 1/5832 (0.0%) |
| 3 | AT | 0.46 | 0/3746 | 0.91 | 4/5832 (0.1%) |
| 4 | CD | 0.37 | 0/1948 | 0.60 | 0/2617 |
| 4 | j | 0.41 | 0/1948 | 0.65 | 1/2617 (0.0%) |
| 5 | CE | 0.45 | 0/3146 | 0.66 | 1/4228 (0.0%) |
| 5 | k | 0.41 | 0/3146 | 0.63 | 0/4228 |
| 6 | CF | 0.40 | 0/2800 | 0.67 | 2/3790 (0.1%) |
| 6 | l | 0.44 | 0/2800 | 0.70 | 3/3790 (0.1%) |
| 7 | CG | 0.39 | 0/2425 | 0.60 | 0/3271 |
| 7 | m | 0.34 | 0/2425 | 0.54 | 0/3271 |
| 8 | CH | 0.40 | 0/1260 | 0.58 | 0/1694 |
| 8 | n | 0.40 | 0/1260 | 0.58 | 0/1694 |
| 9 | CI | 0.43 | 0/1821 | 0.61 | 0/2451 |
| 9 | o | 0.43 | 0/1821 | 0.63 | 1/2451 (0.0%) |
| 10 | CJ | 0.32 | 0/1836 | 0.54 | 1/2481 (0.0%) |
| 10 | p | 0.34 | 0/1836 | 0.58 | 0/2481 |
| 11 | CK | 0.39 | 0/1539 | 0.58 | 0/2073 |
| 11 | q | 0.38 | 0/1539 | 0.58 | 0/2073 |
| 12 | CL | 0.40 | 0/1741 | 0.60 | 0/2335 |
| 12 | r | 0.42 | 0/1741 | 0.64 | 1/2335 (0.0%) |
| 13 | CM | 0.39 | 0/1374 | 0.62 | 1/1842 (0.1%) |
| 13 | s | 0.33 | 0/1374 | 0.57 | 0/1842 |
| 14 | CN | 0.39 | 0/1568 | 0.61 | 0/2106 |
| 14 | t | 0.41 | 0/1568 | 0.64 | 0/2106 |
| 15 | CO | 0.41 | 0/1068 | 0.60 | 0/1438 |
| 15 | u | 0.39 | 0/1068 | 0.59 | 0/1438 |
| 16 | CP | 0.39 | 0/1757 | 0.62 | 1/2354 (0.0%) |
| 16 | v | 0.44 | 0/1757 | 0.66 | 1/2354 (0.0%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 17 | CQ | 0.53 | 0/1585 | 0.63 | 1/2128 (0.0%) |
| 17 | w | 0.47 | 0/1585 | 0.61 | 0/2128 |
| 18 | CR | 0.45 | 0/1443 | 0.66 | 0/1944 |
| 18 | x | 0.43 | 0/1443 | 0.63 | 0/1944 |
| 19 | CS | 0.41 | 0/1465 | 0.66 | 1/1965 (0.1%) |
| 19 | y | 0.44 | 0/1465 | 0.67 | 0/1965 |
| 20 | CT | 0.34 | 0/1538 | 0.55 | 0/2050 |
| 20 | z | 0.33 | 0/1538 | 0.52 | 0/2050 |
| 21 | 0 | 0.40 | 0/1481 | 0.61 | 0/1990 |
| 21 | CU | 0.42 | 0/1481 | 0.60 | 0/1990 |
| 22 | 2 | 0.40 | 0/1300 | 0.60 | 0/1743 |
| 22 | CV | 0.43 | 0/1300 | 0.61 | 0/1743 |
| 23 | 5 | 0.29 | 0/812 | 0.49 | 0/1099 |
| 23 | CW | 0.32 | 0/812 | 0.54 | 0/1099 |
| 24 | 6 | 0.42 | 0/1018 | 0.60 | 0/1369 |
| 24 | CX | 0.44 | 0/1018 | 0.60 | 0/1369 |
| 25 | 7 | 0.35 | 0/712 | 0.51 | 0/958 |
| 25 | CY | 0.37 | 0/712 | 0.60 | 0/958 |
| 26 | 8 | 0.34 | 0/979 | 0.59 | 0/1321 |
| 26 | CZ | 0.36 | 0/979 | 0.60 | 1/1321 (0.1%) |
| 27 | 9 | 0.39 | 0/1004 | 0.67 | 1/1341 (0.1%) |
| 27 | DA | 0.39 | 0/1004 | 0.62 | 0/1341 |
| 28 | AA | 0.33 | 0/1118 | 0.52 | 0/1497 |
| 28 | DB | 0.31 | 0/1118 | 0.54 | 0/1497 |
| 29 | AB | 0.45 | 0/1204 | 0.70 | 1/1612 (0.1%) |
| 29 | DC | 0.44 | 0/1204 | 0.65 | 0/1612 |
| 30 | AC | 0.38 | 0/473 | 0.65 | 1/629 (0.2%) |
| 30 | DD | 0.38 | 0/473 | 0.60 | 0/629 |
| 31 | AD | 0.31 | 0/751 | 0.52 | 0/1008 |
| 31 | DE | 0.30 | 0/751 | 0.52 | 1/1008 (0.1%) |
| 32 | AE | 0.35 | 0/890 | 0.57 | 0/1196 |
| 32 | DF | 0.39 | 0/890 | 0.57 | 0/1196 |
| 33 | AF | 0.43 | 0/1041 | 0.60 | 0/1394 |
| 33 | DG | 0.42 | 0/1041 | 0.62 | 0/1394 |
| 34 | AG | 0.48 | 0/868 | 0.62 | 0/1168 |
| 34 | DH | 0.46 | 0/868 | 0.63 | 0/1168 |
| 35 | AH | 0.37 | 0/890 | 0.60 | 0/1189 |
| 35 | DI | 0.35 | 0/890 | 0.57 | 0/1189 |
| 36 | AI | 0.39 | 0/978 | 0.57 | 0/1301 |
| 36 | DJ | 0.34 | 0/978 | 0.50 | 1/1301 (0.1%) |
| 37 | AJ | 0.37 | 0/778 | 0.59 | 0/1034 |
| 37 | DK | 0.32 | 0/778 | 0.57 | 0/1034 |
| 38 | AK | 0.49 | 0/696 | 0.71 | 0/923 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 38 | DL | 0.41 | 0/696 | 0.65 | 0/923 |
| 39 | AL | 0.33 | 0/618 | 0.51 | 0/826 |
| 39 | DM | 0.30 | 0/618 | 0.52 | 0/826 |
| 40 | AM | 0.42 | 0/443 | 0.67 | 0/588 |
| 40 | DN | 0.35 | 0/443 | 0.63 | 0/588 |
| 41 | AN | 0.44 | 0/423 | 0.65 | 0/562 |
| 41 | DO | 0.44 | 0/423 | 0.66 | 0/562 |
| 42 | AO | 0.36 | 0/234 | 0.57 | 0/300 |
| 42 | DP | 0.37 | 0/234 | 0.56 | 0/300 |
| 43 | AP | 0.42 | 0/860 | 0.64 | 0/1136 |
| 43 | DQ | 0.43 | 0/860 | 0.65 | 0/1136 |
| 44 | AQ | 0.40 | 0/701 | 0.64 | 1/934 (0.1%) |
| 44 | DR | 0.37 | 0/701 | 0.63 | 0/934 |
| 45 | i | 0.33 | 0/1113 | 0.56 | 1/1502 (0.1%) |
| 46 | p0 | 0.31 | 0/1092 | 0.54 | 0/1474 |
| 47 | sM | 0.34 | 0/481 | 0.61 | 0/644 |
| 48 | A | 0.36 | 0/42443 | 0.87 | 45/66134 (0.1%) |
| 48 | sR | 0.40 | 0/42490 | 0.88 | 45/66207 (0.1%) |
| 49 | B | 0.29 | 0/1617 | 0.57 | 0/2215 |
| 49 | s0 | 0.31 | 0/1623 | 0.55 | 0/2222 |
| 50 | C | 0.29 | 0/1735 | 0.58 | 1/2335 (0.0%) |
| 50 | s1 | 0.31 | 0/1748 | 0.59 | 1/2352 (0.0%) |
| 51 | D | 0.30 | 0/1665 | 0.54 | 0/2263 |
| 51 | s2 | 0.33 | 0/1665 | 0.60 | 0/2263 |
| 52 | E | 0.29 | 0/1759 | 0.50 | 1/2368 (0.0%) |
| 52 | s3 | 0.27 | 0/1759 | 0.47 | 0/2368 |
| 53 | F | 0.32 | 0/2109 | 0.60 | 1/2839 (0.0%) |
| 53 | s4 | 0.32 | 0/2109 | 0.60 | 0/2839 |
| 54 | G | 0.27 | 0/1629 | 0.51 | 0/2202 |
| 54 | s5 | 0.28 | 0/1629 | 0.52 | 0/2202 |
| 55 | H | 0.29 | 0/1823 | 0.50 | 0/2439 |
| 55 | s6 | 0.32 | 0/1779 | 0.52 | 0/2379 |
| 56 | I | 0.31 | 0/1506 | 0.54 | 0/2028 |
| 56 | s7 | 0.31 | 0/1516 | 0.53 | 0/2043 |
| 57 | J | 0.33 | 0/1514 | 0.62 | 2/2021 (0.1%) |
| 57 | s8 | 0.34 | 0/1514 | 0.56 | 1/2021 (0.0%) |
| 58 | K | 0.30 | 0/1519 | 0.56 | 0/2035 |
| 58 | s9 | 0.31 | 0/1519 | 0.51 | 0/2035 |
| 59 | L | 0.32 | 0/789 | 0.64 | 1/1067 (0.1%) |
| 59 | c0 | 0.31 | 0/775 | 0.63 | 3/1045 (0.3%) |
| 60 | M | 0.37 | 0/1239 | 0.61 | 0/1673 |
| 60 | c1 | 0.35 | 0/1194 | 0.60 | 0/1610 |
| 61 | N | 0.33 | 0/898 | 0.59 | 0/1220 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 61 | c2 | 0.26 | 0/898 | 0.57 | 1/1220 (0.1%) |
| 62 | O | 0.32 | 0/1215 | 0.52 | 0/1638 |
| 62 | c3 | 0.33 | 0/1215 | 0.55 | 0/1638 |
| 63 | P | 0.29 | 0/901 | 0.59 | 0/1217 |
| 63 | c4 | 0.33 | 0/960 | 0.61 | 0/1290 |
| 64 | Q | 0.31 | 0/998 | 0.56 | 0/1341 |
| 64 | c5 | 0.32 | 0/1060 | 0.58 | 0/1426 |
| 65 | R | 0.29 | 0/1125 | 0.58 | 0/1510 |
| 65 | c6 | 0.30 | 0/1131 | 0.54 | 0/1518 |
| 66 | S | 0.32 | 0/935 | 0.66 | 2/1254 (0.2%) |
| 67 | T | 0.31 | 0/1211 | 0.55 | 0/1628 |
| 67 | c8 | 0.30 | 0/1211 | 0.53 | 1/1628 (0.1%) |
| 68 | U | 0.29 | 0/1130 | 0.49 | 0/1517 |
| 68 | c9 | 0.29 | 0/1130 | 0.55 | 1/1517 (0.1%) |
| 69 | V | 0.29 | 0/865 | 0.54 | 0/1169 |
| 69 | d0 | 0.30 | 0/892 | 0.56 | 0/1205 |
| 70 | W | 0.29 | 0/693 | 0.51 | 0/935 |
| 70 | d1 | 0.29 | 0/693 | 0.56 | 0/935 |
| 71 | X | 0.31 | 0/1038 | 0.61 | 1/1395 (0.1%) |
| 71 | d2 | 0.34 | 0/1038 | 0.57 | 0/1395 |
| 72 | Y | 0.35 | 0/1139 | 0.60 | 0/1518 |
| 72 | d3 | 0.39 | 0/1139 | 0.58 | 0/1518 |
| 73 | Z | 0.30 | 0/1087 | 0.49 | 0/1449 |
| 73 | d4 | 0.33 | 0/1087 | 0.58 | 0/1449 |
| 74 | a | 0.29 | 0/571 | 0.64 | 0/768 |
| 74 | d5 | 0.27 | 0/566 | 0.47 | 0/761 |
| 75 | b | 0.30 | 0/782 | 0.58 | 0/1047 |
| 75 | d6 | 0.33 | 0/782 | 0.55 | 0/1047 |
| 76 | c | 0.27 | 0/620 | 0.52 | 0/838 |
| 76 | d7 | 0.30 | 0/620 | 0.57 | 0/838 |
| 77 | d | 0.25 | 0/499 | 0.49 | 0/670 |
| 77 | d8 | 0.26 | 0/499 | 0.53 | 0/670 |
| 78 | d9 | 0.32 | 0/452 | 0.52 | 0/600 |
| 78 | e | 0.37 | 0/452 | 0.61 | 0/600 |
| 79 | e0 | 0.32 | 0/499 | 0.60 | 0/665 |
| 79 | f | 0.31 | 0/483 | 0.56 | 0/643 |
| 80 | g | 0.39 | 0/577 | 0.76 | 0/770 |
| 81 | Rb | 0.26 | 0/2495 | 0.47 | 0/3395 |
| 81 | h | 0.26 | 0/2490 | 0.49 | 0/3389 |
| 82 | c7 | 0.29 | 0/914 | 0.50 | 0/1224 |
| 83 | e1 | 0.30 | 0/404 | 0.63 | 0/542 |
| All | All | 0.44 | 0/429965 | 0.83 | 366/631328 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 6 | l | 0 | 1 |
| 7 | CG | 0 | 2 |
| 10 | p | 0 | 1 |
| 12 | r | 0 | 1 |
| 17 | CQ | 0 | 1 |
| 17 | w | 0 | 1 |
| 21 | 0 | 0 | 1 |
| 22 | 2 | 0 | 1 |
| 22 | CV | 0 | 1 |
| 25 | CY | 0 | 1 |
| 27 | 9 | 0 | 1 |
| 27 | DA | 0 | 1 |
| 28 | AA | 0 | 1 |
| 28 | DB | 0 | 1 |
| 30 | AC | 0 | 1 |
| 30 | DD | 0 | 1 |
| 32 | DF | 0 | 1 |
| 36 | DJ | 0 | 1 |
| 39 | AL | 0 | 1 |
| 44 | DR | 0 | 1 |
| 51 | D | 0 | 1 |
| 52 | E | 0 | 1 |
| 52 | s3 | 0 | 1 |
| 53 | F | 0 | 1 |
| 53 | s4 | 0 | 1 |
| 54 | G | 0 | 2 |
| 54 | s5 | 0 | 2 |
| 55 | s6 | 0 | 1 |
| 56 | I | 0 | 3 |
| 56 | s7 | 0 | 2 |
| 57 | J | 0 | 1 |
| 61 | c2 | 0 | 1 |
| 63 | P | 0 | 1 |
| 63 | c4 | 0 | 1 |
| 64 | Q | 0 | 1 |
| 64 | c5 | 0 | 2 |
| 65 | R | 0 | 4 |
| 65 | c6 | 0 | 2 |
| 66 | S | 0 | 3 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 67 | T | 0 | 1 |
| 70 | d1 | 0 | 1 |
| 72 | Y | 0 | 1 |
| 73 | d4 | 0 | 1 |
| 75 | b | 0 | 1 |
| 80 | g | 0 | 2 |
| 83 | e1 | 0 | 1 |
| All | All | 0 | 60 |

There are no bond length outliers.

The worst 5 of 366 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 1 | 1308 | A | O5'-P-OP1 | -10.26 | 96.47 | 105.70 |
| 1 | 1 | 1307 | G | P-O3'-C3' | 10.16 | 131.89 | 119.70 |
| 1 | AR | 3217 | C | N1-C2-O2 | 9.74 | 124.75 | 118.90 |
| 1 | 1 | 406 | G | O4'-C1'-N9 | 9.62 | 115.89 | 108.20 |
| 1 | 1 | 3278 | C | N1-C2-O2 | 9.04 | 124.32 | 118.90 |

There are no chirality outliers.

5 of 60 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 21 | 0 | 133 | ALA | Peptide |
| 6 | l | 338 | LYS | Peptide |
| 10 | p | 30 | THR | Peptide |
| 12 | r | 188 | GLY | Peptide |
| 17 | w | 110 | PRO | Peptide |

## 5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 4 | CD | 250/252 (99%) | 237 (95%) | 13 (5%) | 0 | 100 | 100 |
| 4 | j | 250/252 (99%) | 235 (94%) | 15 (6%) | 0 | 100 | 100 |
| 5 | CE | 384/386 (100%) | 357 (93%) | 27 (7%) | 0 | 100 | 100 |
| 5 | k | 384/386 (100%) | 361 (94%) | 22 (6%) | 1 (0%) | 41 | 76 |
| 6 | CF | 359/361 (99%) | 333 (93%) | 25 (7%) | 1 (0%) | 41 | 76 |
| 6 | l | 359/361 (99%) | 334 (93%) | 23 (6%) | 2 (1%) | 25 | 64 |
| 7 | CG | 294/296 (99%) | 274 (93%) | 19 (6%) | 1 (0%) | 41 | 76 |
| 7 | m | 294/296 (99%) | 268 (91%) | 26 (9%) | 0 | 100 | 100 |
| 8 | CH | 152/175 (87%) | 145 (95%) | 6 (4%) | 1 (1%) | 22 | 60 |
| 8 | n | 152/175 (87%) | 146 (96%) | 5 (3%) | 1 (1%) | 22 | 60 |
| 9 | CI | 220/222 (99%) | 207 (94%) | 11 (5%) | 2 (1%) | 17 | 55 |
| 9 | o | 220/222 (99%) | 208 (94%) | 9 (4%) | 3 (1%) | 11 | 43 |
| 10 | CJ | 231/233 (99%) | 208 (90%) | 21 (9%) | 2 (1%) | 17 | 55 |
| 10 | p | 231/233 (99%) | 210 (91%) | 18 (8%) | 3 (1%) | 12 | 45 |
| 11 | CK | 189/191 (99%) | 176 (93%) | 13 (7%) | 0 | 100 | 100 |
| 11 | q | 189/191 (99%) | 176 (93%) | 12 (6%) | 1 (0%) | 29 | 68 |
| 12 | CL | 207/220 (94%) | 194 (94%) | 12 (6%) | 1 (0%) | 29 | 68 |
| 12 | r | 207/220 (94%) | 202 (98%) | 5 (2%) | 0 | 100 | 100 |
| 13 | CM | 167/169 (99%) | 148 (89%) | 16 (10%) | 3 (2%) | 8 | 37 |
| 13 | s | 167/169 (99%) | 149 (89%) | 17 (10%) | 1 (1%) | 25 | 64 |
| 14 | CN | 191/193 (99%) | 175 (92%) | 13 (7%) | 3 (2%) | 9 | 40 |
| 14 | t | 191/193 (99%) | 174 (91%) | 14 (7%) | 3 (2%) | 9 | 40 |
| 15 | CO | 134/136 (98%) | 127 (95%) | 5 (4%) | 2 (2%) | 10 | 42 |
| 15 | u | 134/136 (98%) | 126 (94%) | 6 (4%) | 2 (2%) | 10 | 42 |
| 16 | CP | 201/203 (99%) | 193 (96%) | 8 (4%) | 0 | 100 | 100 |
| 16 | v | 201/203 (99%) | 188 (94%) | 11 (6%) | 2 (1%) | 15 | 53 |
| 17 | CQ | 195/197 (99%) | 189 (97%) | 3 (2%) | 3 (2%) | 10 | 42 |
| 17 | w | 195/197 (99%) | 190 (97%) | 3 (2%) | 2 (1%) | 15 | 53 |
| 18 | CR | 181/183 (99%) | 167 (92%) | 13 (7%) | 1 (1%) | 25 | 64 |
| 18 | x | 181/183 (99%) | 172 (95%) | 8 (4%) | 1 (1%) | 25 | 64 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 19 | CS | 183/185 (99%) | 172 (94%) | 10 (6%) | 1 (0%) | 29 | 68 |
| 19 | y | 183/185 (99%) | 174 (95%) | 8 (4%) | 1 (0%) | 29 | 68 |
| 20 | CT | 186/188 (99%) | 172 (92%) | 13 (7%) | 1 (0%) | 29 | 68 |
| 20 | z | 186/188 (99%) | 181 (97%) | 5 (3%) | 0 | 100 | 100 |
| 21 | 0 | 170/172 (99%) | 159 (94%) | 10 (6%) | 1 (1%) | 25 | 64 |
| 21 | CU | 170/172 (99%) | 163 (96%) | 6 (4%) | 1 (1%) | 25 | 64 |
| 22 | 2 | 157/159 (99%) | 147 (94%) | 9 (6%) | 1 (1%) | 25 | 64 |
| 22 | CV | 157/159 (99%) | 148 (94%) | 8 (5%) | 1 (1%) | 25 | 64 |
| 23 | 5 | 98/100 (98%) | 90 (92%) | 7 (7%) | 1 (1%) | 15 | 53 |
| 23 | CW | 98/100 (98%) | 90 (92%) | 7 (7%) | 1 (1%) | 15 | 53 |
| 24 | 6 | 134/136 (98%) | 133 (99%) | 1 (1%) | 0 | 100 | 100 |
| 24 | CX | 134/136 (98%) | 133 (99%) | 1 (1%) | 0 | 100 | 100 |
| 25 | 7 | 96/98 (98%) | 88 (92%) | 7 (7%) | 1 (1%) | 15 | 53 |
| 25 | CY | 96/98 (98%) | 89 (93%) | 5 (5%) | 2 (2%) | 7 | 33 |
| 26 | 8 | 119/121 (98%) | 114 (96%) | 5 (4%) | 0 | 100 | 100 |
| 26 | CZ | 119/121 (98%) | 112 (94%) | 7 (6%) | 0 | 100 | 100 |
| 27 | 9 | 124/126 (98%) | 118 (95%) | 6 (5%) | 0 | 100 | 100 |
| 27 | DA | 124/126 (98%) | 121 (98%) | 3 (2%) | 0 | 100 | 100 |
| 28 | AA | 133/135 (98%) | 127 (96%) | 6 (4%) | 0 | 100 | 100 |
| 28 | DB | 133/135 (98%) | 121 (91%) | 10 (8%) | 2 (2%) | 10 | 42 |
| 29 | AB | 146/148 (99%) | 127 (87%) | 17 (12%) | 2 (1%) | 11 | 43 |
| 29 | DC | 146/148 (99%) | 133 (91%) | 10 (7%) | 3 (2%) | 7 | 33 |
| 30 | AC | 56/58 (97%) | 52 (93%) | 4 (7%) | 0 | 100 | 100 |
| 30 | DD | 56/58 (97%) | 50 (89%) | 6 (11%) | 0 | 100 | 100 |
| 31 | AD | 95/97 (98%) | 93 (98%) | 2 (2%) | 0 | 100 | 100 |
| 31 | DE | 95/97 (98%) | 93 (98%) | 2 (2%) | 0 | 100 | 100 |
| 32 | AE | 107/109 (98%) | 101 (94%) | 3 (3%) | 3 (3%) | 5 | 25 |
| 32 | DF | 107/109 (98%) | 103 (96%) | 1 (1%) | 3 (3%) | 5 | 25 |
| 33 | AF | 125/127 (98%) | 122 (98%) | 3 (2%) | 0 | 100 | 100 |
| 33 | DG | 125/127 (98%) | 123 (98%) | 2 (2%) | 0 | 100 | 100 |
| 34 | AG | 104/106 (98%) | 101 (97%) | 3 (3%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 34 | DH | 104/106 (98%) | 99 (95%) | 5 (5%) | 0 | 100 | 100 |
| 35 | AH | 110/112 (98%) | 105 (96%) | 4 (4%) | 1 (1%) | 17 | 55 |
| 35 | DI | 110/112 (98%) | 103 (94%) | 6 (6%) | 1 (1%) | 17 | 55 |
| 36 | AI | 117/119 (98%) | 110 (94%) | 7 (6%) | 0 | 100 | 100 |
| 36 | DJ | 117/119 (98%) | 112 (96%) | 5 (4%) | 0 | 100 | 100 |
| 37 | AJ | 97/99 (98%) | 88 (91%) | 8 (8%) | 1 (1%) | 15 | 53 |
| 37 | DK | 97/99 (98%) | 86 (89%) | 10 (10%) | 1 (1%) | 15 | 53 |
| 38 | AK | 85/87 (98%) | 79 (93%) | 6 (7%) | 0 | 100 | 100 |
| 38 | DL | 85/87 (98%) | 79 (93%) | 6 (7%) | 0 | 100 | 100 |
| 39 | AL | 75/77 (97%) | 68 (91%) | 7 (9%) | 0 | 100 | 100 |
| 39 | DM | 75/77 (97%) | 69 (92%) | 5 (7%) | 1 (1%) | 12 | 45 |
| 40 | AM | 48/50 (96%) | 45 (94%) | 3 (6%) | 0 | 100 | 100 |
| 40 | DN | 48/50 (96%) | 47 (98%) | 1 (2%) | 0 | 100 | 100 |
| 41 | AN | 50/52 (96%) | 46 (92%) | 4 (8%) | 0 | 100 | 100 |
| 41 | DO | 50/52 (96%) | 48 (96%) | 2 (4%) | 0 | 100 | 100 |
| 42 | AO | 23/25 (92%) | 22 (96%) | 1 (4%) | 0 | 100 | 100 |
| 42 | DP | 23/25 (92%) | 23 (100%) | 0 | 0 | 100 | 100 |
| 43 | AP | 103/105 (98%) | 90 (87%) | 12 (12%) | 1 (1%) | 15 | 53 |
| 43 | DQ | 103/105 (98%) | 90 (87%) | 13 (13%) | 0 | 100 | 100 |
| 44 | AQ | 89/91 (98%) | 80 (90%) | 9 (10%) | 0 | 100 | 100 |
| 44 | DR | 89/91 (98%) | 81 (91%) | 7 (8%) | 1 (1%) | 14 | 50 |
| 45 | i | 155/168 (92%) | 131 (84%) | 21 (14%) | 3 (2%) | 8 | 36 |
| 46 | p0 | 139/219 (64%) | 123 (88%) | 14 (10%) | 2 (1%) | 11 | 43 |
| 47 | sM | 61/104 (59%) | 50 (82%) | 10 (16%) | 1 (2%) | 9 | 40 |
| 49 | B | 204/206 (99%) | 177 (87%) | 25 (12%) | 2 (1%) | 15 | 53 |
| 49 | s0 | 204/206 (99%) | 179 (88%) | 23 (11%) | 2 (1%) | 15 | 53 |
| 50 | C | 212/216 (98%) | 170 (80%) | 40 (19%) | 2 (1%) | 17 | 55 |
| 50 | s1 | 214/216 (99%) | 193 (90%) | 21 (10%) | 0 | 100 | 100 |
| 51 | D | 215/217 (99%) | 200 (93%) | 13 (6%) | 2 (1%) | 17 | 55 |
| 51 | s2 | 215/217 (99%) | 200 (93%) | 15 (7%) | 0 | 100 | 100 |
| 52 | E | 221/223 (99%) | 203 (92%) | 16 (7%) | 2 (1%) | 17 | 55 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 52 | s3 | 221/223 (99%) | 199 (90%) | 20 (9%) | 2 (1%) | 17 | 55 |
| 53 | F | 258/260 (99%) | 236 (92%) | 21 (8%) | 1 (0%) | 34 | 72 |
| 53 | s4 | 258/260 (99%) | 235 (91%) | 21 (8%) | 2 (1%) | 19 | 57 |
| 54 | G | 204/206 (99%) | 180 (88%) | 21 (10%) | 3 (2%) | 10 | 42 |
| 54 | s5 | 204/206 (99%) | 181 (89%) | 21 (10%) | 2 (1%) | 15 | 53 |
| 55 | H | 224/226 (99%) | 207 (92%) | 14 (6%) | 3 (1%) | 12 | 45 |
| 55 | s6 | 216/226 (96%) | 198 (92%) | 16 (7%) | 2 (1%) | 17 | 55 |
| 56 | I | 182/186 (98%) | 158 (87%) | 18 (10%) | 6 (3%) | 4 | 21 |
| 56 | s7 | 184/186 (99%) | 162 (88%) | 21 (11%) | 1 (0%) | 29 | 68 |
| 57 | J | 184/199 (92%) | 162 (88%) | 20 (11%) | 2 (1%) | 14 | 50 |
| 57 | s8 | 184/199 (92%) | 168 (91%) | 14 (8%) | 2 (1%) | 14 | 50 |
| 58 | K | 183/185 (99%) | 165 (90%) | 17 (9%) | 1 (0%) | 29 | 68 |
| 58 | s9 | 183/185 (99%) | 168 (92%) | 15 (8%) | 0 | 100 | 100 |
| 59 | L | 94/105 (90%) | 77 (82%) | 16 (17%) | 1 (1%) | 14 | 50 |
| 59 | c0 | 92/105 (88%) | 64 (70%) | 21 (23%) | 7 (8%) | 1 | 5 |
| 60 | M | 153/155 (99%) | 135 (88%) | 15 (10%) | 3 (2%) | 7 | 34 |
| 60 | c1 | 144/155 (93%) | 133 (92%) | 9 (6%) | 2 (1%) | 11 | 43 |
| 61 | N | 122/143 (85%) | 88 (72%) | 30 (25%) | 4 (3%) | 4 | 21 |
| 61 | c2 | 122/143 (85%) | 94 (77%) | 24 (20%) | 4 (3%) | 4 | 21 |
| 62 | O | 148/150 (99%) | 138 (93%) | 9 (6%) | 1 (1%) | 22 | 60 |
| 62 | c3 | 148/150 (99%) | 134 (90%) | 11 (7%) | 3 (2%) | 7 | 34 |
| 63 | P | 125/128 (98%) | 112 (90%) | 11 (9%) | 2 (2%) | 9 | 40 |
| 63 | c4 | 126/128 (98%) | 113 (90%) | 11 (9%) | 2 (2%) | 9 | 40 |
| 64 | Q | 122/135 (90%) | 107 (88%) | 12 (10%) | 3 (2%) | 5 | 28 |
| 64 | c5 | 133/135 (98%) | 105 (79%) | 22 (16%) | 6 (4%) | 2 | 14 |
| 65 | R | 139/142 (98%) | 121 (87%) | 15 (11%) | 3 (2%) | 6 | 31 |
| 65 | c6 | 140/142 (99%) | 132 (94%) | 7 (5%) | 1 (1%) | 22 | 60 |
| 66 | S | 116/125 (93%) | 97 (84%) | 15 (13%) | 4 (3%) | 3 | 20 |
| 67 | T | 143/145 (99%) | 124 (87%) | 15 (10%) | 4 (3%) | 5 | 25 |
| 67 | c8 | 143/145 (99%) | 123 (86%) | 16 (11%) | 4 (3%) | 5 | 25 |
| 68 | U | 141/143 (99%) | 125 (89%) | 16 (11%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 68 | c9 | 141/143 (99%) | 131 (93%) | 8 (6%) | 2 (1%) | 11 | 43 |
| 69 | V | 105/110 (96%) | 93 (89%) | 11 (10%) | 1 (1%) | 15 | 53 |
| 69 | d0 | 108/110 (98%) | 92 (85%) | 15 (14%) | 1 (1%) | 17 | 55 |
| 70 | W | 85/87 (98%) | 73 (86%) | 11 (13%) | 1 (1%) | 13 | 48 |
| 70 | d1 | 85/87 (98%) | 77 (91%) | 8 (9%) | 0 | 100 | 100 |
| 71 | X | 127/129 (98%) | 116 (91%) | 8 (6%) | 3 (2%) | 6 | 29 |
| 71 | d2 | 127/129 (98%) | 120 (94%) | 6 (5%) | 1 (1%) | 19 | 57 |
| 72 | Y | 142/144 (99%) | 121 (85%) | 20 (14%) | 1 (1%) | 22 | 60 |
| 72 | d3 | 142/144 (99%) | 134 (94%) | 8 (6%) | 0 | 100 | 100 |
| 73 | Z | 132/134 (98%) | 121 (92%) | 8 (6%) | 3 (2%) | 6 | 30 |
| 73 | d4 | 132/134 (98%) | 120 (91%) | 11 (8%) | 1 (1%) | 19 | 57 |
| 74 | a | 68/70 (97%) | 55 (81%) | 9 (13%) | 4 (6%) | 1 | 9 |
| 74 | d5 | 67/70 (96%) | 62 (92%) | 4 (6%) | 1 (2%) | 10 | 42 |
| 75 | b | 95/97 (98%) | 71 (75%) | 21 (22%) | 3 (3%) | 4 | 22 |
| 75 | d6 | 95/97 (98%) | 78 (82%) | 15 (16%) | 2 (2%) | 7 | 33 |
| 76 | c | 79/81 (98%) | 70 (89%) | 8 (10%) | 1 (1%) | 12 | 45 |
| 76 | d7 | 79/81 (98%) | 69 (87%) | 8 (10%) | 2 (2%) | 5 | 28 |
| 77 | d | 61/63 (97%) | 55 (90%) | 6 (10%) | 0 | 100 | 100 |
| 77 | d8 | 61/63 (97%) | 50 (82%) | 11 (18%) | 0 | 100 | 100 |
| 78 | d9 | 51/53 (96%) | 44 (86%) | 6 (12%) | 1 (2%) | 7 | 34 |
| 78 | e | 51/53 (96%) | 46 (90%) | 5 (10%) | 0 | 100 | 100 |
| 79 | e0 | 60/62 (97%) | 52 (87%) | 7 (12%) | 1 (2%) | 9 | 39 |
| 79 | f | 58/62 (94%) | 49 (84%) | 7 (12%) | 2 (3%) | 3 | 20 |
| 80 | g | 69/71 (97%) | 44 (64%) | 19 (28%) | 6 (9%) | 1 | 3 |
| 81 | Rb | 316/318 (99%) | 294 (93%) | 22 (7%) | 0 | 100 | 100 |
| 81 | h | 316/318 (99%) | 295 (93%) | 21 (7%) | 0 | 100 | 100 |
| 82 | c7 | 113/121 (93%) | 101 (89%) | 10 (9%) | 2 (2%) | 8 | 37 |
| 83 | e1 | 49/51 (96%) | 37 (76%) | 12 (24%) | 0 | 100 | 100 |
| All | All | 22260/22893 (97%) | 20326 (91%) | 1724 (8%) | 210 (1%) | 17 | 55 |

5 of 210 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | l | 339 | LEU |
| 8 | n | 98 | VAL |
| 11 | q | 50 | ASN |
| 16 | v | 75 | VAL |
| 17 | w | 111 | PRO |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 4 | CD | 193/194 (100%) | 165 (86%) | 28 (14%) | 3 | 15 |
| 4 | j | 193/194 (100%) | 164 (85%) | 29 (15%) | 3 | 14 |
| 5 | CE | 320/322 (99%) | 269 (84%) | 51 (16%) | 2 | 12 |
| 5 | k | 320/322 (99%) | 266 (83%) | 54 (17%) | 2 | 11 |
| 6 | CF | 288/288 (100%) | 249 (86%) | 39 (14%) | 4 | 17 |
| 6 | l | 288/288 (100%) | 243 (84%) | 45 (16%) | 2 | 13 |
| 7 | CG | 244/244 (100%) | 206 (84%) | 38 (16%) | 2 | 13 |
| 7 | m | 244/244 (100%) | 207 (85%) | 37 (15%) | 3 | 14 |
| 8 | CH | 134/152 (88%) | 119 (89%) | 15 (11%) | 6 | 24 |
| 8 | n | 134/152 (88%) | 116 (87%) | 18 (13%) | 4 | 17 |
| 9 | CI | 186/186 (100%) | 169 (91%) | 17 (9%) | 9 | 34 |
| 9 | o | 186/186 (100%) | 164 (88%) | 22 (12%) | 5 | 22 |
| 10 | CJ | 187/191 (98%) | 169 (90%) | 18 (10%) | 8 | 32 |
| 10 | p | 187/191 (98%) | 157 (84%) | 30 (16%) | 2 | 12 |
| 11 | CK | 171/171 (100%) | 146 (85%) | 25 (15%) | 3 | 15 |
| 11 | q | 171/171 (100%) | 145 (85%) | 26 (15%) | 3 | 14 |
| 12 | CL | 177/186 (95%) | 157 (89%) | 20 (11%) | 6 | 24 |
| 12 | r | 177/186 (95%) | 151 (85%) | 26 (15%) | 3 | 15 |
| 13 | CM | 147/147 (100%) | 123 (84%) | 24 (16%) | 2 | 11 |
| 13 | s | 147/147 (100%) | 122 (83%) | 25 (17%) | 2 | 10 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 14 | CN | 154/154 (100%) | 135 (88%) | 19 (12%) | 4 | 21 |
| 14 | t | 154/154 (100%) | 130 (84%) | 24 (16%) | 2 | 13 |
| 15 | CO | 107/107 (100%) | 96 (90%) | 11 (10%) | 7 | 28 |
| 15 | u | 107/107 (100%) | 92 (86%) | 15 (14%) | 3 | 16 |
| 16 | CP | 175/175 (100%) | 153 (87%) | 22 (13%) | 4 | 20 |
| 16 | v | 175/175 (100%) | 156 (89%) | 19 (11%) | 6 | 25 |
| 17 | CQ | 160/160 (100%) | 142 (89%) | 18 (11%) | 6 | 24 |
| 17 | w | 160/160 (100%) | 143 (89%) | 17 (11%) | 6 | 26 |
| 18 | CR | 140/145 (97%) | 116 (83%) | 24 (17%) | 2 | 10 |
| 18 | x | 140/145 (97%) | 122 (87%) | 18 (13%) | 4 | 19 |
| 19 | CS | 150/150 (100%) | 125 (83%) | 25 (17%) | 2 | 11 |
| 19 | y | 150/150 (100%) | 125 (83%) | 25 (17%) | 2 | 11 |
| 20 | CT | 153/153 (100%) | 125 (82%) | 28 (18%) | 1 | 9 |
| 20 | z | 153/153 (100%) | 136 (89%) | 17 (11%) | 6 | 25 |
| 21 | 0 | 156/156 (100%) | 131 (84%) | 25 (16%) | 2 | 12 |
| 21 | CU | 156/156 (100%) | 132 (85%) | 24 (15%) | 2 | 13 |
| 22 | 2 | 136/136 (100%) | 110 (81%) | 26 (19%) | 1 | 8 |
| 22 | CV | 136/136 (100%) | 111 (82%) | 25 (18%) | 1 | 9 |
| 23 | 5 | 87/87 (100%) | 77 (88%) | 10 (12%) | 5 | 24 |
| 23 | CW | 87/87 (100%) | 76 (87%) | 11 (13%) | 4 | 20 |
| 24 | 6 | 104/104 (100%) | 88 (85%) | 16 (15%) | 2 | 13 |
| 24 | CX | 104/104 (100%) | 91 (88%) | 13 (12%) | 4 | 20 |
| 25 | 7 | 57/86 (66%) | 51 (90%) | 6 (10%) | 7 | 27 |
| 25 | CY | 57/86 (66%) | 51 (90%) | 6 (10%) | 7 | 27 |
| 26 | 8 | 104/105 (99%) | 87 (84%) | 17 (16%) | 2 | 11 |
| 26 | CZ | 104/105 (99%) | 86 (83%) | 18 (17%) | 2 | 10 |
| 27 | 9 | 109/109 (100%) | 90 (83%) | 19 (17%) | 2 | 10 |
| 27 | DA | 109/109 (100%) | 94 (86%) | 15 (14%) | 3 | 17 |
| 28 | AA | 115/115 (100%) | 98 (85%) | 17 (15%) | 3 | 14 |
| 28 | DB | 115/115 (100%) | 105 (91%) | 10 (9%) | 10 | 37 |
| 29 | AB | 118/118 (100%) | 98 (83%) | 20 (17%) | 2 | 11 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 29 | DC | 118/118 (100%) | 102 (86%) | 16 (14%) | 3 | 17 |
| 30 | AC | 46/46 (100%) | 40 (87%) | 6 (13%) | 4 | 19 |
| 30 | DD | 46/46 (100%) | 39 (85%) | 7 (15%) | 3 | 14 |
| 31 | AD | 81/81 (100%) | 69 (85%) | 12 (15%) | 3 | 14 |
| 31 | DE | 81/81 (100%) | 75 (93%) | 6 (7%) | 13 | 44 |
| 32 | AE | 92/96 (96%) | 79 (86%) | 13 (14%) | 3 | 16 |
| 32 | DF | 92/96 (96%) | 74 (80%) | 18 (20%) | 1 | 7 |
| 33 | AF | 109/109 (100%) | 94 (86%) | 15 (14%) | 3 | 17 |
| 33 | DG | 109/109 (100%) | 98 (90%) | 11 (10%) | 7 | 29 |
| 34 | AG | 90/90 (100%) | 84 (93%) | 6 (7%) | 16 | 49 |
| 34 | DH | 90/90 (100%) | 80 (89%) | 10 (11%) | 6 | 25 |
| 35 | AH | 95/95 (100%) | 80 (84%) | 15 (16%) | 2 | 12 |
| 35 | DI | 95/95 (100%) | 86 (90%) | 9 (10%) | 8 | 32 |
| 36 | AI | 104/104 (100%) | 89 (86%) | 15 (14%) | 3 | 15 |
| 36 | DJ | 104/104 (100%) | 81 (78%) | 23 (22%) | 1 | 4 |
| 37 | AJ | 81/81 (100%) | 66 (82%) | 15 (18%) | 1 | 8 |
| 37 | DK | 81/81 (100%) | 65 (80%) | 16 (20%) | 1 | 7 |
| 38 | AK | 70/70 (100%) | 61 (87%) | 9 (13%) | 4 | 19 |
| 38 | DL | 70/70 (100%) | 59 (84%) | 11 (16%) | 2 | 13 |
| 39 | AL | 68/68 (100%) | 57 (84%) | 11 (16%) | 2 | 12 |
| 39 | DM | 68/68 (100%) | 56 (82%) | 12 (18%) | 2 | 10 |
| 40 | AM | 45/45 (100%) | 38 (84%) | 7 (16%) | 2 | 13 |
| 40 | DN | 45/45 (100%) | 40 (89%) | 5 (11%) | 6 | 25 |
| 41 | AN | 47/47 (100%) | 38 (81%) | 9 (19%) | 1 | 8 |
| 41 | DO | 47/47 (100%) | 40 (85%) | 7 (15%) | 3 | 14 |
| 42 | AO | 23/23 (100%) | 19 (83%) | 4 (17%) | 2 | 10 |
| 42 | DP | 23/23 (100%) | 19 (83%) | 4 (17%) | 2 | 10 |
| 43 | AP | 90/90 (100%) | 80 (89%) | 10 (11%) | 6 | 25 |
| 43 | DQ | 90/90 (100%) | 73 (81%) | 17 (19%) | 1 | 8 |
| 44 | AQ | 71/71 (100%) | 58 (82%) | 13 (18%) | 1 | 9 |
| 44 | DR | 71/71 (100%) | 64 (90%) | 7 (10%) | 8 | 30 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 45 | i | 97/137 (71%) | 81 (84%) | 16 (16%) | 2 | 11 |
| 46 | p0 | 105/186 (56%) | 88 (84%) | 17 (16%) | 2 | 12 |
| 47 | sM | 54/54 (100%) | 47 (87%) | 7 (13%) | 4 | 19 |
| 49 | B | 164/173 (95%) | 149 (91%) | 15 (9%) | 9 | 34 |
| 49 | s0 | 165/173 (95%) | 139 (84%) | 26 (16%) | 2 | 12 |
| 50 | C | 191/192 (100%) | 160 (84%) | 31 (16%) | 2 | 12 |
| 50 | s1 | 192/192 (100%) | 164 (85%) | 28 (15%) | 3 | 15 |
| 51 | D | 176/176 (100%) | 140 (80%) | 36 (20%) | 1 | 6 |
| 51 | s2 | 176/176 (100%) | 141 (80%) | 35 (20%) | 1 | 7 |
| 52 | E | 182/182 (100%) | 157 (86%) | 25 (14%) | 3 | 17 |
| 52 | s3 | 182/182 (100%) | 163 (90%) | 19 (10%) | 7 | 27 |
| 53 | F | 221/221 (100%) | 194 (88%) | 27 (12%) | 5 | 21 |
| 53 | s4 | 221/221 (100%) | 191 (86%) | 30 (14%) | 3 | 17 |
| 54 | G | 173/173 (100%) | 158 (91%) | 15 (9%) | 10 | 37 |
| 54 | s5 | 173/173 (100%) | 153 (88%) | 20 (12%) | 5 | 23 |
| 55 | H | 188/193 (97%) | 159 (85%) | 29 (15%) | 2 | 13 |
| 55 | s6 | 187/193 (97%) | 165 (88%) | 22 (12%) | 5 | 22 |
| 56 | I | 165/166 (99%) | 144 (87%) | 21 (13%) | 4 | 19 |
| 56 | s7 | 165/166 (99%) | 148 (90%) | 17 (10%) | 7 | 28 |
| 57 | J | 150/160 (94%) | 135 (90%) | 15 (10%) | 7 | 29 |
| 57 | s8 | 150/160 (94%) | 136 (91%) | 14 (9%) | 9 | 33 |
| 58 | K | 158/158 (100%) | 129 (82%) | 29 (18%) | 1 | 9 |
| 58 | s9 | 158/158 (100%) | 137 (87%) | 21 (13%) | 4 | 17 |
| 59 | L | 77/98 (79%) | 70 (91%) | 7 (9%) | 9 | 34 |
| 59 | c0 | 73/98 (74%) | 67 (92%) | 6 (8%) | 11 | 39 |
| 60 | M | 129/136 (95%) | 108 (84%) | 21 (16%) | 2 | 11 |
| 60 | c1 | 129/136 (95%) | 110 (85%) | 19 (15%) | 3 | 15 |
| 61 | N | 88/119 (74%) | 68 (77%) | 20 (23%) | 1 | 4 |
| 61 | c2 | 88/119 (74%) | 68 (77%) | 20 (23%) | 1 | 4 |
| 62 | O | 127/127 (100%) | 106 (84%) | 21 (16%) | 2 | 11 |
| 62 | c3 | 127/127 (100%) | 110 (87%) | 17 (13%) | 4 | 17 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 63 | P | 81/97 (84%) | 69 (85%) | 12 (15%) | 3 | 14 |
| 63 | c4 | 97/97 (100%) | 83 (86%) | 14 (14%) | 3 | 15 |
| 64 | Q | 101/111 (91%) | 86 (85%) | 15 (15%) | 3 | 14 |
| 64 | c5 | 103/111 (93%) | 94 (91%) | 9 (9%) | 10 | 37 |
| 65 | R | 117/118 (99%) | 100 (86%) | 17 (14%) | 3 | 15 |
| 65 | c6 | 118/118 (100%) | 102 (86%) | 16 (14%) | 3 | 17 |
| 66 | S | 94/113 (83%) | 77 (82%) | 17 (18%) | 1 | 9 |
| 67 | T | 128/128 (100%) | 104 (81%) | 24 (19%) | 1 | 8 |
| 67 | c8 | 128/128 (100%) | 111 (87%) | 17 (13%) | 4 | 17 |
| 68 | U | 115/115 (100%) | 94 (82%) | 21 (18%) | 1 | 9 |
| 68 | c9 | 115/115 (100%) | 105 (91%) | 10 (9%) | 10 | 37 |
| 69 | V | 100/103 (97%) | 84 (84%) | 16 (16%) | 2 | 12 |
| 69 | d0 | 103/103 (100%) | 89 (86%) | 14 (14%) | 3 | 17 |
| 70 | W | 74/74 (100%) | 61 (82%) | 13 (18%) | 2 | 10 |
| 70 | d1 | 74/74 (100%) | 63 (85%) | 11 (15%) | 3 | 14 |
| 71 | X | 110/110 (100%) | 91 (83%) | 19 (17%) | 2 | 10 |
| 71 | d2 | 110/110 (100%) | 99 (90%) | 11 (10%) | 7 | 29 |
| 72 | Y | 119/119 (100%) | 101 (85%) | 18 (15%) | 3 | 14 |
| 72 | d3 | 119/119 (100%) | 106 (89%) | 13 (11%) | 6 | 25 |
| 73 | Z | 112/112 (100%) | 99 (88%) | 13 (12%) | 5 | 23 |
| 73 | d4 | 112/112 (100%) | 101 (90%) | 11 (10%) | 8 | 30 |
| 74 | a | 61/61 (100%) | 44 (72%) | 17 (28%) | 0 | 2 |
| 74 | d5 | 61/61 (100%) | 57 (93%) | 4 (7%) | 16 | 49 |
| 75 | b | 83/83 (100%) | 73 (88%) | 10 (12%) | 5 | 22 |
| 75 | d6 | 83/83 (100%) | 77 (93%) | 6 (7%) | 14 | 45 |
| 76 | c | 70/70 (100%) | 63 (90%) | 7 (10%) | 7 | 29 |
| 76 | d7 | 70/70 (100%) | 63 (90%) | 7 (10%) | 7 | 29 |
| 77 | d | 56/56 (100%) | 49 (88%) | 7 (12%) | 4 | 20 |
| 77 | d8 | 56/56 (100%) | 50 (89%) | 6 (11%) | 6 | 26 |
| 78 | d9 | 47/47 (100%) | 37 (79%) | 10 (21%) | 1 | 5 |
| 78 | e | 47/47 (100%) | 39 (83%) | 8 (17%) | 2 | 10 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 79 | e0 | 53/53 (100%) | 44 (83%) | 9 (17%) | 2 10 |
| 79 | f | 51/53 (96%) | 44 (86%) | 7 (14%) | 3 17 |
| 80 | g | 62/62 (100%) | 55 (89%) | 7 (11%) | 6 24 |
| 81 | Rb | 260/261 (100%) | 243 (94%) | 17 (6%) | 17 50 |
| 81 | h | 259/261 (99%) | 241 (93%) | 18 (7%) | 15 48 |
| 82 | c7 | 92/110 (84%) | 82 (89%) | 10 (11%) | 6 25 |
| 83 | e1 | 43/43 (100%) | 33 (77%) | 10 (23%) | 1 4 |
| All | All | 18683/19203 (97%) | 16080 (86%) | 2603 (14%) | 3 16 |

5 of 2603 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 64 | Q | 26 | LEU |
| 55 | s6 | 129 | VAL |
| 67 | T | 25 | ASN |
| 64 | Q | 11 | VAL |
| 80 | g | 91 | ILE |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 58 | K | 110 | GLN |
| 56 | s7 | 71 | HIS |
| 67 | T | 25 | ASN |
| 49 | s0 | 32 | HIS |
| 66 | S | 105 | GLN |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | 1 | 3145/3149 (99%) | 550 (17%) | 62 (1%) |
| 1 | AR | 3145/3149 (99%) | 548 (17%) | 63 (2%) |
| 2 | 3 | 120/121 (99%) | 14 (11%) | 1 (0%) |
| 2 | AS | 120/121 (99%) | 14 (11%) | 1 (0%) |
| 3 | 4 | 157/158 (99%) | 31 (19%) | 3 (1%) |
| 3 | AT | 157/158 (99%) | 30 (19%) | 3 (1%) |
| 48 | A | 1778/1800 (98%) | 417 (23%) | 50 (2%) |

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| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 48 | sR | 1780/1800 (98%) | 372 (20%) | 0 |
| All | All | 10402/10456 (99%) | 1976 (18%) | 183 (1%) |

5 of 1976 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 26 | A |
| 1 | 1 | 40 | A |
| 1 | 1 | 49 | A |
| 1 | 1 | 59 | G |
| 1 | 1 | 60 | A |

5 of 183 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | AR | 2801 | A |
| 48 | A | 240 | U |
| 1 | AR | 3121 | U |
| 3 | AT | 82 | U |
| 48 | A | 503 | G |

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 2486 ligands modelled in this entry, 1 is modelled with single atom and 1410 are monoatomic - leaving 1075 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 | $\#\|Z\| > 2$ |
| 84 | OHX | 1 | 3480 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3525 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3599 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3491 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3659 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1990 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3725 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3559 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1910 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | v | 301 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3549 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3578 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3640 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3689 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3532 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AS | 210 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3628 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1995 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3690 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1939 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3416 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3526 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3574 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3455 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3557 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3473 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3446 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3512 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3588 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3423 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1902 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3667 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3606 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3657 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2020 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3451 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3734 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | e | 101 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2032 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3648 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2014 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3482 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2042 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 84 | OHX | 1 | 3603 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3617 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3569 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1981 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2048 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1989 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3506 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3700 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3570 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3416 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2047 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3559 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3716 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1941 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3683 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3670 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1912 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1958 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1972 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3610 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AT | 213 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1987 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3607 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3498 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1966 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 4 | 212 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3561 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2020 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3508 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3454 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3740 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3570 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3686 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3444 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2023 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1905 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3456 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1974 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3568 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3402 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3620 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3721 | 84 | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3677 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 84 | OHX | 1 | 3702 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1922 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 4 | 210 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3501 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3703 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3704 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3431 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3682 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3710 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3573 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3631 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3654 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1957 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3720 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1949 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1971 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3691 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3518 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AT | 215 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3499 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3411 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3655 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AS | 203 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3688 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2011 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3524 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3575 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1956 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1985 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3672 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3519 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3455 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3647 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1959 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3637 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 4 | 205 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3691 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1935 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AT | 206 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2018 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3694 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3402 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3600 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 84 | OHX | 1 | 3533 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | CE | 401 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3419 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3583 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3409 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3555 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2032 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2033 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AG | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3459 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3491 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3635 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3726 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AC | 101 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1926 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | c5 | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1965 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3507 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2040 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1977 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3453 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 4 | 208 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3448 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3437 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1960 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3457 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1932 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3662 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1946 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3463 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | J | 301 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1928 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1997 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3461 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3583 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1973 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3464 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1955 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3535 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3510 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3610 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3526 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3449 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 84 | OHX | 1 | 3579 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3612 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3493 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3538 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3728 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1945 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1970 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3667 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1937 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2010 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2033 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3637 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3537 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1916 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3653 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3409 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2037 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3721 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3428 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3401 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1996 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3561 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1920 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1923 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3501 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3560 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3704 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3573 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1931 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3531 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1940 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3629 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3479 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3689 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3685 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3621 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1925 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2046 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3529 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3592 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3414 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3499 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3718 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 84 | OHX | 1 | 3540 | 84 | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3563 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3634 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 4 | 211 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3684 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3572 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3666 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3711 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3467 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1964 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3534 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3418 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3697 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3541 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3622 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3604 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3698 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 3 | 203 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1975 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3611 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3420 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3520 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3575 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3707 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3451 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3695 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1917 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3582 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | x | 202 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1915 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3554 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AT | 214 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3548 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | CG | 303 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3588 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3616 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AT | 204 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3682 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1969 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3483 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3609 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AS | 208 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2009 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 84 | OHX | 1 | 3493 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3406 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | CX | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AT | 209 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1925 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3530 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3457 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3471 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3652 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1930 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3674 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3414 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3601 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AT | 218 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2027 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3641 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3642 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3698 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AT | 211 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3546 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1956 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1931 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 3 | 206 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1939 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3553 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3538 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 3 | 202 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3522 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3632 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | CG | 302 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1902 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3550 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3487 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3442 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3438 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1973 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3452 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1993 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3422 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1955 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2050 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3494 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1959 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 84 | OHX | A | 2003 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3428 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3638 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3439 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3523 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3503 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3537 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3433 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3615 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 4 | 206 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3515 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3630 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 4 | 202 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3551 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3636 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3465 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3594 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3720 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3739 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1985 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3522 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1903 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3661 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3717 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3486 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3629 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3479 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3744 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3685 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3449 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1994 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3536 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3676 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3619 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3407 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3592 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3475 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3590 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3519 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | y | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3585 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1928 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | l | 401 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 84 | OHX | AR | 3664 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3543 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2016 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2011 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2003 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2010 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3426 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3633 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3430 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3521 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3565 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3567 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1999 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3517 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3497 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3421 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3656 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3693 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1996 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1978 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AS | 206 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2025 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3654 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3554 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1946 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1958 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1974 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1988 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3458 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3515 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3548 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AT | 202 | 84 | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3545 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3680 | - | 0,6,6 | - | - | - | | |
| 86 | 7AL | AR | 4246 | - | 28,28,28 | 0.37 | 0 | 35,45,45 | 0.36 | 0 |
| 84 | OHX | sR | 1963 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3687 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1908 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3421 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2022 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3468 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1957 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3484 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 84 | OHX | A | 1937 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3713 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2028 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3492 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3641 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3725 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3405 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3664 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3612 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 3 | 208 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3446 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3496 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3597 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3530 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2036 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3593 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3738 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3540 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1936 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3410 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3436 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3497 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3553 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3434 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3465 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3638 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3709 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1927 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3595 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AT | 207 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1998 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3448 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3542 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AT | 216 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1979 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3406 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3438 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2009 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | H | 301 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3551 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3419 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3636 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1919 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 84 | OHX | 1 | 3512 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3605 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3635 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 4 | 214 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3602 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3673 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3681 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3442 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3653 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3730 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3475 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3560 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2012 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3645 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3593 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3618 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | CP | 501 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3470 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3488 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3401 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3477 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1911 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3498 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1910 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1907 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 4 | 215 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2007 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3580 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3494 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3520 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3656 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3703 | 84 | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2044 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3480 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2013 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1906 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3587 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1989 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2008 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3433 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3669 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3686 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1913 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 84 | OHX | sR | 1930 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3727 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3578 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3620 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2029 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1934 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1963 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3476 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1903 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3607 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3470 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1943 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3711 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1929 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3407 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3723 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1924 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | d4 | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3639 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3468 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1916 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1994 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AS | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2049 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1969 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3604 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3403 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1987 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3714 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3695 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3589 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3440 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3574 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3678 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2000 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3443 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3569 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 3 | 204 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | x | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3576 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3644 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3660 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1998 | 48 | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 84 | OHX | A | 2000 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3665 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3606 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AS | 202 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3508 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3550 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3601 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1979 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1976 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1968 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3640 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3648 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3435 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3408 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3671 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3735 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | CV | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | c3 | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3544 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3675 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2005 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1967 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2035 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1964 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2039 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3613 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1920 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3651 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1921 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3427 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3605 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3514 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3564 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3597 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3616 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3630 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1947 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2038 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3437 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3745 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1983 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3681 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3594 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 84 | OHX | AR | 3456 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2043 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1948 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3422 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3568 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | z | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3513 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3596 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3541 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3464 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3645 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3603 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3556 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3642 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3705 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3673 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2015 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3581 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3650 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | DD | 102 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2024 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 4 | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | DH | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3461 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3679 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2027 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1984 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2001 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2002 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | M | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3525 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2019 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3472 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3571 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3518 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1941 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3426 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1944 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2051 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1918 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3565 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3460 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2036 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 86 | 7AL | 1 | 4210 | - | 28,28,28 | 0.38 | 0 | 35,45,45 | 0.68 | 1 (2%) |
| 84 | OHX | AR | 3539 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1978 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3517 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3688 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3450 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3723 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3708 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3474 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 4 | 207 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3567 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3476 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3528 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1962 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3694 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3706 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3580 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1905 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2004 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1977 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3459 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3608 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3429 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3492 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3562 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3405 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3436 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3722 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3590 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3709 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3423 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1912 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3503 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1927 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1953 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1914 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3617 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3511 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3736 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | CM | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3644 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1950 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1954 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 84 | OHX | sR | 2013 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1943 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3668 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3732 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1921 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1940 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2012 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2017 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2026 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3729 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3579 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3450 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 4 | 204 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | DQ | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1951 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3417 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3663 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3410 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1962 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3513 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3652 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1942 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3701 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 3 | 207 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3563 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2034 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1972 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3546 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3413 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3542 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1950 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3557 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1908 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | CF | 401 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | O | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3478 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1909 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1913 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3531 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1904 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | d9 | 101 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3556 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3679 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 84 | OHX | sR | 1924 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3488 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1986 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | s4 | 301 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 4 | 213 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3589 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3631 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1967 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3502 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3624 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3587 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2008 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2039 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3625 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1932 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3514 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3523 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3454 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AP | 502 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3614 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3716 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AS | 207 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2042 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3586 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3477 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3507 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3655 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2041 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1970 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3528 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3622 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1926 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | CE | 402 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2038 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3439 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3581 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3463 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3715 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1942 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3543 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3415 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3625 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3584 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 84 | OHX | sR | 2040 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1952 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3577 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1982 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3742 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1923 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2005 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3717 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | r | 301 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3533 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2006 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3447 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3435 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3582 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2021 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | CX | 202 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1935 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3547 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3432 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2015 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AS | 205 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2021 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3614 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1936 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3453 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3462 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3662 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3500 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3715 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3683 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3474 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3549 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AS | 204 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1995 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3626 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1976 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3444 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2018 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3586 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3489 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | Rb | 401 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1982 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3627 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 84 | OHX | AR | 3441 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3702 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3432 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3726 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | c8 | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3608 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3660 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1999 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3675 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3547 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3676 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1947 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1933 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3524 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1975 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2022 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3496 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | CL | 302 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3545 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3408 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3731 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1909 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1944 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3687 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3478 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3485 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3511 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1986 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2031 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3746 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1914 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AT | 212 | 84 | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3509 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3413 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3713 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3502 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3596 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3624 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3699 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3733 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3404 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3462 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3504 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 84 | OHX | AT | 203 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2034 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3619 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1981 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1951 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3621 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2004 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3495 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3591 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3633 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3701 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3418 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3572 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3555 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3585 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3521 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3697 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1961 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3696 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1919 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2024 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1952 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3651 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3719 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3632 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3427 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3646 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1953 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AK | 103 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3598 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3460 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3707 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3615 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2007 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3529 | 84 | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3445 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AS | 211 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3481 | 84 | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3680 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3659 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1938 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3628 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3613 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 84 | OHX | sR | 2002 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3434 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1980 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3712 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | k | 401 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3708 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3699 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3728 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3558 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3643 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3534 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3425 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3506 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3700 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3618 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3500 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3490 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3420 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3706 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3674 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3429 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3692 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3566 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | T | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3412 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1933 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1992 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1915 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3415 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3584 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | CO | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2035 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3741 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3527 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3452 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3417 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AT | 205 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 3 | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3727 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1929 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3483 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3646 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2030 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 84 | OHX | A | 2014 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2030 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1901 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2025 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1991 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3595 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3445 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3668 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3509 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3424 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3481 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1991 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3558 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3552 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3505 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3690 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3665 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | s8 | 301 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1949 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3527 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2041 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2045 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3487 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | CG | 301 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3466 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3724 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3669 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3495 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3536 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3602 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | CL | 301 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1990 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3516 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3692 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3441 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1960 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3576 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | v | 302 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1961 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1980 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1984 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3649 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3431 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 84 | OHX | sR | 1992 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1918 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1901 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1948 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3469 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3710 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3671 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3647 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1965 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3719 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3609 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1954 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1945 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3714 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3598 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2052 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3599 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1938 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2017 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1904 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3678 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | CK | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 4 | 209 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3482 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 3 | 205 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3623 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3471 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3649 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3458 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3505 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3696 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3504 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3712 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1922 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3532 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1971 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1906 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1934 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3484 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3472 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3626 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3411 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1988 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 84 | OHX | sR | 2029 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3412 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1983 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3490 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3591 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3403 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2037 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3473 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3661 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3486 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3672 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2016 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3566 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1997 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3425 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2023 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3539 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 4 | 203 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1911 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3657 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3564 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2031 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2006 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3489 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3443 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3650 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3658 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3571 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3467 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AS | 209 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3544 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3430 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3424 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3623 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 2001 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3718 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3611 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AK | 102 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3627 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AT | 217 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3684 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3643 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3639 | - | 0,6,6 | - | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 84 | OHX | AR | 3693 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3552 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3404 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3737 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3577 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3670 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | h | 401 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1917 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1993 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3724 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1907 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3658 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3743 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3466 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3562 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3722 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2026 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3447 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3535 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3510 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | Q | 201 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | DL | 101 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3730 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 1968 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | sR | 1966 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3731 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3729 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3634 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3677 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | CF | 402 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | s1 | 301 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3485 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3663 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AT | 208 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AT | 210 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | AR | 3666 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2019 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3469 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3516 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3600 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | A | 2028 | - | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3705 | 84 | 0,6,6 | - | - | - | | |
| 84 | OHX | 1 | 3440 | - | 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 |
|---|---|---|---|---|---|---|---|
| 86 | 7AL | AR | 4246 | - | - | 2/8/60/60 | 0/3/3/3 |
| 86 | 7AL | 1 | 4210 | - | - | 2/8/60/60 | 0/3/3/3 |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 86 | 1 | 4210 | 7AL | O4-C8-C7 | 2.33 | 114.89 | 109.92 |

There are no chirality outliers.

All (4) torsion outliers are listed below:

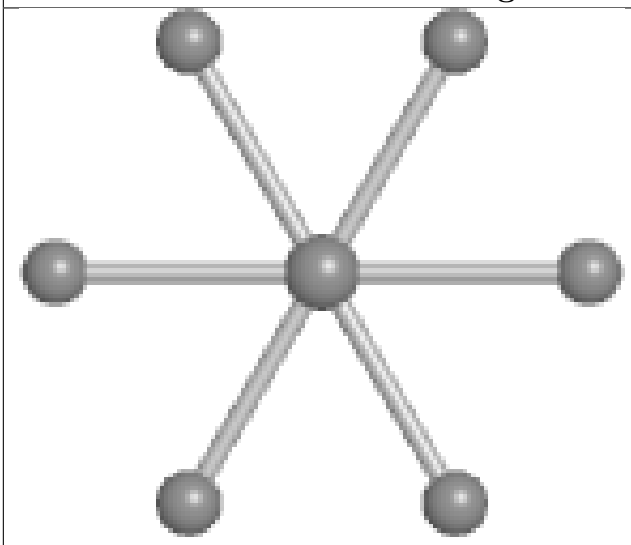
| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 86 | 1 | 4210 | 7AL | C10-C14-C15-C16 |
| 86 | AR | 4246 | 7AL | C10-C14-C15-C16 |
| 86 | 1 | 4210 | 7AL | C10-C14-C15-O1 |
| 86 | AR | 4246 | 7AL | C10-C14-C15-O1 |

There are no ring outliers.

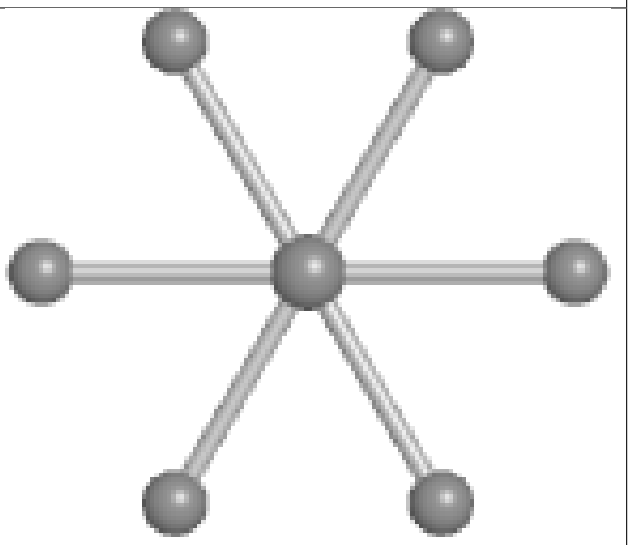
No monomer is involved in short contacts.

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 then 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.

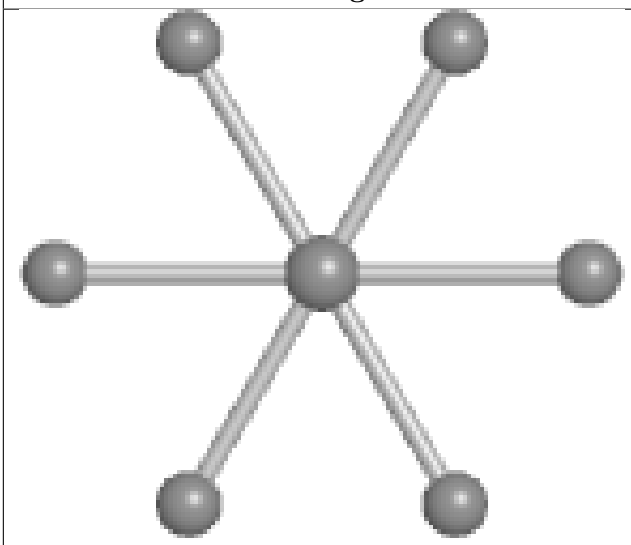
**Ligand OHX AR 3740**



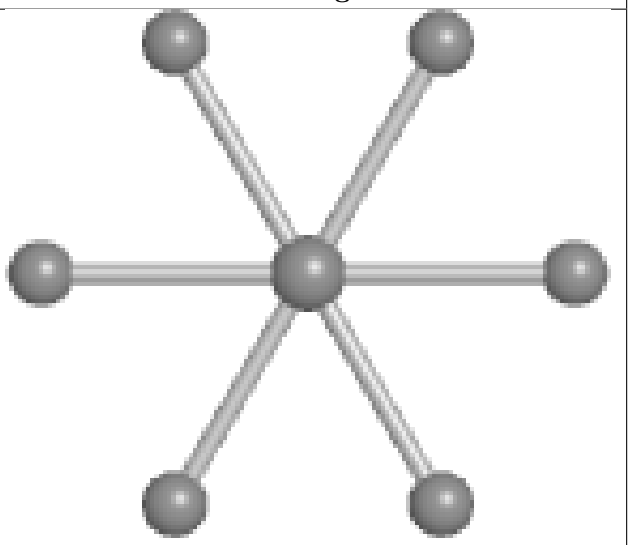
**Bond lengths**



**Bond angles**

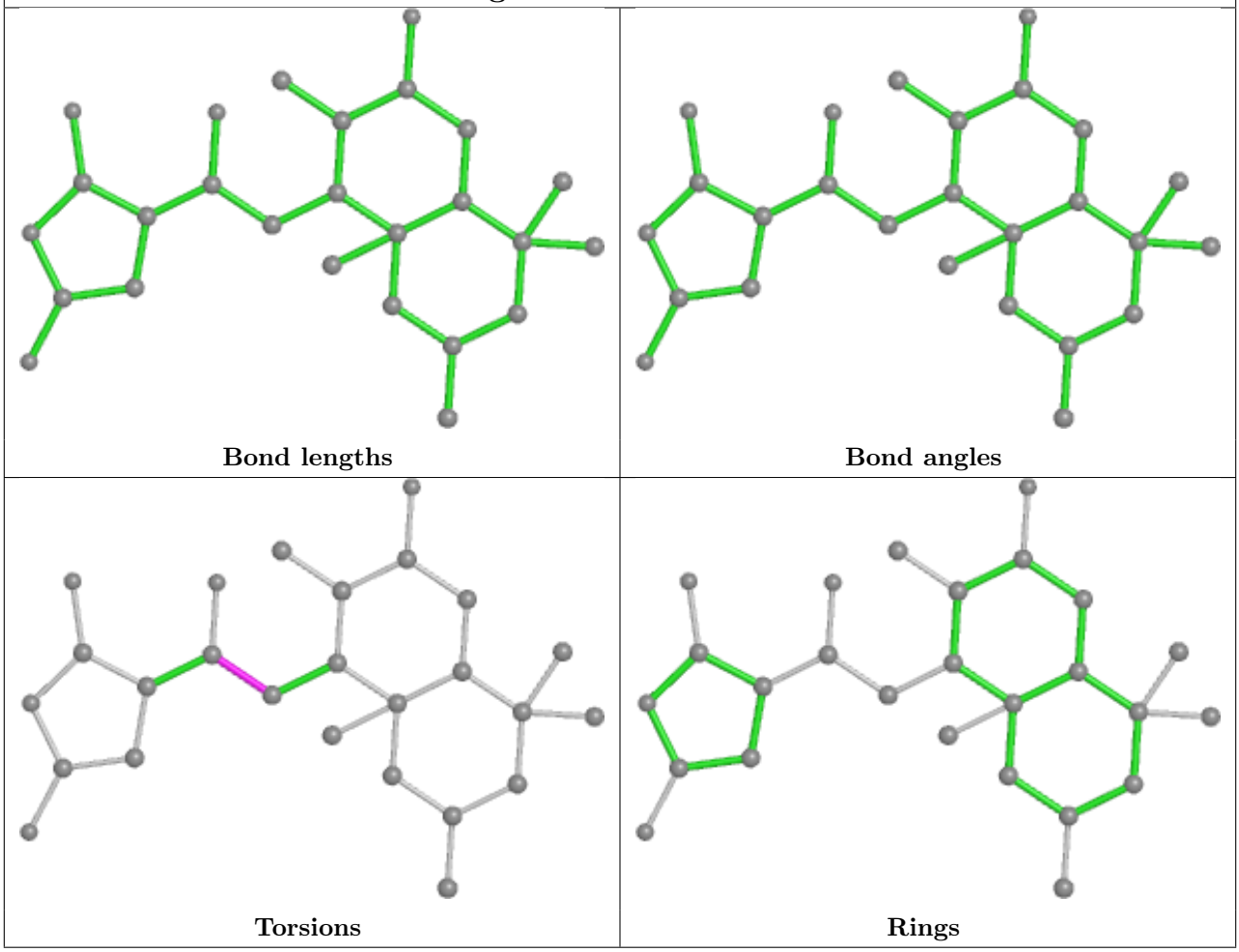


**Torsions**

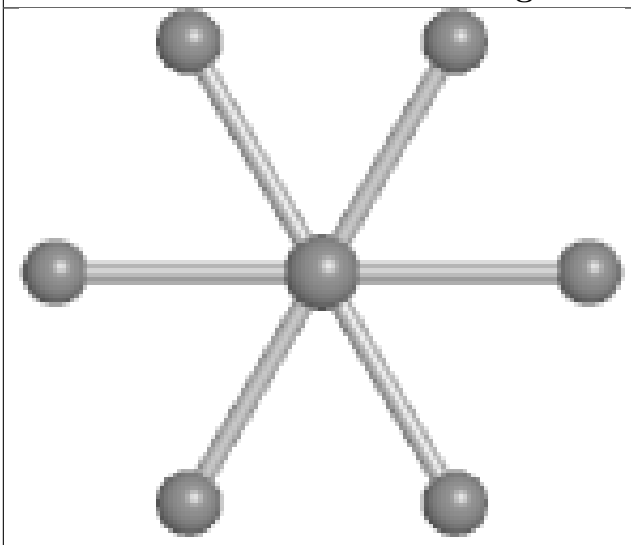


**Rings**

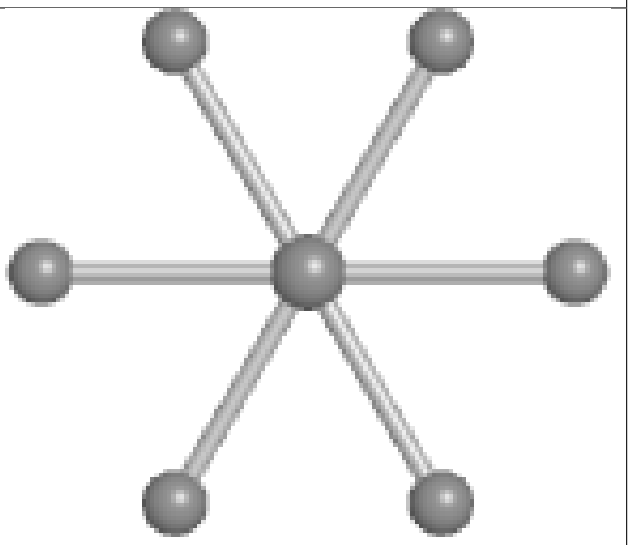
**Ligand 7AL AR 4246**



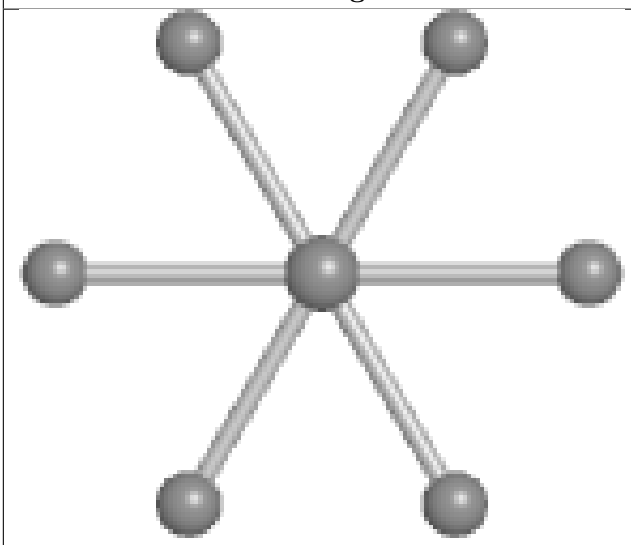
**Ligand OHX 1 3673**



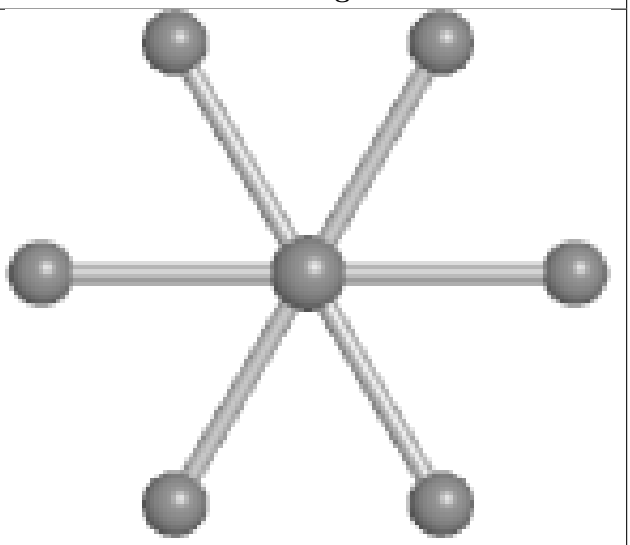
**Bond lengths**



**Bond angles**

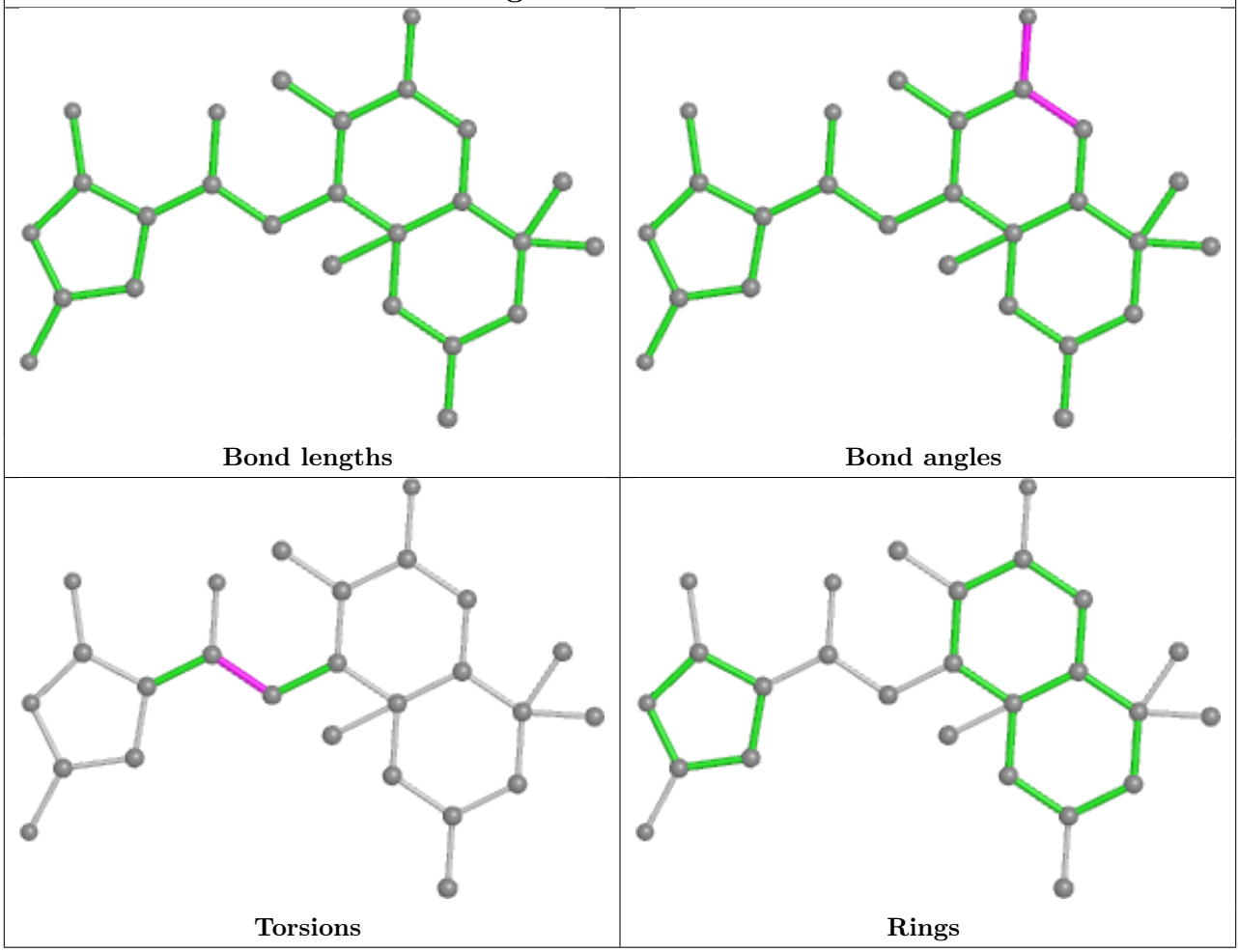


**Torsions**

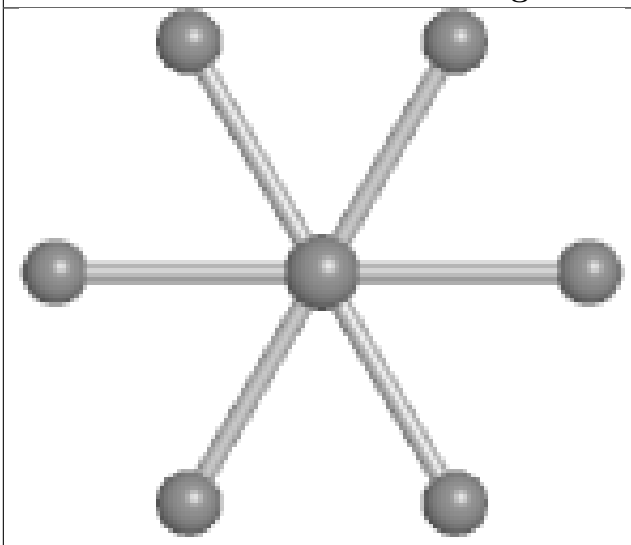


**Rings**

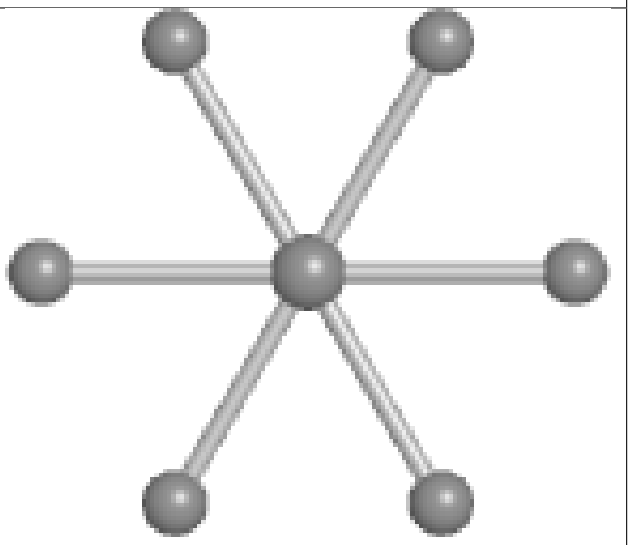
**Ligand 7AL 1 4210**



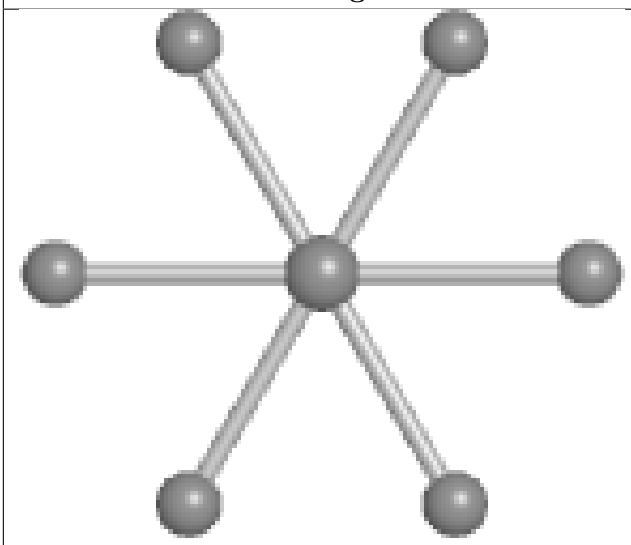
**Ligand OHX A 2039**



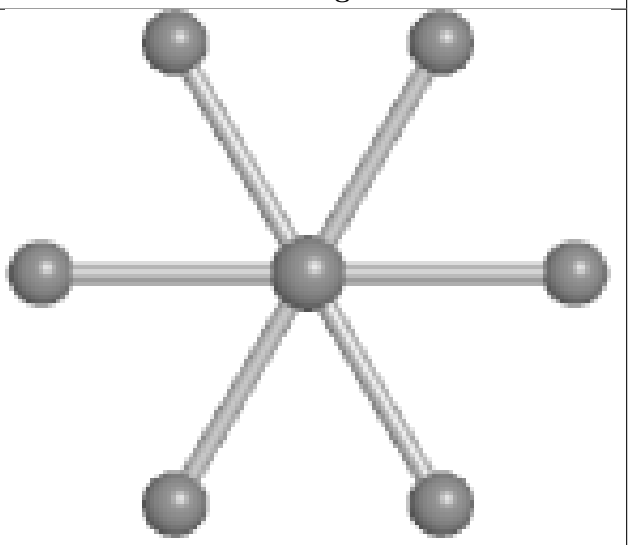
**Bond lengths**



**Bond angles**

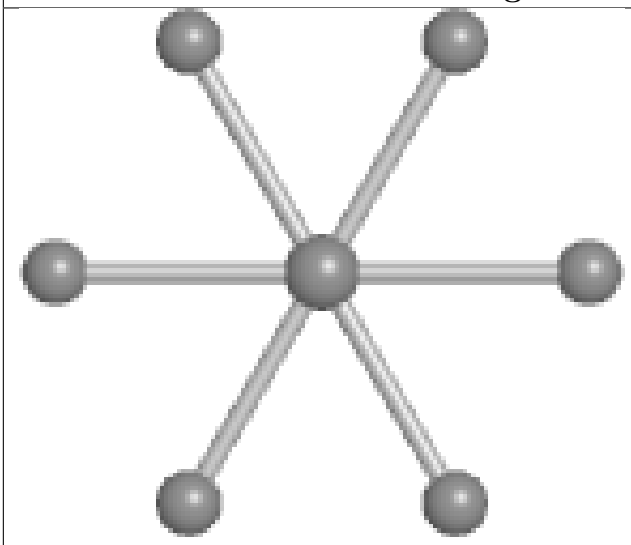


**Torsions**

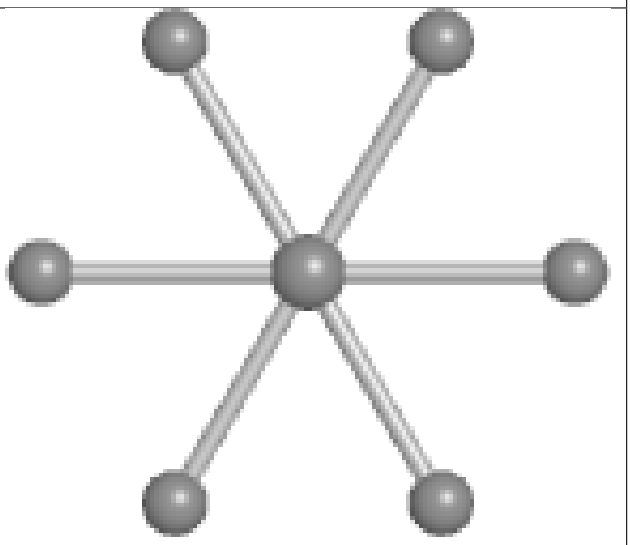


**Rings**

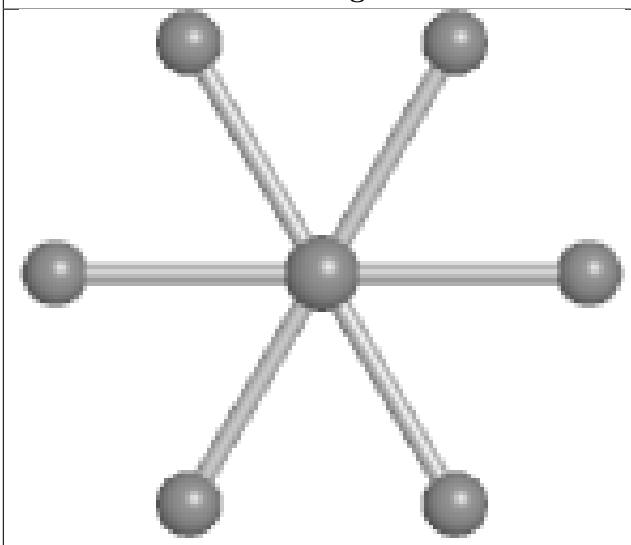
**Ligand OHX sR 2040**



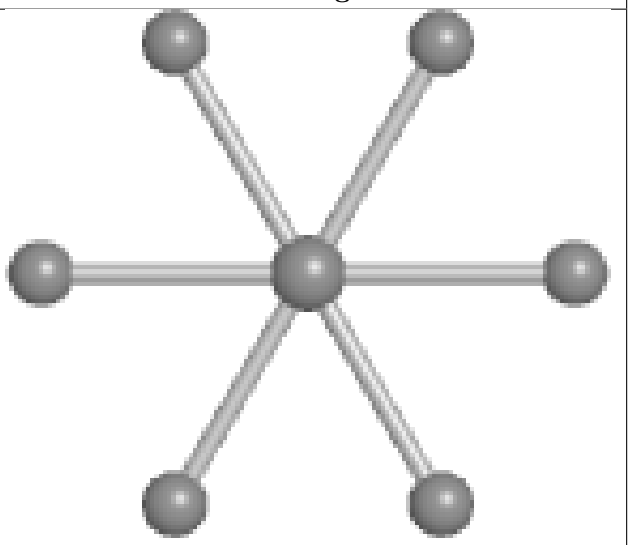
**Bond lengths**



**Bond angles**

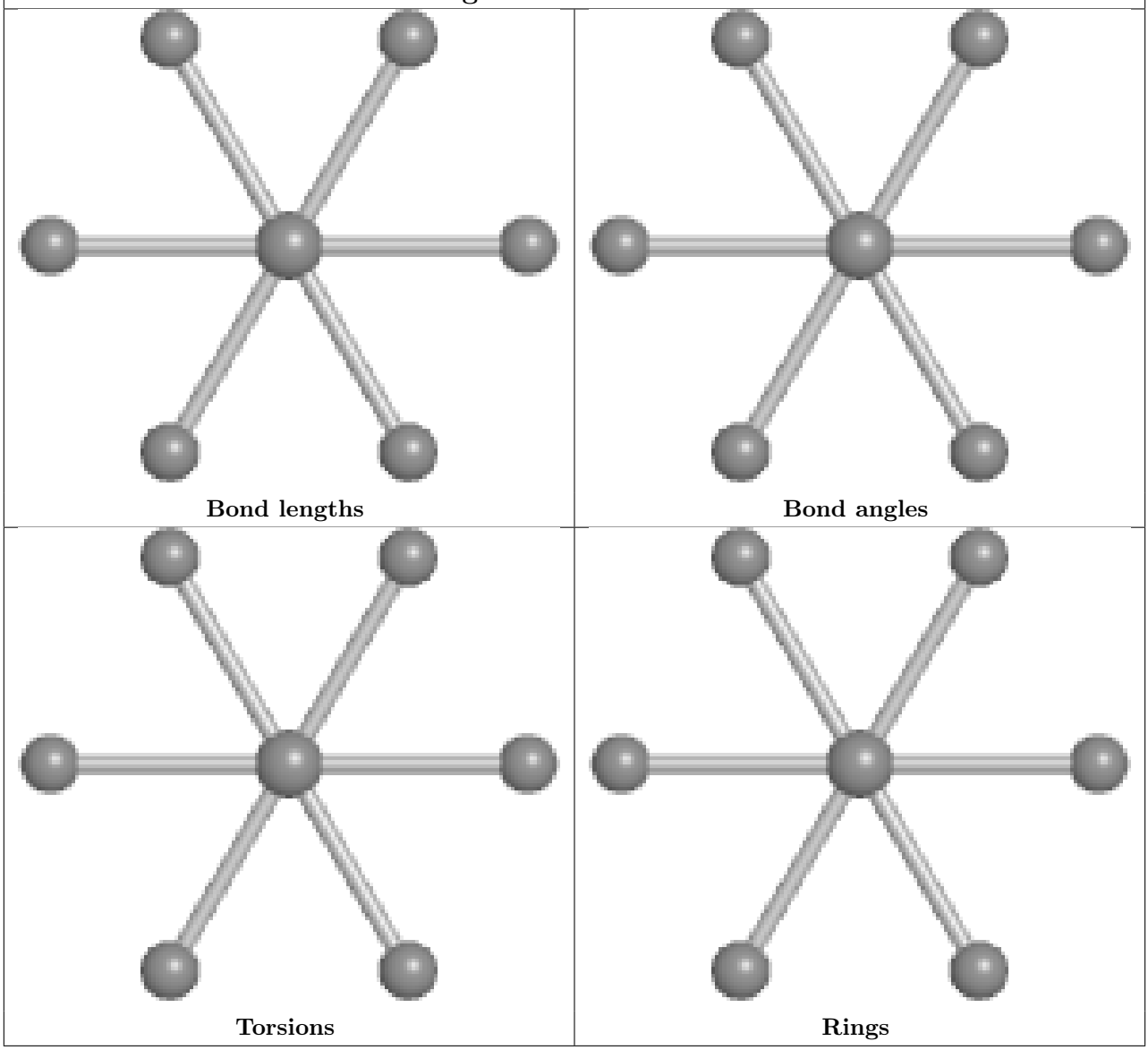


**Torsions**



**Rings**

**Ligand OHX 1 3718**




## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 1 | 1 | 3 |
| 1 | AR | 3 |
| 47 | sM | 2 |

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| Mol | Chain | Number of breaks |
|---|---|---|
| 48 | A | 1 |

The worst 5 of 9 chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | sM | 85:SER | C | 119:UNK | N | 43.91 |
| 1 | sM | 139:UNK | C | 155:UNK | N | 37.53 |
| 1 | 1 | 1955:U | O3' | 2093:A | P | 25.84 |
| 1 | AR | 1955:U | O3' | 2093:A | P | 24.08 |
| 1 | 1 | 2445:A | O3' | 2501:U | P | 15.80 |

# 6 Fit of model and data (i)

## 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, $95^{th}$ 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$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 3149/3149 (100%) | -0.02 | 78 (2%) | 57 | 29 | 23, 45, 148, 258 | 0 |
| 1 | AR | 3149/3149 (100%) | -0.00 | 87 (2%) | 53 | 25 | 24, 48, 147, 276 | 0 |
| 2 | 3 | 121/121 (100%) | -0.34 | 0 | 100 | 100 | 33, 61, 76, 92 | 0 |
| 2 | AS | 121/121 (100%) | -0.33 | 0 | 100 | 100 | 30, 54, 69, 103 | 0 |
| 3 | 4 | 158/158 (100%) | -0.10 | 1 (0%) | 89 | 72 | 28, 46, 98, 165 | 0 |
| 3 | AT | 158/158 (100%) | -0.06 | 2 (1%) | 77 | 51 | 35, 57, 112, 166 | 0 |
| 4 | CD | 252/252 (100%) | -0.27 | 2 (0%) | 86 | 65 | 31, 51, 76, 131 | 0 |
| 4 | j | 252/252 (100%) | -0.27 | 0 | 100 | 100 | 26, 45, 64, 113 | 0 |
| 5 | CE | 386/386 (100%) | -0.35 | 2 (0%) | 91 | 75 | 24, 42, 66, 121 | 0 |
| 5 | k | 386/386 (100%) | -0.36 | 1 (0%) | 94 | 84 | 26, 49, 69, 116 | 0 |
| 6 | CF | 361/361 (100%) | -0.33 | 0 | 100 | 100 | 28, 48, 75, 107 | 0 |
| 6 | l | 361/361 (100%) | -0.34 | 0 | 100 | 100 | 24, 43, 72, 92 | 0 |
| 7 | CG | 296/296 (100%) | -0.14 | 4 (1%) | 75 | 49 | 40, 56, 94, 133 | 0 |
| 7 | m | 296/296 (100%) | 0.09 | 6 (2%) | 65 | 36 | 42, 70, 104, 152 | 0 |
| 8 | CH | 156/175 (89%) | -0.25 | 3 (1%) | 66 | 37 | 36, 47, 85, 108 | 0 |
| 8 | n | 156/175 (89%) | -0.34 | 0 | 100 | 100 | 33, 44, 74, 119 | 0 |
| 9 | CI | 222/222 (100%) | -0.30 | 3 (1%) | 75 | 49 | 28, 38, 86, 165 | 0 |
| 9 | o | 222/222 (100%) | -0.33 | 2 (0%) | 84 | 63 | 28, 38, 75, 155 | 0 |
| 10 | CJ | 233/233 (100%) | 0.73 | 22 (9%) | 8 | 3 | 65, 82, 141, 172 | 0 |
| 10 | p | 233/233 (100%) | 0.18 | 4 (1%) | 70 | 41 | 50, 68, 138, 161 | 0 |
| 11 | CK | 191/191 (100%) | -0.22 | 3 (1%) | 72 | 44 | 36, 47, 78, 142 | 0 |
| 11 | q | 191/191 (100%) | -0.31 | 1 (0%) | 91 | 75 | 41, 56, 75, 141 | 0 |
| 12 | CL | 211/220 (95%) | 0.02 | 6 (2%) | 53 | 25 | 29, 55, 91, 155 | 0 |
| 12 | r | 211/220 (95%) | -0.24 | 0 | 100 | 100 | 28, 48, 95, 119 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 13 | CM | 169/169 (100%) | -0.21 | 1 (0%) | 89 | 72 | 42, 62, 82, 103 | 0 |
| 13 | s | 169/169 (100%) | -0.04 | 1 (0%) | 89 | 72 | 50, 73, 91, 114 | 0 |
| 14 | CN | 193/193 (100%) | 0.10 | 5 (2%) | 56 | 27 | 31, 61, 121, 150 | 0 |
| 14 | t | 193/193 (100%) | -0.16 | 2 (1%) | 82 | 59 | 25, 51, 110, 138 | 0 |
| 15 | CO | 136/136 (100%) | -0.42 | 1 (0%) | 87 | 69 | 35, 43, 72, 91 | 0 |
| 15 | u | 136/136 (100%) | -0.42 | 0 | 100 | 100 | 38, 46, 70, 86 | 0 |
| 16 | CP | 203/203 (100%) | -0.22 | 0 | 100 | 100 | 34, 52, 66, 70 | 0 |
| 16 | v | 203/203 (100%) | -0.36 | 0 | 100 | 100 | 26, 42, 54, 71 | 0 |
| 17 | CQ | 197/197 (100%) | -0.26 | 3 (1%) | 73 | 46 | 24, 35, 75, 89 | 0 |
| 17 | w | 197/197 (100%) | -0.37 | 0 | 100 | 100 | 27, 38, 65, 71 | 0 |
| 18 | CR | 183/183 (100%) | 1.09 | 29 (15%) | 2 | 1 | 27, 40, 169, 211 | 0 |
| 18 | x | 183/183 (100%) | 0.18 | 14 (7%) | 13 | 4 | 30, 39, 137, 171 | 0 |
| 19 | CS | 185/185 (100%) | -0.35 | 0 | 100 | 100 | 31, 45, 60, 78 | 0 |
| 19 | y | 185/185 (100%) | -0.29 | 0 | 100 | 100 | 30, 42, 79, 117 | 0 |
| 20 | CT | 188/188 (100%) | 0.12 | 11 (5%) | 22 | 7 | 44, 63, 165, 184 | 0 |
| 20 | z | 188/188 (100%) | 0.19 | 13 (6%) | 16 | 5 | 44, 60, 163, 180 | 0 |
| 21 | 0 | 172/172 (100%) | -0.30 | 2 (1%) | 79 | 54 | 33, 43, 64, 89 | 0 |
| 21 | CU | 172/172 (100%) | -0.38 | 2 (1%) | 79 | 54 | 29, 40, 62, 77 | 0 |
| 22 | 2 | 159/159 (100%) | -0.20 | 2 (1%) | 77 | 51 | 29, 44, 105, 121 | 0 |
| 22 | CV | 159/159 (100%) | -0.21 | 0 | 100 | 100 | 29, 42, 100, 120 | 0 |
| 23 | 5 | 100/100 (100%) | 0.72 | 11 (11%) | 5 | 2 | 76, 99, 124, 160 | 0 |
| 23 | CW | 100/100 (100%) | 1.19 | 19 (19%) | 1 | 0 | 74, 95, 120, 141 | 0 |
| 24 | 6 | 136/136 (100%) | -0.15 | 1 (0%) | 87 | 69 | 33, 46, 73, 108 | 0 |
| 24 | CX | 136/136 (100%) | 0.02 | 3 (2%) | 62 | 33 | 28, 42, 67, 92 | 0 |
| 25 | 7 | 98/98 (100%) | 1.70 | 32 (32%) | 0 | 0 | 42, 58, 175, 180 | 0 |
| 25 | CY | 98/98 (100%) | 1.01 | 17 (17%) | 1 | 0 | 39, 54, 177, 215 | 0 |
| 26 | 8 | 121/121 (100%) | -0.14 | 0 | 100 | 100 | 40, 57, 79, 136 | 0 |
| 26 | CZ | 121/121 (100%) | -0.01 | 2 (1%) | 70 | 41 | 46, 63, 89, 142 | 0 |
| 27 | 9 | 126/126 (100%) | -0.15 | 1 (0%) | 86 | 65 | 33, 50, 69, 92 | 0 |
| 27 | DA | 126/126 (100%) | -0.02 | 2 (1%) | 72 | 44 | 37, 55, 79, 96 | 0 |
| 28 | AA | 135/135 (100%) | 0.66 | 6 (4%) | 34 | 13 | 65, 80, 103, 111 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 28 | DB | 135/135 (100%) | 0.65 | 9 (6%) 17 5 | 75, 97, 119, 125 | 0 |
| 29 | AB | 148/148 (100%) | -0.22 | 0 100 100 | 24, 42, 79, 92 | 0 |
| 29 | DC | 148/148 (100%) | -0.15 | 0 100 100 | 26, 49, 78, 89 | 0 |
| 30 | AC | 58/58 (100%) | -0.20 | 0 100 100 | 27, 47, 111, 141 | 0 |
| 30 | DD | 58/58 (100%) | -0.21 | 1 (1%) 70 41 | 30, 53, 92, 108 | 0 |
| 31 | AD | 97/97 (100%) | 0.27 | 3 (3%) 49 21 | 62, 75, 101, 127 | 0 |
| 31 | DE | 97/97 (100%) | 0.35 | 5 (5%) 27 10 | 69, 84, 117, 131 | 0 |
| 32 | AE | 109/109 (100%) | -0.06 | 3 (2%) 53 25 | 40, 58, 116, 136 | 0 |
| 32 | DF | 109/109 (100%) | -0.02 | 5 (4%) 32 12 | 39, 53, 120, 142 | 0 |
| 33 | AF | 127/127 (100%) | -0.14 | 2 (1%) 72 44 | 24, 37, 56, 121 | 0 |
| 33 | DG | 127/127 (100%) | -0.05 | 3 (2%) 59 30 | 25, 41, 59, 124 | 0 |
| 34 | AG | 106/106 (100%) | -0.42 | 0 100 100 | 28, 36, 62, 95 | 0 |
| 34 | DH | 106/106 (100%) | -0.34 | 0 100 100 | 28, 36, 68, 120 | 0 |
| 35 | AH | 112/112 (100%) | -0.01 | 4 (3%) 42 17 | 39, 59, 119, 136 | 0 |
| 35 | DI | 112/112 (100%) | -0.00 | 2 (1%) 68 40 | 44, 67, 126, 145 | 0 |
| 36 | AI | 119/119 (100%) | -0.06 | 1 (0%) 86 65 | 36, 59, 75, 83 | 0 |
| 36 | DJ | 119/119 (100%) | -0.06 | 2 (1%) 70 41 | 45, 68, 84, 91 | 0 |
| 37 | AJ | 99/99 (100%) | 0.07 | 6 (6%) 21 7 | 46, 60, 108, 143 | 0 |
| 37 | DK | 99/99 (100%) | 0.41 | 6 (6%) 21 7 | 59, 72, 112, 151 | 0 |
| 38 | AK | 87/87 (100%) | -0.11 | 2 (2%) 60 31 | 29, 36, 59, 114 | 0 |
| 38 | DL | 87/87 (100%) | 0.05 | 2 (2%) 60 31 | 34, 43, 74, 156 | 0 |
| 39 | AL | 77/77 (100%) | 0.43 | 1 (1%) 77 51 | 64, 84, 120, 132 | 0 |
| 39 | DM | 77/77 (100%) | 1.47 | 20 (25%) 0 0 | 67, 91, 127, 132 | 0 |
| 40 | AM | 50/50 (100%) | -0.25 | 1 (2%) 65 36 | 33, 47, 58, 65 | 0 |
| 40 | DN | 50/50 (100%) | -0.26 | 0 100 100 | 42, 52, 65, 77 | 0 |
| 41 | AN | 52/52 (100%) | -0.22 | 1 (1%) 66 37 | 36, 45, 69, 100 | 0 |
| 41 | DO | 52/52 (100%) | -0.37 | 0 100 100 | 30, 36, 59, 92 | 0 |
| 42 | AO | 25/25 (100%) | -0.14 | 0 100 100 | 50, 55, 64, 71 | 0 |
| 42 | DP | 25/25 (100%) | -0.17 | 0 100 100 | 45, 53, 65, 76 | 0 |
| 43 | AP | 105/105 (100%) | 0.04 | 2 (1%) 66 37 | 28, 49, 81, 150 | 0 |
| 43 | DQ | 105/105 (100%) | -0.10 | 1 (0%) 82 59 | 33, 50, 81, 142 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 44 | AQ | 91/91 (100%) | -0.31 | 0 | 100 | 100 | 36, 49, 81, 96 | 0 |
| 44 | DR | 91/91 (100%) | -0.31 | 0 | 100 | 100 | 36, 54, 76, 84 | 0 |
| 45 | i | 159/168 (94%) | 0.90 | 25 (15%) | 2 | 1 | 49, 98, 163, 168 | 0 |
| 46 | p0 | 143/219 (65%) | 1.32 | 37 (25%) | 0 | 0 | 85, 106, 174, 178 | 0 |
| 47 | sM | 63/104 (60%) | 0.89 | 12 (19%) | 1 | 0 | 55, 105, 131, 138 | 0 |
| 48 | A | 1781/1800 (98%) | 0.16 | 89 (4%) | 28 | 10 | 45, 84, 220, 289 | 0 |
| 48 | sR | 1783/1800 (99%) | 0.14 | 88 (4%) | 29 | 11 | 39, 76, 187, 269 | 0 |
| 49 | B | 206/206 (100%) | 0.73 | 24 (11%) | 4 | 1 | 90, 114, 140, 174 | 0 |
| 49 | s0 | 206/206 (100%) | 0.47 | 14 (6%) | 17 | 5 | 76, 100, 125, 142 | 0 |
| 50 | C | 214/216 (99%) | 1.23 | 44 (20%) | 1 | 0 | 93, 128, 163, 175 | 0 |
| 50 | s1 | 216/216 (100%) | 0.54 | 12 (5%) | 24 | 8 | 66, 85, 121, 152 | 0 |
| 51 | D | 217/217 (100%) | 0.13 | 4 (1%) | 68 | 40 | 71, 90, 113, 136 | 0 |
| 51 | s2 | 217/217 (100%) | 0.16 | 6 (2%) | 53 | 25 | 59, 79, 101, 128 | 0 |
| 52 | E | 223/223 (100%) | 0.48 | 13 (5%) | 23 | 7 | 74, 93, 131, 173 | 0 |
| 52 | s3 | 223/223 (100%) | 0.42 | 10 (4%) | 33 | 12 | 73, 106, 139, 159 | 0 |
| 53 | F | 260/260 (100%) | 0.41 | 8 (3%) | 49 | 21 | 65, 85, 104, 157 | 0 |
| 53 | s4 | 260/260 (100%) | 0.19 | 6 (2%) | 60 | 31 | 54, 80, 100, 152 | 0 |
| 54 | G | 206/206 (100%) | 0.96 | 30 (14%) | 2 | 1 | 89, 114, 139, 171 | 0 |
| 54 | s5 | 206/206 (100%) | 0.94 | 27 (13%) | 3 | 1 | 78, 106, 139, 163 | 0 |
| 55 | H | 226/226 (100%) | 0.50 | 17 (7%) | 14 | 4 | 61, 95, 135, 168 | 0 |
| 55 | s6 | 218/226 (96%) | 0.29 | 13 (5%) | 21 | 7 | 49, 80, 118, 141 | 0 |
| 56 | I | 184/186 (98%) | 0.85 | 24 (13%) | 3 | 1 | 81, 117, 151, 173 | 0 |
| 56 | s7 | 186/186 (100%) | 0.91 | 25 (13%) | 3 | 1 | 74, 111, 152, 173 | 0 |
| 57 | J | 188/199 (94%) | 0.17 | 6 (3%) | 47 | 20 | 47, 65, 105, 130 | 0 |
| 57 | s8 | 188/199 (94%) | 0.35 | 9 (4%) | 30 | 11 | 43, 71, 119, 137 | 0 |
| 58 | K | 185/185 (100%) | 0.79 | 20 (10%) | 5 | 2 | 81, 98, 138, 175 | 0 |
| 58 | s9 | 185/185 (100%) | 0.49 | 10 (5%) | 25 | 9 | 67, 83, 126, 178 | 0 |
| 59 | L | 96/105 (91%) | 0.55 | 1 (1%) | 82 | 59 | 74, 102, 139, 163 | 0 |
| 59 | c0 | 96/105 (91%) | 1.48 | 24 (25%) | 0 | 0 | 92, 127, 157, 175 | 0 |
| 60 | M | 155/155 (100%) | 0.57 | 18 (11%) | 4 | 1 | 52, 65, 151, 176 | 0 |
| 60 | c1 | 146/155 (94%) | 0.35 | 10 (6%) | 17 | 5 | 49, 68, 116, 134 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 61 | N | 124/143 (86%) | 1.78 | 50 (40%) | 0 | 0 | 124, 148, 177, 187 | 0 |
| 61 | c2 | 124/143 (86%) | 2.68 | 77 (62%) | 0 | 0 | 167, 178, 203, 219 | 0 |
| 62 | O | 150/150 (100%) | 0.20 | 4 (2%) | 54 | 26 | 58, 84, 107, 127 | 0 |
| 62 | c3 | 150/150 (100%) | -0.07 | 0 | 100 | 100 | 56, 77, 102, 126 | 0 |
| 63 | P | 127/128 (99%) | 1.28 | 31 (24%) | 0 | 0 | 67, 131, 155, 163 | 0 |
| 63 | c4 | 128/128 (100%) | 0.66 | 12 (9%) | 8 | 3 | 53, 87, 102, 110 | 0 |
| 64 | Q | 124/135 (91%) | 0.49 | 6 (4%) | 30 | 11 | 69, 86, 147, 175 | 0 |
| 64 | c5 | 135/135 (100%) | 0.75 | 16 (11%) | 4 | 1 | 77, 100, 139, 149 | 0 |
| 65 | R | 141/142 (99%) | 0.80 | 19 (13%) | 3 | 1 | 76, 104, 114, 121 | 0 |
| 65 | c6 | 142/142 (100%) | 0.66 | 13 (9%) | 9 | 3 | 65, 99, 118, 149 | 0 |
| 66 | S | 120/125 (96%) | 0.40 | 11 (9%) | 9 | 3 | 83, 111, 155, 165 | 0 |
| 67 | T | 145/145 (100%) | 0.56 | 15 (10%) | 6 | 2 | 66, 100, 134, 148 | 0 |
| 67 | c8 | 145/145 (100%) | 0.50 | 13 (8%) | 9 | 3 | 78, 95, 133, 156 | 0 |
| 68 | U | 143/143 (100%) | 0.53 | 10 (6%) | 16 | 5 | 78, 99, 125, 149 | 0 |
| 68 | c9 | 143/143 (100%) | 0.53 | 12 (8%) | 11 | 3 | 71, 93, 120, 146 | 0 |
| 69 | V | 107/110 (97%) | 1.02 | 24 (22%) | 0 | 0 | 66, 107, 159, 169 | 0 |
| 69 | d0 | 110/110 (100%) | 1.34 | 28 (25%) | 0 | 0 | 68, 113, 164, 172 | 0 |
| 70 | W | 87/87 (100%) | 0.56 | 7 (8%) | 12 | 4 | 89, 98, 123, 140 | 0 |
| 70 | d1 | 87/87 (100%) | 0.29 | 5 (5%) | 23 | 8 | 70, 83, 115, 136 | 0 |
| 71 | X | 129/129 (100%) | 0.20 | 1 (0%) | 86 | 65 | 64, 80, 92, 97 | 0 |
| 71 | d2 | 129/129 (100%) | -0.19 | 0 | 100 | 100 | 54, 68, 77, 86 | 0 |
| 72 | Y | 144/144 (100%) | -0.06 | 0 | 100 | 100 | 52, 62, 77, 113 | 0 |
| 72 | d3 | 144/144 (100%) | -0.11 | 1 (0%) | 87 | 69 | 43, 52, 71, 108 | 0 |
| 73 | Z | 134/134 (100%) | 0.58 | 7 (5%) | 27 | 10 | 63, 97, 136, 156 | 0 |
| 73 | d4 | 134/134 (100%) | 0.18 | 5 (3%) | 41 | 17 | 58, 86, 117, 146 | 0 |
| 74 | a | 70/70 (100%) | 1.49 | 23 (32%) | 0 | 0 | 110, 129, 149, 159 | 0 |
| 74 | d5 | 69/70 (98%) | 1.45 | 22 (31%) | 0 | 0 | 90, 122, 141, 152 | 0 |
| 75 | b | 97/97 (100%) | 0.86 | 15 (15%) | 2 | 1 | 73, 101, 162, 171 | 0 |
| 75 | d6 | 97/97 (100%) | 0.15 | 2 (2%) | 63 | 34 | 55, 76, 112, 124 | 0 |
| 76 | c | 81/81 (100%) | 0.86 | 10 (12%) | 4 | 1 | 77, 96, 147, 155 | 0 |
| 76 | d7 | 81/81 (100%) | 0.69 | 12 (14%) | 2 | 1 | 68, 84, 146, 162 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 77 | d | 63/63 (100%) | 1.22 | 11 (17%) | 1 | 0 | 106, 124, 145, 152 | 0 |
| 77 | d8 | 63/63 (100%) | 1.59 | 20 (31%) | 0 | 0 | 94, 117, 146, 163 | 0 |
| 78 | d9 | 53/53 (100%) | 0.40 | 2 (3%) | 40 | 16 | 68, 80, 127, 157 | 0 |
| 78 | e | 53/53 (100%) | -0.08 | 1 (1%) | 66 | 37 | 68, 75, 95, 120 | 0 |
| 79 | e0 | 62/62 (100%) | 0.71 | 6 (9%) | 7 | 2 | 55, 83, 146, 149 | 0 |
| 79 | f | 60/62 (96%) | 1.21 | 8 (13%) | 3 | 1 | 55, 92, 162, 167 | 0 |
| 80 | g | 71/71 (100%) | 1.15 | 15 (21%) | 1 | 0 | 100, 130, 157, 167 | 0 |
| 81 | Rb | 318/318 (100%) | 1.31 | 80 (25%) | 0 | 0 | 103, 125, 145, 164 | 0 |
| 81 | h | 318/318 (100%) | 0.89 | 43 (13%) | 3 | 1 | 92, 114, 155, 188 | 0 |
| 82 | c7 | 117/121 (96%) | 0.32 | 6 (5%) | 28 | 10 | 76, 101, 137, 150 | 0 |
| 83 | e1 | 51/51 (100%) | 1.49 | 15 (29%) | 0 | 0 | 145, 158, 171, 177 | 0 |
| All | All | 33004/33349 (98%) | 0.19 | 1773 (5%) | 25 | 9 | 23, 66, 144, 289 | 0 |

The worst 5 of 1773 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 18 | CR | 161 | ALA | 21.9 |
| 18 | CR | 160 | ALA | 18.7 |
| 25 | 7 | 76 | VAL | 16.1 |
| 25 | 7 | 75 | THR | 15.5 |
| 18 | CR | 162 | GLU | 15.3 |

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

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

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95$^{th}$ 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$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | AR | 3834 | 1/1 | 0.28 | 0.47 | 61,61,61,61 | 0 |
| 85 | MG | 1 | 4165 | 1/1 | 0.32 | 0.36 | 153,153,153,153 | 0 |
| 85 | MG | AR | 4138 | 1/1 | 0.39 | 0.48 | 75,75,75,75 | 0 |
| 85 | MG | AR | 4055 | 1/1 | 0.40 | 0.54 | 72,72,72,72 | 0 |
| 85 | MG | 1 | 3970 | 1/1 | 0.41 | 0.29 | 82,82,82,82 | 0 |
| 85 | MG | sR | 2066 | 1/1 | 0.41 | 0.43 | 73,73,73,73 | 0 |
| 85 | MG | AR | 4156 | 1/1 | 0.43 | 0.66 | 56,56,56,56 | 0 |
| 85 | MG | 4 | 229 | 1/1 | 0.47 | 0.37 | 55,55,55,55 | 0 |
| 85 | MG | sR | 2157 | 1/1 | 0.47 | 0.66 | 71,71,71,71 | 0 |
| 85 | MG | 3 | 210 | 1/1 | 0.52 | 0.45 | 46,46,46,46 | 0 |
| 85 | MG | AR | 4006 | 1/1 | 0.53 | 0.20 | 54,54,54,54 | 0 |
| 85 | MG | 1 | 3822 | 1/1 | 0.55 | 0.73 | 69,69,69,69 | 0 |
| 85 | MG | AR | 4102 | 1/1 | 0.56 | 0.69 | 53,53,53,53 | 0 |
| 85 | MG | 3 | 216 | 1/1 | 0.57 | 0.49 | 78,78,78,78 | 0 |
| 85 | MG | AR | 4126 | 1/1 | 0.57 | 0.79 | 46,46,46,46 | 0 |
| 85 | MG | AR | 4230 | 1/1 | 0.58 | 0.40 | 59,59,59,59 | 0 |
| 85 | MG | A | 2119 | 1/1 | 0.59 | 0.67 | 66,66,66,66 | 0 |
| 85 | MG | AR | 3957 | 1/1 | 0.59 | 0.30 | 57,57,57,57 | 0 |
| 85 | MG | sR | 2142 | 1/1 | 0.59 | 0.28 | 65,65,65,65 | 0 |
| 85 | MG | AR | 4113 | 1/1 | 0.59 | 0.52 | 63,63,63,63 | 0 |
| 84 | OHX | AR | 3742 | 7/7 | 0.60 | 0.35 | 225,225,226,226 | 0 |
| 85 | MG | AR | 4004 | 1/1 | 0.60 | 0.36 | 68,68,68,68 | 0 |
| 85 | MG | 1 | 4076 | 1/1 | 0.61 | 0.34 | 82,82,82,82 | 0 |
| 85 | MG | 1 | 4116 | 1/1 | 0.61 | 0.51 | 52,52,52,52 | 0 |
| 85 | MG | l | 404 | 1/1 | 0.61 | 0.57 | 44,44,44,44 | 0 |
| 85 | MG | sR | 2185 | 1/1 | 0.61 | 0.60 | 68,68,68,68 | 0 |
| 85 | MG | AR | 4236 | 1/1 | 0.62 | 0.53 | 58,58,58,58 | 0 |
| 85 | MG | s | 300 | 1/1 | 0.62 | 0.18 | 63,63,63,63 | 0 |
| 85 | MG | 1 | 4115 | 1/1 | 0.62 | 0.31 | 60,60,60,60 | 0 |
| 85 | MG | AR | 4091 | 1/1 | 0.64 | 0.49 | 70,70,70,70 | 0 |
| 84 | OHX | CG | 302 | 7/7 | 0.64 | 0.33 | 208,208,209,209 | 0 |
| 85 | MG | sR | 2082 | 1/1 | 0.64 | 0.60 | 63,63,63,63 | 0 |
| 85 | MG | A | 2098 | 1/1 | 0.65 | 0.21 | 96,96,96,96 | 0 |
| 85 | MG | x | 206 | 1/1 | 0.65 | 0.56 | 47,47,47,47 | 0 |
| 85 | MG | AR | 4038 | 1/1 | 0.65 | 0.47 | 57,57,57,57 | 0 |
| 85 | MG | AR | 4186 | 1/1 | 0.65 | 0.45 | 60,60,60,60 | 0 |
| 85 | MG | 1 | 4155 | 1/1 | 0.65 | 0.68 | 71,71,71,71 | 0 |
| 85 | MG | AR | 4085 | 1/1 | 0.65 | 0.41 | 73,73,73,73 | 0 |
| 85 | MG | A | 2068 | 1/1 | 0.65 | 0.44 | 73,73,73,73 | 0 |
| 85 | MG | AR | 3817 | 1/1 | 0.66 | 0.18 | 106,106,106,106 | 0 |
| 85 | MG | sR | 2151 | 1/1 | 0.66 | 0.40 | 63,63,63,63 | 0 |
| 85 | MG | AR | 4059 | 1/1 | 0.66 | 0.19 | 68,68,68,68 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | A | 2113 | 1/1 | 0.66 | 0.41 | 78,78,78,78 | 0 |
| 85 | MG | AR | 3777 | 1/1 | 0.67 | 0.25 | 78,78,78,78 | 0 |
| 85 | MG | AR | 4183 | 1/1 | 0.67 | 0.14 | 102,102,102,102 | 0 |
| 85 | MG | 1 | 3979 | 1/1 | 0.67 | 0.35 | 59,59,59,59 | 0 |
| 85 | MG | AR | 4130 | 1/1 | 0.67 | 0.24 | 64,64,64,64 | 0 |
| 85 | MG | sR | 2170 | 1/1 | 0.67 | 0.39 | 59,59,59,59 | 0 |
| 85 | MG | 1 | 3802 | 1/1 | 0.67 | 0.47 | 52,52,52,52 | 0 |
| 85 | MG | 1 | 3921 | 1/1 | 0.68 | 0.39 | 39,39,39,39 | 0 |
| 85 | MG | AR | 3908 | 1/1 | 0.68 | 0.39 | 41,41,41,41 | 0 |
| 85 | MG | AR | 4145 | 1/1 | 0.68 | 0.27 | 48,48,48,48 | 0 |
| 85 | MG | AR | 4048 | 1/1 | 0.68 | 0.33 | 68,68,68,68 | 0 |
| 85 | MG | 1 | 4033 | 1/1 | 0.68 | 0.32 | 73,73,73,73 | 0 |
| 85 | MG | A | 2115 | 1/1 | 0.68 | 0.34 | 69,69,69,69 | 0 |
| 84 | OHX | AR | 3740 | 7/7 | 0.68 | 0.55 | 212,212,213,213 | 0 |
| 85 | MG | AR | 4037 | 1/1 | 0.69 | 0.30 | 70,70,70,70 | 0 |
| 85 | MG | 1 | 4045 | 1/1 | 0.69 | 0.26 | 58,58,58,58 | 0 |
| 85 | MG | d3 | 202 | 1/1 | 0.69 | 0.30 | 59,59,59,59 | 0 |
| 84 | OHX | sR | 2041 | 7/7 | 0.70 | 0.30 | 238,238,239,240 | 0 |
| 85 | MG | AR | 4124 | 1/1 | 0.70 | 0.17 | 73,73,73,73 | 0 |
| 85 | MG | AR | 4027 | 1/1 | 0.70 | 0.12 | 105,105,105,105 | 0 |
| 85 | MG | AR | 4049 | 1/1 | 0.71 | 0.20 | 52,52,52,52 | 0 |
| 85 | MG | 1 | 4104 | 1/1 | 0.71 | 0.57 | 47,47,47,47 | 0 |
| 85 | MG | AR | 3796 | 1/1 | 0.71 | 0.34 | 62,62,62,62 | 0 |
| 85 | MG | AR | 4227 | 1/1 | 0.71 | 0.60 | 78,78,78,78 | 0 |
| 85 | MG | A | 2104 | 1/1 | 0.71 | 0.59 | 67,67,67,67 | 0 |
| 85 | MG | sR | 2121 | 1/1 | 0.71 | 0.32 | 69,69,69,69 | 0 |
| 85 | MG | AR | 4169 | 1/1 | 0.72 | 0.99 | 101,101,101,101 | 0 |
| 85 | MG | 1 | 3994 | 1/1 | 0.72 | 0.59 | 45,45,45,45 | 0 |
| 85 | MG | 1 | 4183 | 1/1 | 0.72 | 0.14 | 67,67,67,67 | 0 |
| 85 | MG | sR | 2069 | 1/1 | 0.72 | 0.33 | 53,53,53,53 | 0 |
| 85 | MG | AR | 4014 | 1/1 | 0.72 | 0.19 | 53,53,53,53 | 0 |
| 85 | MG | AR | 3972 | 1/1 | 0.72 | 0.64 | 52,52,52,52 | 0 |
| 85 | MG | 1 | 3834 | 1/1 | 0.73 | 0.45 | 42,42,42,42 | 0 |
| 85 | MG | A | 2110 | 1/1 | 0.73 | 0.25 | 78,78,78,78 | 0 |
| 85 | MG | AR | 4110 | 1/1 | 0.73 | 0.30 | 56,56,56,56 | 0 |
| 85 | MG | DA | 201 | 1/1 | 0.73 | 0.22 | 52,52,52,52 | 0 |
| 85 | MG | A | 2046 | 1/1 | 0.73 | 0.27 | 55,55,55,55 | 0 |
| 85 | MG | A | 2150 | 1/1 | 0.73 | 0.39 | 51,51,51,51 | 0 |
| 85 | MG | AR | 4155 | 1/1 | 0.73 | 0.35 | 46,46,46,46 | 0 |
| 85 | MG | sR | 2187 | 1/1 | 0.73 | 0.59 | 70,70,70,70 | 0 |
| 85 | MG | AR | 3989 | 1/1 | 0.73 | 0.72 | 58,58,58,58 | 0 |
| 84 | OHX | 1 | 3673 | 7/7 | 0.74 | 0.47 | 183,183,183,183 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | AR | 3974 | 1/1 | 0.74 | 0.41 | 71,71,71,71 | 0 |
| 85 | MG | 1 | 4125 | 1/1 | 0.74 | 0.38 | 49,49,49,49 | 0 |
| 85 | MG | 1 | 4138 | 1/1 | 0.74 | 0.35 | 44,44,44,44 | 0 |
| 85 | MG | 1 | 4003 | 1/1 | 0.74 | 0.43 | 62,62,62,62 | 0 |
| 85 | MG | AR | 4176 | 1/1 | 0.74 | 0.22 | 60,60,60,60 | 0 |
| 85 | MG | 1 | 4032 | 1/1 | 0.74 | 0.58 | 66,66,66,66 | 0 |
| 85 | MG | 1 | 3988 | 1/1 | 0.74 | 0.44 | 44,44,44,44 | 0 |
| 85 | MG | sR | 2074 | 1/1 | 0.75 | 0.37 | 51,51,51,51 | 0 |
| 85 | MG | A | 2134 | 1/1 | 0.75 | 0.55 | 53,53,53,53 | 0 |
| 84 | OHX | AR | 3746 | 7/7 | 0.75 | 0.20 | 269,269,270,270 | 0 |
| 85 | MG | 1 | 4100 | 1/1 | 0.75 | 0.28 | 46,46,46,46 | 0 |
| 85 | MG | AT | 221 | 1/1 | 0.75 | 0.77 | 57,57,57,57 | 0 |
| 85 | MG | l | 402 | 1/1 | 0.76 | 0.20 | 39,39,39,39 | 0 |
| 84 | OHX | AR | 3735 | 7/7 | 0.76 | 0.34 | 208,208,208,209 | 0 |
| 85 | MG | AR | 4171 | 1/1 | 0.76 | 0.45 | 50,50,50,50 | 0 |
| 85 | MG | A | 2082 | 1/1 | 0.76 | 0.26 | 69,69,69,69 | 0 |
| 85 | MG | A | 2097 | 1/1 | 0.76 | 0.25 | 75,75,75,75 | 0 |
| 85 | MG | AR | 3966 | 1/1 | 0.76 | 0.55 | 55,55,55,55 | 0 |
| 85 | MG | 1 | 4167 | 1/1 | 0.76 | 0.24 | 57,57,57,57 | 0 |
| 84 | OHX | sR | 2052 | 7/7 | 0.76 | 0.22 | 208,209,210,210 | 0 |
| 85 | MG | 1 | 4187 | 1/1 | 0.76 | 0.33 | 52,52,52,52 | 0 |
| 85 | MG | 1 | 3772 | 1/1 | 0.76 | 0.43 | 50,50,50,50 | 0 |
| 85 | MG | 1 | 4152 | 1/1 | 0.76 | 0.35 | 37,37,37,37 | 0 |
| 85 | MG | 1 | 3790 | 1/1 | 0.76 | 0.79 | 72,72,72,72 | 0 |
| 85 | MG | A | 2138 | 1/1 | 0.76 | 0.33 | 74,74,74,74 | 0 |
| 85 | MG | CP | 504 | 1/1 | 0.77 | 0.40 | 51,51,51,51 | 0 |
| 85 | MG | 1 | 3824 | 1/1 | 0.77 | 0.34 | 53,53,53,53 | 0 |
| 85 | MG | sR | 2094 | 1/1 | 0.77 | 0.29 | 33,33,33,33 | 0 |
| 85 | MG | DC | 205 | 1/1 | 0.77 | 0.40 | 34,34,34,34 | 0 |
| 85 | MG | sR | 2132 | 1/1 | 0.77 | 0.21 | 59,59,59,59 | 0 |
| 85 | MG | AR | 4157 | 1/1 | 0.77 | 0.44 | 62,62,62,62 | 0 |
| 85 | MG | AR | 4161 | 1/1 | 0.77 | 0.27 | 52,52,52,52 | 0 |
| 85 | MG | 1 | 4093 | 1/1 | 0.77 | 0.13 | 68,68,68,68 | 0 |
| 85 | MG | sR | 2159 | 1/1 | 0.77 | 0.63 | 58,58,58,58 | 0 |
| 85 | MG | AR | 4233 | 1/1 | 0.77 | 0.44 | 54,54,54,54 | 0 |
| 85 | MG | J | 302 | 1/1 | 0.77 | 0.30 | 55,55,55,55 | 0 |
| 84 | OHX | 1 | 3718 | 7/7 | 0.77 | 0.42 | 254,254,255,255 | 0 |
| 85 | MG | 1 | 3875 | 1/1 | 0.77 | 0.28 | 32,32,32,32 | 0 |
| 85 | MG | AR | 4187 | 1/1 | 0.78 | 0.29 | 50,50,50,50 | 0 |
| 85 | MG | l | 406 | 1/1 | 0.78 | 0.81 | 72,72,72,72 | 0 |
| 85 | MG | AR | 4118 | 1/1 | 0.78 | 0.15 | 55,55,55,55 | 0 |
| 85 | MG | 1 | 3785 | 1/1 | 0.78 | 0.37 | 30,30,30,30 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | w | 201 | 1/1 | 0.78 | 0.40 | 54,54,54,54 | 0 |
| 85 | MG | e | 102 | 1/1 | 0.78 | 0.17 | 81,81,81,81 | 0 |
| 84 | OHX | A | 2039 | 7/7 | 0.78 | 0.40 | 234,235,236,236 | 0 |
| 85 | MG | AT | 224 | 1/1 | 0.78 | 0.29 | 70,70,70,70 | 0 |
| 85 | MG | 6 | 202 | 1/1 | 0.78 | 0.30 | 67,67,67,67 | 0 |
| 85 | MG | sR | 2076 | 1/1 | 0.78 | 0.37 | 77,77,77,77 | 0 |
| 85 | MG | 1 | 3985 | 1/1 | 0.78 | 0.46 | 85,85,85,85 | 0 |
| 85 | MG | AR | 4150 | 1/1 | 0.78 | 0.31 | 63,63,63,63 | 0 |
| 85 | MG | 1 | 4184 | 1/1 | 0.78 | 0.26 | 48,48,48,48 | 0 |
| 85 | MG | AR | 3803 | 1/1 | 0.78 | 0.51 | 43,43,43,43 | 0 |
| 85 | MG | 1 | 3866 | 1/1 | 0.78 | 0.41 | 44,44,44,44 | 0 |
| 85 | MG | A | 2087 | 1/1 | 0.78 | 0.30 | 70,70,70,70 | 0 |
| 85 | MG | 1 | 4130 | 1/1 | 0.78 | 0.33 | 69,69,69,69 | 0 |
| 85 | MG | 1 | 4088 | 1/1 | 0.78 | 0.28 | 53,53,53,53 | 0 |
| 84 | OHX | AR | 3670 | 7/7 | 0.78 | 0.37 | 245,245,245,245 | 0 |
| 85 | MG | 1 | 3784 | 1/1 | 0.78 | 0.39 | 54,54,54,54 | 0 |
| 85 | MG | l | 403 | 1/1 | 0.78 | 0.45 | 63,63,63,63 | 0 |
| 85 | MG | 1 | 4162 | 1/1 | 0.78 | 0.49 | 32,32,32,32 | 0 |
| 84 | OHX | AR | 3725 | 7/7 | 0.79 | 0.37 | 178,178,178,178 | 0 |
| 85 | MG | A | 2084 | 1/1 | 0.79 | 0.28 | 66,66,66,66 | 0 |
| 85 | MG | 1 | 3878 | 1/1 | 0.79 | 0.49 | 53,53,53,53 | 0 |
| 85 | MG | 1 | 4001 | 1/1 | 0.79 | 0.58 | 61,61,61,61 | 0 |
| 85 | MG | 1 | 4094 | 1/1 | 0.79 | 0.32 | 59,59,59,59 | 0 |
| 85 | MG | AR | 4100 | 1/1 | 0.79 | 0.32 | 63,63,63,63 | 0 |
| 84 | OHX | sR | 2040 | 7/7 | 0.79 | 0.42 | 165,166,166,167 | 0 |
| 85 | MG | 1 | 4004 | 1/1 | 0.79 | 0.13 | 66,66,66,66 | 0 |
| 85 | MG | AT | 225 | 1/1 | 0.79 | 0.71 | 72,72,72,72 | 0 |
| 85 | MG | AR | 4029 | 1/1 | 0.79 | 0.16 | 51,51,51,51 | 0 |
| 85 | MG | A | 2124 | 1/1 | 0.79 | 0.25 | 67,67,67,67 | 0 |
| 85 | MG | sR | 2158 | 1/1 | 0.79 | 0.20 | 62,62,62,62 | 0 |
| 84 | OHX | 1 | 3698 | 7/7 | 0.79 | 0.29 | 245,245,246,246 | 0 |
| 85 | MG | 1 | 3787 | 1/1 | 0.79 | 0.49 | 63,63,63,63 | 0 |
| 85 | MG | 1 | 4123 | 1/1 | 0.79 | 0.28 | 53,53,53,53 | 0 |
| 85 | MG | A | 2051 | 1/1 | 0.79 | 0.35 | 69,69,69,69 | 0 |
| 85 | MG | sR | 2188 | 1/1 | 0.79 | 0.43 | 62,62,62,62 | 0 |
| 84 | OHX | AR | 3693 | 7/7 | 0.79 | 0.30 | 221,222,222,223 | 0 |
| 85 | MG | sR | 2087 | 1/1 | 0.80 | 0.33 | 53,53,53,53 | 0 |
| 85 | MG | 1 | 3913 | 1/1 | 0.80 | 0.44 | 40,40,40,40 | 0 |
| 85 | MG | 1 | 4194 | 1/1 | 0.80 | 0.41 | 29,29,29,29 | 0 |
| 85 | MG | AR | 4234 | 1/1 | 0.80 | 0.40 | 59,59,59,59 | 0 |
| 85 | MG | 1 | 4005 | 1/1 | 0.80 | 0.30 | 49,49,49,49 | 0 |
| 84 | OHX | 1 | 3682 | 7/7 | 0.80 | 0.28 | 179,179,180,180 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | 1 | 4108 | 1/1 | 0.80 | 0.51 | 69,69,69,69 | 0 |
| 85 | MG | AR | 4182 | 1/1 | 0.80 | 0.28 | 40,40,40,40 | 0 |
| 85 | MG | A | 2102 | 1/1 | 0.80 | 0.61 | 75,75,75,75 | 0 |
| 85 | MG | 4 | 232 | 1/1 | 0.80 | 0.17 | 52,52,52,52 | 0 |
| 85 | MG | 1 | 4110 | 1/1 | 0.80 | 0.34 | 76,76,76,76 | 0 |
| 85 | MG | 1 | 3871 | 1/1 | 0.80 | 0.33 | 70,70,70,70 | 0 |
| 85 | MG | AR | 3983 | 1/1 | 0.80 | 0.28 | 71,71,71,71 | 0 |
| 85 | MG | sR | 2086 | 1/1 | 0.80 | 0.28 | 81,81,81,81 | 0 |
| 84 | OHX | sR | 2051 | 7/7 | 0.81 | 0.29 | 196,196,197,198 | 0 |
| 85 | MG | A | 2129 | 1/1 | 0.81 | 0.61 | 65,65,65,65 | 0 |
| 85 | MG | A | 2132 | 1/1 | 0.81 | 0.23 | 68,68,68,68 | 0 |
| 85 | MG | 1 | 3935 | 1/1 | 0.81 | 0.26 | 38,38,38,38 | 0 |
| 85 | MG | AR | 4043 | 1/1 | 0.81 | 0.39 | 45,45,45,45 | 0 |
| 85 | MG | AR | 3899 | 1/1 | 0.81 | 0.43 | 32,32,32,32 | 0 |
| 85 | MG | AT | 227 | 1/1 | 0.81 | 0.79 | 75,75,75,75 | 0 |
| 85 | MG | CE | 403 | 1/1 | 0.81 | 0.39 | 31,31,31,31 | 0 |
| 85 | MG | CF | 403 | 1/1 | 0.81 | 0.38 | 37,37,37,37 | 0 |
| 84 | OHX | 4 | 215 | 7/7 | 0.81 | 0.27 | 167,168,168,168 | 0 |
| 85 | MG | 1 | 4176 | 1/1 | 0.81 | 0.32 | 66,66,66,66 | 0 |
| 85 | MG | 1 | 3738 | 1/1 | 0.81 | 0.40 | 36,36,36,36 | 0 |
| 85 | MG | AR | 4162 | 1/1 | 0.81 | 0.40 | 69,69,69,69 | 0 |
| 85 | MG | AR | 4082 | 1/1 | 0.81 | 0.23 | 37,37,37,37 | 0 |
| 85 | MG | 1 | 3762 | 1/1 | 0.81 | 0.50 | 45,45,45,45 | 0 |
| 85 | MG | A | 2069 | 1/1 | 0.81 | 0.53 | 65,65,65,65 | 0 |
| 85 | MG | 1 | 4185 | 1/1 | 0.81 | 0.35 | 42,42,42,42 | 0 |
| 85 | MG | 1 | 4132 | 1/1 | 0.81 | 0.36 | 54,54,54,54 | 0 |
| 85 | MG | sR | 2141 | 1/1 | 0.81 | 0.15 | 62,62,62,62 | 0 |
| 85 | MG | AR | 3985 | 1/1 | 0.81 | 0.37 | 61,61,61,61 | 0 |
| 85 | MG | 1 | 4192 | 1/1 | 0.81 | 0.20 | 32,32,32,32 | 0 |
| 84 | OHX | AR | 3669 | 7/7 | 0.81 | 0.21 | 188,189,189,189 | 0 |
| 85 | MG | AR | 4194 | 1/1 | 0.81 | 0.29 | 54,54,54,54 | 0 |
| 85 | MG | AR | 3751 | 1/1 | 0.81 | 0.50 | 33,33,33,33 | 0 |
| 85 | MG | sR | 2161 | 1/1 | 0.81 | 0.35 | 58,58,58,58 | 0 |
| 85 | MG | A | 2106 | 1/1 | 0.81 | 0.47 | 71,71,71,71 | 0 |
| 85 | MG | sR | 2179 | 1/1 | 0.81 | 0.45 | 64,64,64,64 | 0 |
| 85 | MG | sR | 2180 | 1/1 | 0.81 | 0.46 | 68,68,68,68 | 0 |
| 84 | OHX | A | 2015 | 7/7 | 0.81 | 0.46 | 213,214,216,216 | 0 |
| 85 | MG | 1 | 4047 | 1/1 | 0.81 | 0.65 | 63,63,63,63 | 0 |
| 85 | MG | 3 | 219 | 1/1 | 0.81 | 0.16 | 68,68,68,68 | 0 |
| 85 | MG | AR | 4235 | 1/1 | 0.81 | 0.37 | 66,66,66,66 | 0 |
| 85 | MG | AR | 3980 | 1/1 | 0.82 | 0.41 | 66,66,66,66 | 0 |
| 85 | MG | AR | 3982 | 1/1 | 0.82 | 0.30 | 45,45,45,45 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | 1 | 3971 | 1/1 | 0.82 | 0.23 | 41,41,41,41 | 0 |
| 85 | MG | sR | 2085 | 1/1 | 0.82 | 0.68 | 64,64,64,64 | 0 |
| 85 | MG | 1 | 3808 | 1/1 | 0.82 | 0.32 | 52,52,52,52 | 0 |
| 85 | MG | 1 | 3984 | 1/1 | 0.82 | 0.36 | 54,54,54,54 | 0 |
| 85 | MG | 1 | 4020 | 1/1 | 0.82 | 0.24 | 62,62,62,62 | 0 |
| 85 | MG | sR | 2110 | 1/1 | 0.82 | 0.48 | 61,61,61,61 | 0 |
| 84 | OHX | A | 2034 | 7/7 | 0.82 | 0.16 | 261,262,263,263 | 0 |
| 85 | MG | AR | 3876 | 1/1 | 0.82 | 0.20 | 50,50,50,50 | 0 |
| 85 | MG | 1 | 3952 | 1/1 | 0.82 | 0.45 | 75,75,75,75 | 0 |
| 85 | MG | x | 203 | 1/1 | 0.82 | 0.43 | 65,65,65,65 | 0 |
| 85 | MG | 4 | 226 | 1/1 | 0.82 | 0.36 | 55,55,55,55 | 0 |
| 85 | MG | 1 | 3960 | 1/1 | 0.82 | 0.64 | 47,47,47,47 | 0 |
| 85 | MG | CM | 202 | 1/1 | 0.82 | 0.17 | 60,60,60,60 | 0 |
| 84 | OHX | 1 | 3704 | 7/7 | 0.82 | 0.45 | 181,181,181,181 | 0 |
| 85 | MG | AR | 4046 | 1/1 | 0.82 | 0.46 | 63,63,63,63 | 0 |
| 85 | MG | DC | 204 | 1/1 | 0.82 | 0.62 | 47,47,47,47 | 0 |
| 85 | MG | AR | 3774 | 1/1 | 0.82 | 0.34 | 48,48,48,48 | 0 |
| 85 | MG | AR | 4200 | 1/1 | 0.82 | 0.36 | 46,46,46,46 | 0 |
| 85 | MG | AR | 4202 | 1/1 | 0.82 | 0.42 | 50,50,50,50 | 0 |
| 85 | MG | A | 2061 | 1/1 | 0.82 | 0.44 | 68,68,68,68 | 0 |
| 85 | MG | AR | 4207 | 1/1 | 0.82 | 0.23 | 54,54,54,54 | 0 |
| 85 | MG | AR | 4222 | 1/1 | 0.82 | 0.33 | 73,73,73,73 | 0 |
| 85 | MG | d6 | 102 | 1/1 | 0.82 | 0.40 | 59,59,59,59 | 0 |
| 85 | MG | 1 | 3981 | 1/1 | 0.83 | 0.25 | 49,49,49,49 | 0 |
| 85 | MG | n | 201 | 1/1 | 0.83 | 0.21 | 48,48,48,48 | 0 |
| 85 | MG | sR | 2116 | 1/1 | 0.83 | 0.32 | 64,64,64,64 | 0 |
| 85 | MG | AR | 3819 | 1/1 | 0.83 | 0.37 | 56,56,56,56 | 0 |
| 85 | MG | sR | 2124 | 1/1 | 0.83 | 0.52 | 54,54,54,54 | 0 |
| 85 | MG | 1 | 4180 | 1/1 | 0.83 | 0.20 | 58,58,58,58 | 0 |
| 85 | MG | sR | 2138 | 1/1 | 0.83 | 0.26 | 65,65,65,65 | 0 |
| 85 | MG | 1 | 4181 | 1/1 | 0.83 | 0.16 | 50,50,50,50 | 0 |
| 85 | MG | A | 2053 | 1/1 | 0.83 | 0.50 | 49,49,49,49 | 0 |
| 84 | OHX | 1 | 3719 | 7/7 | 0.83 | 0.28 | 176,176,177,177 | 0 |
| 85 | MG | AR | 4022 | 1/1 | 0.83 | 0.42 | 36,36,36,36 | 0 |
| 85 | MG | 1 | 4051 | 1/1 | 0.83 | 0.32 | 44,44,44,44 | 0 |
| 85 | MG | AR | 4238 | 1/1 | 0.83 | 0.39 | 54,54,54,54 | 0 |
| 85 | MG | 4 | 230 | 1/1 | 0.83 | 0.50 | 60,60,60,60 | 0 |
| 85 | MG | 1 | 4160 | 1/1 | 0.83 | 0.22 | 51,51,51,51 | 0 |
| 85 | MG | A | 2088 | 1/1 | 0.83 | 0.28 | 55,55,55,55 | 0 |
| 85 | MG | AR | 3968 | 1/1 | 0.83 | 0.31 | 47,47,47,47 | 0 |
| 85 | MG | sR | 2183 | 1/1 | 0.83 | 0.58 | 68,68,68,68 | 0 |
| 85 | MG | 1 | 4062 | 1/1 | 0.83 | 0.37 | 47,47,47,47 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 84 | OHX | CM | 201 | 7/7 | 0.83 | 0.31 | 200,200,201,201 | 0 |
| 85 | MG | AR | 3778 | 1/1 | 0.83 | 0.39 | 52,52,52,52 | 0 |
| 85 | MG | sR | 2191 | 1/1 | 0.83 | 0.16 | 67,67,67,67 | 0 |
| 85 | MG | AR | 4140 | 1/1 | 0.83 | 0.26 | 64,64,64,64 | 0 |
| 84 | OHX | AS | 209 | 7/7 | 0.83 | 0.25 | 182,183,183,184 | 0 |
| 85 | MG | 1 | 4061 | 1/1 | 0.84 | 0.44 | 55,55,55,55 | 0 |
| 84 | OHX | AR | 3732 | 7/7 | 0.84 | 0.27 | 227,228,228,228 | 0 |
| 85 | MG | AR | 4122 | 1/1 | 0.84 | 0.47 | 62,62,62,62 | 0 |
| 85 | MG | A | 2135 | 1/1 | 0.84 | 0.56 | 70,70,70,70 | 0 |
| 85 | MG | 1 | 4066 | 1/1 | 0.84 | 0.27 | 45,45,45,45 | 0 |
| 84 | OHX | z | 201 | 7/7 | 0.84 | 0.39 | 229,229,229,230 | 0 |
| 85 | MG | AR | 4245 | 1/1 | 0.84 | 0.26 | 56,56,56,56 | 0 |
| 85 | MG | 1 | 4195 | 1/1 | 0.84 | 0.39 | 25,25,25,25 | 0 |
| 85 | MG | AR | 4134 | 1/1 | 0.84 | 0.35 | 46,46,46,46 | 0 |
| 85 | MG | AR | 3753 | 1/1 | 0.84 | 0.27 | 39,39,39,39 | 0 |
| 84 | OHX | AR | 3711 | 7/7 | 0.84 | 0.29 | 180,181,181,181 | 0 |
| 85 | MG | 1 | 3896 | 1/1 | 0.84 | 0.56 | 35,35,35,35 | 0 |
| 85 | MG | AR | 4149 | 1/1 | 0.84 | 0.29 | 53,53,53,53 | 0 |
| 85 | MG | CG | 304 | 1/1 | 0.84 | 0.20 | 59,59,59,59 | 0 |
| 85 | MG | 1 | 4021 | 1/1 | 0.84 | 0.39 | 46,46,46,46 | 0 |
| 85 | MG | AR | 4023 | 1/1 | 0.84 | 0.29 | 73,73,73,73 | 0 |
| 85 | MG | 1 | 4097 | 1/1 | 0.84 | 0.25 | 55,55,55,55 | 0 |
| 85 | MG | 1 | 3757 | 1/1 | 0.84 | 0.16 | 63,63,63,63 | 0 |
| 84 | OHX | A | 2040 | 7/7 | 0.84 | 0.27 | 215,216,216,216 | 0 |
| 84 | OHX | A | 2041 | 7/7 | 0.84 | 0.45 | 182,182,183,183 | 0 |
| 85 | MG | sR | 2122 | 1/1 | 0.84 | 0.23 | 71,71,71,71 | 0 |
| 85 | MG | AR | 4165 | 1/1 | 0.84 | 0.34 | 43,43,43,43 | 0 |
| 85 | MG | AR | 4166 | 1/1 | 0.84 | 0.11 | 91,91,91,91 | 0 |
| 85 | MG | AR | 3828 | 1/1 | 0.84 | 0.74 | 64,64,64,64 | 0 |
| 85 | MG | AR | 3830 | 1/1 | 0.84 | 0.24 | 47,47,47,47 | 0 |
| 85 | MG | AR | 4172 | 1/1 | 0.84 | 0.17 | 73,73,73,73 | 0 |
| 85 | MG | A | 2070 | 1/1 | 0.84 | 0.41 | 70,70,70,70 | 0 |
| 85 | MG | k | 402 | 1/1 | 0.84 | 0.25 | 57,57,57,57 | 0 |
| 85 | MG | AR | 3842 | 1/1 | 0.84 | 0.20 | 42,42,42,42 | 0 |
| 85 | MG | AR | 4053 | 1/1 | 0.84 | 0.14 | 47,47,47,47 | 0 |
| 85 | MG | k | 403 | 1/1 | 0.84 | 0.37 | 37,37,37,37 | 0 |
| 85 | MG | 1 | 4109 | 1/1 | 0.84 | 0.36 | 40,40,40,40 | 0 |
| 85 | MG | sR | 2172 | 1/1 | 0.84 | 0.39 | 101,101,101,101 | 0 |
| 85 | MG | sR | 2176 | 1/1 | 0.84 | 0.32 | 64,64,64,64 | 0 |
| 85 | MG | 1 | 4178 | 1/1 | 0.84 | 0.33 | 39,39,39,39 | 0 |
| 85 | MG | AR | 4196 | 1/1 | 0.84 | 0.20 | 72,72,72,72 | 0 |
| 85 | MG | AR | 4197 | 1/1 | 0.84 | 0.17 | 82,82,82,82 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 84 | OHX | AR | 3653 | 7/7 | 0.84 | 0.32 | 167,167,168,168 | 0 |
| 85 | MG | AR | 4087 | 1/1 | 0.84 | 0.28 | 72,72,72,72 | 0 |
| 84 | OHX | A | 1971 | 7/7 | 0.84 | 0.18 | 164,165,166,166 | 0 |
| 85 | MG | 1 | 4058 | 1/1 | 0.84 | 0.25 | 45,45,45,45 | 0 |
| 85 | MG | 1 | 4122 | 1/1 | 0.84 | 0.24 | 51,51,51,51 | 0 |
| 85 | MG | d5 | 201 | 1/1 | 0.84 | 0.08 | 74,74,74,74 | 0 |
| 85 | MG | t | 203 | 1/1 | 0.84 | 0.66 | 41,41,41,41 | 0 |
| 85 | MG | A | 2105 | 1/1 | 0.85 | 0.40 | 58,58,58,58 | 0 |
| 85 | MG | 3 | 220 | 1/1 | 0.85 | 0.23 | 58,58,58,58 | 0 |
| 85 | MG | A | 2109 | 1/1 | 0.85 | 0.53 | 60,60,60,60 | 0 |
| 85 | MG | AR | 4052 | 1/1 | 0.85 | 0.46 | 42,42,42,42 | 0 |
| 84 | OHX | sR | 2050 | 7/7 | 0.85 | 0.31 | 224,224,225,225 | 0 |
| 85 | MG | 1 | 3982 | 1/1 | 0.85 | 0.24 | 46,46,46,46 | 0 |
| 85 | MG | AR | 4056 | 1/1 | 0.85 | 0.25 | 55,55,55,55 | 0 |
| 85 | MG | AR | 3835 | 1/1 | 0.85 | 0.63 | 58,58,58,58 | 0 |
| 85 | MG | AR | 4061 | 1/1 | 0.85 | 0.22 | 56,56,56,56 | 0 |
| 85 | MG | A | 2131 | 1/1 | 0.85 | 0.20 | 90,90,90,90 | 0 |
| 85 | MG | AR | 4079 | 1/1 | 0.85 | 0.10 | 57,57,57,57 | 0 |
| 85 | MG | A | 2133 | 1/1 | 0.85 | 0.24 | 68,68,68,68 | 0 |
| 85 | MG | AR | 4081 | 1/1 | 0.85 | 0.15 | 107,107,107,107 | 0 |
| 84 | OHX | 1 | 3697 | 7/7 | 0.85 | 0.40 | 154,155,155,155 | 0 |
| 84 | OHX | A | 1946 | 7/7 | 0.85 | 0.16 | 181,182,183,183 | 0 |
| 85 | MG | j | 301 | 1/1 | 0.85 | 0.36 | 33,33,33,33 | 0 |
| 85 | MG | AR | 4089 | 1/1 | 0.85 | 0.31 | 52,52,52,52 | 0 |
| 85 | MG | 1 | 4065 | 1/1 | 0.85 | 0.20 | 46,46,46,46 | 0 |
| 85 | MG | AR | 3920 | 1/1 | 0.85 | 0.56 | 27,27,27,27 | 0 |
| 85 | MG | AR | 3921 | 1/1 | 0.85 | 0.57 | 31,31,31,31 | 0 |
| 85 | MG | AR | 4104 | 1/1 | 0.85 | 0.26 | 49,49,49,49 | 0 |
| 85 | MG | AR | 4247 | 1/1 | 0.85 | 0.30 | 31,31,31,31 | 0 |
| 85 | MG | sR | 2079 | 1/1 | 0.85 | 0.40 | 46,46,46,46 | 0 |
| 85 | MG | AS | 228 | 1/1 | 0.85 | 0.07 | 72,72,72,72 | 0 |
| 85 | MG | 1 | 4154 | 1/1 | 0.85 | 0.31 | 69,69,69,69 | 0 |
| 85 | MG | 1 | 3987 | 1/1 | 0.85 | 0.23 | 51,51,51,51 | 0 |
| 85 | MG | 1 | 4073 | 1/1 | 0.85 | 0.63 | 47,47,47,47 | 0 |
| 85 | MG | 1 | 4161 | 1/1 | 0.85 | 0.29 | 54,54,54,54 | 0 |
| 85 | MG | 1 | 3880 | 1/1 | 0.85 | 0.59 | 48,48,48,48 | 0 |
| 85 | MG | CE | 404 | 1/1 | 0.85 | 0.32 | 31,31,31,31 | 0 |
| 85 | MG | sR | 2117 | 1/1 | 0.85 | 0.16 | 88,88,88,88 | 0 |
| 85 | MG | 1 | 4083 | 1/1 | 0.85 | 0.43 | 56,56,56,56 | 0 |
| 84 | OHX | s1 | 301 | 7/7 | 0.85 | 0.41 | 188,189,190,190 | 0 |
| 84 | OHX | 1 | 3709 | 7/7 | 0.85 | 0.33 | 189,190,190,190 | 0 |
| 85 | MG | 1 | 3753 | 1/1 | 0.85 | 0.39 | 30,30,30,30 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | CR | 203 | 1/1 | 0.85 | 0.37 | 112,112,112,112 | 0 |
| 85 | MG | 1 | 3820 | 1/1 | 0.85 | 0.29 | 51,51,51,51 | 0 |
| 85 | MG | AR | 3996 | 1/1 | 0.85 | 0.20 | 63,63,63,63 | 0 |
| 85 | MG | 1 | 4098 | 1/1 | 0.85 | 0.44 | 50,50,50,50 | 0 |
| 85 | MG | DD | 101 | 1/1 | 0.85 | 0.47 | 41,41,41,41 | 0 |
| 85 | MG | 1 | 3949 | 1/1 | 0.85 | 0.20 | 46,46,46,46 | 0 |
| 85 | MG | AR | 4012 | 1/1 | 0.85 | 0.37 | 60,60,60,60 | 0 |
| 85 | MG | 1 | 4103 | 1/1 | 0.85 | 0.24 | 48,48,48,48 | 0 |
| 84 | OHX | sR | 2022 | 7/7 | 0.85 | 0.22 | 215,216,217,218 | 0 |
| 85 | MG | AR | 3759 | 1/1 | 0.85 | 0.38 | 50,50,50,50 | 0 |
| 85 | MG | 1 | 3954 | 1/1 | 0.85 | 0.32 | 38,38,38,38 | 0 |
| 85 | MG | AR | 4163 | 1/1 | 0.85 | 0.18 | 50,50,50,50 | 0 |
| 85 | MG | AR | 4028 | 1/1 | 0.85 | 0.23 | 48,48,48,48 | 0 |
| 85 | MG | 1 | 4029 | 1/1 | 0.85 | 0.36 | 46,46,46,46 | 0 |
| 85 | MG | A | 2085 | 1/1 | 0.85 | 0.15 | 75,75,75,75 | 0 |
| 85 | MG | AR | 4036 | 1/1 | 0.85 | 0.30 | 61,61,61,61 | 0 |
| 84 | OHX | AS | 211 | 7/7 | 0.85 | 0.25 | 190,191,192,192 | 0 |
| 84 | OHX | 4 | 214 | 7/7 | 0.85 | 0.33 | 187,187,187,187 | 0 |
| 85 | MG | 1 | 3855 | 1/1 | 0.85 | 0.26 | 31,31,31,31 | 0 |
| 85 | MG | 1 | 4046 | 1/1 | 0.85 | 0.11 | 48,48,48,48 | 0 |
| 85 | MG | d6 | 101 | 1/1 | 0.85 | 0.62 | 50,50,50,50 | 0 |
| 85 | MG | 1 | 3780 | 1/1 | 0.85 | 0.23 | 43,43,43,43 | 0 |
| 84 | OHX | A | 2036 | 7/7 | 0.86 | 0.13 | 277,278,279,279 | 0 |
| 85 | MG | 1 | 3939 | 1/1 | 0.86 | 0.43 | 55,55,55,55 | 0 |
| 85 | MG | sR | 2068 | 1/1 | 0.86 | 0.41 | 60,60,60,60 | 0 |
| 85 | MG | 1 | 4036 | 1/1 | 0.86 | 0.59 | 55,55,55,55 | 0 |
| 85 | MG | sR | 2070 | 1/1 | 0.86 | 0.41 | 65,65,65,65 | 0 |
| 85 | MG | 1 | 3859 | 1/1 | 0.86 | 0.33 | 43,43,43,43 | 0 |
| 85 | MG | AR | 4003 | 1/1 | 0.86 | 0.26 | 45,45,45,45 | 0 |
| 85 | MG | AR | 3826 | 1/1 | 0.86 | 0.35 | 69,69,69,69 | 0 |
| 85 | MG | sR | 2080 | 1/1 | 0.86 | 0.52 | 70,70,70,70 | 0 |
| 84 | OHX | AR | 3652 | 7/7 | 0.86 | 0.28 | 140,141,141,141 | 0 |
| 85 | MG | sR | 2083 | 1/1 | 0.86 | 0.47 | 69,69,69,69 | 0 |
| 85 | MG | A | 2064 | 1/1 | 0.86 | 0.24 | 69,69,69,69 | 0 |
| 85 | MG | AR | 4008 | 1/1 | 0.86 | 0.43 | 58,58,58,58 | 0 |
| 85 | MG | 1 | 3806 | 1/1 | 0.86 | 0.23 | 77,77,77,77 | 0 |
| 84 | OHX | CO | 201 | 7/7 | 0.86 | 0.25 | 244,244,245,245 | 0 |
| 85 | MG | sR | 2102 | 1/1 | 0.86 | 0.44 | 45,45,45,45 | 0 |
| 85 | MG | A | 2081 | 1/1 | 0.86 | 0.42 | 61,61,61,61 | 0 |
| 85 | MG | 1 | 3966 | 1/1 | 0.86 | 0.20 | 70,70,70,70 | 0 |
| 84 | OHX | A | 2024 | 7/7 | 0.86 | 0.51 | 164,165,166,166 | 0 |
| 85 | MG | sR | 2118 | 1/1 | 0.86 | 0.28 | 72,72,72,72 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | AR | 4024 | 1/1 | 0.86 | 0.55 | 48,48,48,48 | 0 |
| 85 | MG | A | 2086 | 1/1 | 0.86 | 0.23 | 50,50,50,50 | 0 |
| 85 | MG | sR | 2123 | 1/1 | 0.86 | 0.31 | 65,65,65,65 | 0 |
| 85 | MG | AR | 3869 | 1/1 | 0.86 | 0.48 | 28,28,28,28 | 0 |
| 84 | OHX | A | 2042 | 7/7 | 0.86 | 0.19 | 211,213,213,214 | 0 |
| 85 | MG | A | 2094 | 1/1 | 0.86 | 0.46 | 62,62,62,62 | 0 |
| 85 | MG | AR | 4129 | 1/1 | 0.86 | 0.26 | 91,91,91,91 | 0 |
| 85 | MG | 1 | 4163 | 1/1 | 0.86 | 0.22 | 45,45,45,45 | 0 |
| 85 | MG | AR | 4131 | 1/1 | 0.86 | 0.13 | 65,65,65,65 | 0 |
| 85 | MG | AR | 4034 | 1/1 | 0.86 | 0.12 | 52,52,52,52 | 0 |
| 84 | OHX | A | 2029 | 7/7 | 0.86 | 0.18 | 219,220,221,221 | 0 |
| 85 | MG | AR | 3909 | 1/1 | 0.86 | 0.30 | 22,22,22,22 | 0 |
| 85 | MG | sR | 2160 | 1/1 | 0.86 | 0.30 | 51,51,51,51 | 0 |
| 85 | MG | AR | 3911 | 1/1 | 0.86 | 0.67 | 35,35,35,35 | 0 |
| 85 | MG | AS | 217 | 1/1 | 0.86 | 0.32 | 50,50,50,50 | 0 |
| 85 | MG | AR | 3916 | 1/1 | 0.86 | 0.46 | 49,49,49,49 | 0 |
| 85 | MG | AB | 204 | 1/1 | 0.86 | 0.24 | 35,35,35,35 | 0 |
| 85 | MG | 1 | 3831 | 1/1 | 0.86 | 0.77 | 66,66,66,66 | 0 |
| 85 | MG | 1 | 4027 | 1/1 | 0.86 | 0.43 | 41,41,41,41 | 0 |
| 85 | MG | AR | 4051 | 1/1 | 0.86 | 0.39 | 43,43,43,43 | 0 |
| 85 | MG | 4 | 231 | 1/1 | 0.86 | 0.28 | 66,66,66,66 | 0 |
| 85 | MG | sR | 2186 | 1/1 | 0.86 | 0.33 | 86,86,86,86 | 0 |
| 85 | MG | AR | 3772 | 1/1 | 0.86 | 0.24 | 36,36,36,36 | 0 |
| 85 | MG | 1 | 4117 | 1/1 | 0.86 | 0.34 | 60,60,60,60 | 0 |
| 84 | OHX | AR | 3726 | 7/7 | 0.86 | 0.33 | 214,215,215,216 | 0 |
| 85 | MG | AR | 3976 | 1/1 | 0.86 | 0.45 | 39,39,39,39 | 0 |
| 85 | MG | AR | 4168 | 1/1 | 0.86 | 0.30 | 44,44,44,44 | 0 |
| 85 | MG | 1 | 4030 | 1/1 | 0.86 | 0.35 | 60,60,60,60 | 0 |
| 85 | MG | AR | 3789 | 1/1 | 0.86 | 0.38 | 25,25,25,25 | 0 |
| 85 | MG | AR | 3783 | 1/1 | 0.87 | 0.34 | 33,33,33,33 | 0 |
| 85 | MG | A | 2137 | 1/1 | 0.87 | 0.33 | 60,60,60,60 | 0 |
| 84 | OHX | x | 201 | 7/7 | 0.87 | 0.46 | 143,144,144,144 | 0 |
| 85 | MG | A | 2146 | 1/1 | 0.87 | 0.62 | 50,50,50,50 | 0 |
| 85 | MG | 1 | 4050 | 1/1 | 0.87 | 0.20 | 55,55,55,55 | 0 |
| 85 | MG | 3 | 218 | 1/1 | 0.87 | 0.24 | 64,64,64,64 | 0 |
| 85 | MG | O | 202 | 1/1 | 0.87 | 0.47 | 55,55,55,55 | 0 |
| 85 | MG | AR | 3812 | 1/1 | 0.87 | 0.53 | 39,39,39,39 | 0 |
| 85 | MG | sR | 2060 | 1/1 | 0.87 | 0.41 | 46,46,46,46 | 0 |
| 85 | MG | sR | 2064 | 1/1 | 0.87 | 0.77 | 60,60,60,60 | 0 |
| 84 | OHX | AR | 3676 | 7/7 | 0.87 | 0.21 | 193,193,193,193 | 0 |
| 85 | MG | 1 | 4055 | 1/1 | 0.87 | 0.17 | 41,41,41,41 | 0 |
| 84 | OHX | AS | 210 | 7/7 | 0.87 | 0.34 | 153,153,154,154 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 84 | OHX | AR | 3687 | 7/7 | 0.87 | 0.23 | 167,168,168,168 | 0 |
| 85 | MG | CP | 502 | 1/1 | 0.87 | 0.34 | 49,49,49,49 | 0 |
| 85 | MG | 1 | 4149 | 1/1 | 0.87 | 0.41 | 27,27,27,27 | 0 |
| 85 | MG | 1 | 4151 | 1/1 | 0.87 | 0.24 | 51,51,51,51 | 0 |
| 85 | MG | CX | 204 | 1/1 | 0.87 | 0.18 | 57,57,57,57 | 0 |
| 84 | OHX | sR | 1960 | 7/7 | 0.87 | 0.21 | 140,140,141,141 | 0 |
| 85 | MG | AR | 4042 | 1/1 | 0.87 | 0.36 | 58,58,58,58 | 0 |
| 85 | MG | 1 | 3884 | 1/1 | 0.87 | 0.25 | 45,45,45,45 | 0 |
| 84 | OHX | 1 | 3727 | 7/7 | 0.87 | 0.38 | 167,168,168,168 | 0 |
| 84 | OHX | AR | 3569 | 7/7 | 0.87 | 0.19 | 143,143,144,144 | 0 |
| 84 | OHX | AR | 3718 | 7/7 | 0.87 | 0.44 | 158,158,159,159 | 0 |
| 85 | MG | AR | 3902 | 1/1 | 0.87 | 0.49 | 44,44,44,44 | 0 |
| 84 | OHX | AR | 3607 | 7/7 | 0.87 | 0.19 | 168,169,169,169 | 0 |
| 84 | OHX | AR | 3637 | 7/7 | 0.87 | 0.16 | 213,213,213,214 | 0 |
| 85 | MG | 1 | 3941 | 1/1 | 0.87 | 0.18 | 44,44,44,44 | 0 |
| 85 | MG | 1 | 3944 | 1/1 | 0.87 | 0.29 | 46,46,46,46 | 0 |
| 85 | MG | 1 | 4172 | 1/1 | 0.87 | 0.26 | 44,44,44,44 | 0 |
| 85 | MG | A | 2076 | 1/1 | 0.87 | 0.50 | 72,72,72,72 | 0 |
| 85 | MG | 1 | 4173 | 1/1 | 0.87 | 0.34 | 51,51,51,51 | 0 |
| 85 | MG | AR | 4067 | 1/1 | 0.87 | 0.29 | 51,51,51,51 | 0 |
| 85 | MG | 1 | 3948 | 1/1 | 0.87 | 0.18 | 50,50,50,50 | 0 |
| 85 | MG | 1 | 4024 | 1/1 | 0.87 | 0.41 | 43,43,43,43 | 0 |
| 85 | MG | sR | 2140 | 1/1 | 0.87 | 0.23 | 69,69,69,69 | 0 |
| 85 | MG | x | 204 | 1/1 | 0.87 | 0.37 | 33,33,33,33 | 0 |
| 84 | OHX | AR | 3646 | 7/7 | 0.87 | 0.28 | 162,162,163,163 | 0 |
| 85 | MG | z | 202 | 1/1 | 0.87 | 0.27 | 63,63,63,63 | 0 |
| 85 | MG | A | 2089 | 1/1 | 0.87 | 0.43 | 72,72,72,72 | 0 |
| 85 | MG | AR | 4088 | 1/1 | 0.87 | 0.34 | 46,46,46,46 | 0 |
| 84 | OHX | 1 | 3729 | 7/7 | 0.87 | 0.46 | 178,179,179,179 | 0 |
| 85 | MG | AR | 4209 | 1/1 | 0.87 | 0.31 | 58,58,58,58 | 0 |
| 85 | MG | AR | 4090 | 1/1 | 0.87 | 0.46 | 50,50,50,50 | 0 |
| 85 | MG | sR | 2164 | 1/1 | 0.87 | 0.23 | 107,107,107,107 | 0 |
| 85 | MG | AR | 4224 | 1/1 | 0.87 | 0.20 | 79,79,79,79 | 0 |
| 84 | OHX | c3 | 201 | 7/7 | 0.87 | 0.21 | 189,190,191,191 | 0 |
| 84 | OHX | 1 | 3710 | 7/7 | 0.87 | 0.18 | 243,243,244,244 | 0 |
| 84 | OHX | 1 | 3726 | 7/7 | 0.87 | 0.45 | 182,183,183,183 | 0 |
| 85 | MG | 1 | 3967 | 1/1 | 0.87 | 0.44 | 53,53,53,53 | 0 |
| 85 | MG | AR | 3762 | 1/1 | 0.87 | 0.31 | 37,37,37,37 | 0 |
| 85 | MG | AR | 4112 | 1/1 | 0.87 | 0.33 | 54,54,54,54 | 0 |
| 85 | MG | AR | 3768 | 1/1 | 0.87 | 0.38 | 40,40,40,40 | 0 |
| 85 | MG | AR | 4244 | 1/1 | 0.87 | 0.21 | 52,52,52,52 | 0 |
| 85 | MG | A | 2127 | 1/1 | 0.87 | 0.25 | 72,72,72,72 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | 1 | 4191 | 1/1 | 0.87 | 0.09 | 52,52,52,52 | 0 |
| 85 | MG | c8 | 202 | 1/1 | 0.87 | 0.30 | 80,80,80,80 | 0 |
| 85 | MG | 1 | 4038 | 1/1 | 0.87 | 0.30 | 47,47,47,47 | 0 |
| 85 | MG | AR | 4248 | 1/1 | 0.87 | 0.73 | 45,45,45,45 | 0 |
| 85 | MG | 1 | 3754 | 1/1 | 0.87 | 0.48 | 50,50,50,50 | 0 |
| 84 | OHX | AR | 3744 | 7/7 | 0.87 | 0.51 | 196,196,197,197 | 0 |
| 85 | MG | AR | 4035 | 1/1 | 0.88 | 0.19 | 38,38,38,38 | 0 |
| 85 | MG | AR | 4181 | 1/1 | 0.88 | 0.47 | 51,51,51,51 | 0 |
| 84 | OHX | 1 | 3607 | 7/7 | 0.88 | 0.23 | 152,152,153,153 | 0 |
| 85 | MG | 1 | 4200 | 1/1 | 0.88 | 0.61 | 49,49,49,49 | 0 |
| 85 | MG | AR | 3814 | 1/1 | 0.88 | 0.33 | 82,82,82,82 | 0 |
| 85 | MG | AR | 4041 | 1/1 | 0.88 | 0.45 | 48,48,48,48 | 0 |
| 85 | MG | AR | 3815 | 1/1 | 0.88 | 0.35 | 35,35,35,35 | 0 |
| 84 | OHX | AR | 3730 | 7/7 | 0.88 | 0.17 | 207,207,208,208 | 0 |
| 85 | MG | 1 | 4111 | 1/1 | 0.88 | 0.29 | 50,50,50,50 | 0 |
| 84 | OHX | AR | 3522 | 7/7 | 0.88 | 0.17 | 164,165,165,165 | 0 |
| 84 | OHX | AR | 3674 | 7/7 | 0.88 | 0.23 | 153,153,153,154 | 0 |
| 84 | OHX | 1 | 3716 | 7/7 | 0.88 | 0.39 | 164,164,165,165 | 0 |
| 85 | MG | 1 | 3733 | 1/1 | 0.88 | 0.80 | 50,50,50,50 | 0 |
| 85 | MG | AR | 4210 | 1/1 | 0.88 | 0.32 | 44,44,44,44 | 0 |
| 85 | MG | AR | 4214 | 1/1 | 0.88 | 0.26 | 50,50,50,50 | 0 |
| 85 | MG | AR | 4215 | 1/1 | 0.88 | 0.54 | 38,38,38,38 | 0 |
| 85 | MG | AR | 4219 | 1/1 | 0.88 | 0.21 | 40,40,40,40 | 0 |
| 85 | MG | 1 | 3829 | 1/1 | 0.88 | 0.42 | 41,41,41,41 | 0 |
| 85 | MG | AR | 3840 | 1/1 | 0.88 | 0.29 | 68,68,68,68 | 0 |
| 85 | MG | 1 | 4124 | 1/1 | 0.88 | 0.33 | 71,71,71,71 | 0 |
| 85 | MG | A | 2147 | 1/1 | 0.88 | 0.19 | 103,103,103,103 | 0 |
| 85 | MG | AR | 4057 | 1/1 | 0.88 | 0.12 | 50,50,50,50 | 0 |
| 85 | MG | AR | 3851 | 1/1 | 0.88 | 0.51 | 50,50,50,50 | 0 |
| 84 | OHX | AR | 3677 | 7/7 | 0.88 | 0.36 | 146,146,147,147 | 0 |
| 85 | MG | AR | 4065 | 1/1 | 0.88 | 0.55 | 45,45,45,45 | 0 |
| 85 | MG | 1 | 4127 | 1/1 | 0.88 | 0.20 | 64,64,64,64 | 0 |
| 85 | MG | AR | 4069 | 1/1 | 0.88 | 0.43 | 51,51,51,51 | 0 |
| 85 | MG | AR | 4075 | 1/1 | 0.88 | 0.23 | 58,58,58,58 | 0 |
| 85 | MG | 1 | 3963 | 1/1 | 0.88 | 0.29 | 33,33,33,33 | 0 |
| 85 | MG | 1 | 3746 | 1/1 | 0.88 | 0.31 | 46,46,46,46 | 0 |
| 85 | MG | AR | 3905 | 1/1 | 0.88 | 0.56 | 49,49,49,49 | 0 |
| 85 | MG | sR | 2071 | 1/1 | 0.88 | 0.43 | 38,38,38,38 | 0 |
| 85 | MG | 1 | 3848 | 1/1 | 0.88 | 0.44 | 43,43,43,43 | 0 |
| 85 | MG | 1 | 4146 | 1/1 | 0.88 | 0.24 | 76,76,76,76 | 0 |
| 85 | MG | AT | 219 | 1/1 | 0.88 | 0.39 | 38,38,38,38 | 0 |
| 85 | MG | 1 | 3852 | 1/1 | 0.88 | 0.43 | 73,73,73,73 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | AT | 223 | 1/1 | 0.88 | 0.70 | 58,58,58,58 | 0 |
| 84 | OHX | AR | 3743 | 7/7 | 0.88 | 0.16 | 160,161,161,162 | 0 |
| 85 | MG | 1 | 3977 | 1/1 | 0.88 | 0.21 | 48,48,48,48 | 0 |
| 85 | MG | 1 | 4054 | 1/1 | 0.88 | 0.44 | 45,45,45,45 | 0 |
| 85 | MG | AR | 4094 | 1/1 | 0.88 | 0.29 | 56,56,56,56 | 0 |
| 85 | MG | sR | 2092 | 1/1 | 0.88 | 0.45 | 77,77,77,77 | 0 |
| 85 | MG | AR | 3953 | 1/1 | 0.88 | 0.58 | 48,48,48,48 | 0 |
| 85 | MG | sR | 2096 | 1/1 | 0.88 | 0.51 | 60,60,60,60 | 0 |
| 85 | MG | 1 | 3978 | 1/1 | 0.88 | 0.38 | 47,47,47,47 | 0 |
| 84 | OHX | 1 | 3708 | 7/7 | 0.88 | 0.31 | 195,196,197,197 | 0 |
| 85 | MG | CJ | 301 | 1/1 | 0.88 | 0.28 | 75,75,75,75 | 0 |
| 85 | MG | v | 304 | 1/1 | 0.88 | 0.47 | 46,46,46,46 | 0 |
| 84 | OHX | 3 | 208 | 7/7 | 0.88 | 0.18 | 190,190,191,191 | 0 |
| 84 | OHX | 1 | 3617 | 7/7 | 0.88 | 0.33 | 165,165,166,166 | 0 |
| 85 | MG | CR | 202 | 1/1 | 0.88 | 0.35 | 39,39,39,39 | 0 |
| 85 | MG | 1 | 4064 | 1/1 | 0.88 | 0.20 | 57,57,57,57 | 0 |
| 85 | MG | CR | 206 | 1/1 | 0.88 | 0.29 | 46,46,46,46 | 0 |
| 85 | MG | sR | 2126 | 1/1 | 0.88 | 0.36 | 58,58,58,58 | 0 |
| 85 | MG | AR | 3977 | 1/1 | 0.88 | 0.23 | 24,24,24,24 | 0 |
| 85 | MG | sR | 2137 | 1/1 | 0.88 | 0.15 | 61,61,61,61 | 0 |
| 84 | OHX | AR | 3713 | 7/7 | 0.88 | 0.29 | 164,164,164,164 | 0 |
| 85 | MG | 1 | 3877 | 1/1 | 0.88 | 0.25 | 56,56,56,56 | 0 |
| 85 | MG | 1 | 3775 | 1/1 | 0.88 | 0.18 | 72,72,72,72 | 0 |
| 84 | OHX | 1 | 3720 | 7/7 | 0.88 | 0.45 | 163,163,163,163 | 0 |
| 85 | MG | AP | 503 | 1/1 | 0.88 | 0.14 | 68,68,68,68 | 0 |
| 85 | MG | 1 | 4081 | 1/1 | 0.88 | 0.34 | 52,52,52,52 | 0 |
| 85 | MG | A | 2052 | 1/1 | 0.88 | 0.51 | 53,53,53,53 | 0 |
| 84 | OHX | AT | 218 | 7/7 | 0.88 | 0.34 | 162,162,163,163 | 0 |
| 85 | MG | A | 2056 | 1/1 | 0.88 | 0.38 | 47,47,47,47 | 0 |
| 85 | MG | A | 2060 | 1/1 | 0.88 | 0.56 | 45,45,45,45 | 0 |
| 85 | MG | 1 | 3888 | 1/1 | 0.88 | 0.10 | 54,54,54,54 | 0 |
| 84 | OHX | CF | 402 | 7/7 | 0.88 | 0.51 | 190,191,192,192 | 0 |
| 85 | MG | AR | 3766 | 1/1 | 0.88 | 0.32 | 58,58,58,58 | 0 |
| 85 | MG | sR | 2174 | 1/1 | 0.88 | 0.29 | 53,53,53,53 | 0 |
| 85 | MG | 1 | 4182 | 1/1 | 0.88 | 0.55 | 75,75,75,75 | 0 |
| 85 | MG | 1 | 3786 | 1/1 | 0.88 | 0.40 | 44,44,44,44 | 0 |
| 85 | MG | AR | 4018 | 1/1 | 0.88 | 0.53 | 50,50,50,50 | 0 |
| 84 | OHX | AR | 3720 | 7/7 | 0.88 | 0.37 | 169,170,170,170 | 0 |
| 85 | MG | 1 | 4010 | 1/1 | 0.88 | 0.57 | 51,51,51,51 | 0 |
| 85 | MG | 1 | 4011 | 1/1 | 0.88 | 0.54 | 53,53,53,53 | 0 |
| 85 | MG | AR | 4026 | 1/1 | 0.88 | 0.24 | 46,46,46,46 | 0 |
| 85 | MG | 1 | 4015 | 1/1 | 0.88 | 0.21 | 56,56,56,56 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | 1 | 4016 | 1/1 | 0.88 | 0.34 | 51,51,51,51 | 0 |
| 85 | MG | s8 | 302 | 1/1 | 0.88 | 0.31 | 54,54,54,54 | 0 |
| 85 | MG | AR | 4167 | 1/1 | 0.88 | 0.30 | 44,44,44,44 | 0 |
| 85 | MG | d3 | 201 | 1/1 | 0.88 | 0.30 | 55,55,55,55 | 0 |
| 84 | OHX | 1 | 3721 | 7/7 | 0.88 | 0.42 | 172,172,173,173 | 0 |
| 85 | MG | AR | 4030 | 1/1 | 0.88 | 0.21 | 34,34,34,34 | 0 |
| 85 | MG | AR | 4031 | 1/1 | 0.88 | 0.24 | 73,73,73,73 | 0 |
| 85 | MG | AR | 3797 | 1/1 | 0.88 | 0.47 | 56,56,56,56 | 0 |
| 87 | ZN | c | 101 | 1/1 | 0.88 | 0.39 | 190,190,190,190 | 0 |
| 87 | ZN | e1 | 501 | 1/1 | 0.88 | 0.03 | 156,156,156,156 | 0 |
| 85 | MG | AR | 4019 | 1/1 | 0.89 | 0.25 | 35,35,35,35 | 0 |
| 85 | MG | AR | 3757 | 1/1 | 0.89 | 0.33 | 29,29,29,29 | 0 |
| 84 | OHX | A | 2038 | 7/7 | 0.89 | 0.52 | 164,164,166,166 | 0 |
| 85 | MG | A | 2103 | 1/1 | 0.89 | 0.40 | 89,89,89,89 | 0 |
| 85 | MG | AR | 4173 | 1/1 | 0.89 | 0.26 | 54,54,54,54 | 0 |
| 84 | OHX | 1 | 3728 | 7/7 | 0.89 | 0.33 | 211,212,212,212 | 0 |
| 85 | MG | AR | 4178 | 1/1 | 0.89 | 0.06 | 94,94,94,94 | 0 |
| 84 | OHX | 1 | 3713 | 7/7 | 0.89 | 0.27 | 138,139,139,139 | 0 |
| 84 | OHX | 1 | 3730 | 7/7 | 0.89 | 0.36 | 159,160,160,160 | 0 |
| 85 | MG | 1 | 3957 | 1/1 | 0.89 | 0.21 | 56,56,56,56 | 0 |
| 84 | OHX | AR | 3602 | 7/7 | 0.89 | 0.27 | 173,174,174,175 | 0 |
| 85 | MG | AR | 3776 | 1/1 | 0.89 | 0.22 | 31,31,31,31 | 0 |
| 85 | MG | AR | 4193 | 1/1 | 0.89 | 0.28 | 57,57,57,57 | 0 |
| 84 | OHX | AR | 3723 | 7/7 | 0.89 | 0.34 | 168,168,168,169 | 0 |
| 84 | OHX | sR | 1991 | 7/7 | 0.89 | 0.31 | 174,175,175,176 | 0 |
| 84 | OHX | sR | 2003 | 7/7 | 0.89 | 0.21 | 188,188,189,189 | 0 |
| 85 | MG | AR | 4198 | 1/1 | 0.89 | 0.55 | 54,54,54,54 | 0 |
| 84 | OHX | AR | 3724 | 7/7 | 0.89 | 0.39 | 217,218,219,219 | 0 |
| 85 | MG | 1 | 3816 | 1/1 | 0.89 | 0.31 | 47,47,47,47 | 0 |
| 84 | OHX | AT | 213 | 7/7 | 0.89 | 0.29 | 187,187,187,187 | 0 |
| 85 | MG | 1 | 4075 | 1/1 | 0.89 | 0.26 | 75,75,75,75 | 0 |
| 84 | OHX | 1 | 3671 | 7/7 | 0.89 | 0.44 | 152,153,154,154 | 0 |
| 85 | MG | AR | 4211 | 1/1 | 0.89 | 0.41 | 69,69,69,69 | 0 |
| 85 | MG | 1 | 4186 | 1/1 | 0.89 | 0.32 | 59,59,59,59 | 0 |
| 84 | OHX | sR | 2042 | 7/7 | 0.89 | 0.29 | 179,180,180,181 | 0 |
| 84 | OHX | sR | 2046 | 7/7 | 0.89 | 0.40 | 178,178,178,179 | 0 |
| 85 | MG | AR | 3818 | 1/1 | 0.89 | 0.33 | 32,32,32,32 | 0 |
| 85 | MG | Y | 201 | 1/1 | 0.89 | 0.17 | 55,55,55,55 | 0 |
| 85 | MG | b | 101 | 1/1 | 0.89 | 0.22 | 75,75,75,75 | 0 |
| 84 | OHX | sR | 2047 | 7/7 | 0.89 | 0.26 | 195,195,196,196 | 0 |
| 85 | MG | AR | 4226 | 1/1 | 0.89 | 0.28 | 38,38,38,38 | 0 |
| 85 | MG | 1 | 3832 | 1/1 | 0.89 | 0.44 | 57,57,57,57 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 84 | OHX | 1 | 3724 | 7/7 | 0.89 | 0.47 | 186,186,187,188 | 0 |
| 85 | MG | 1 | 4199 | 1/1 | 0.89 | 0.40 | 31,31,31,31 | 0 |
| 84 | OHX | AR | 3729 | 7/7 | 0.89 | 0.31 | 177,177,178,178 | 0 |
| 85 | MG | 1 | 4216 | 1/1 | 0.89 | 0.12 | 53,53,53,53 | 0 |
| 84 | OHX | 1 | 3699 | 7/7 | 0.89 | 0.32 | 151,151,152,152 | 0 |
| 85 | MG | AR | 4237 | 1/1 | 0.89 | 0.71 | 59,59,59,59 | 0 |
| 84 | OHX | AR | 3688 | 7/7 | 0.89 | 0.42 | 182,182,182,183 | 0 |
| 85 | MG | 1 | 4000 | 1/1 | 0.89 | 0.32 | 60,60,60,60 | 0 |
| 84 | OHX | AR | 3733 | 7/7 | 0.89 | 0.38 | 153,153,154,154 | 0 |
| 85 | MG | 1 | 4107 | 1/1 | 0.89 | 0.19 | 43,43,43,43 | 0 |
| 85 | MG | AR | 3884 | 1/1 | 0.89 | 0.24 | 46,46,46,46 | 0 |
| 85 | MG | AR | 4251 | 1/1 | 0.89 | 0.09 | 45,45,45,45 | 0 |
| 85 | MG | AR | 3893 | 1/1 | 0.89 | 0.39 | 32,32,32,32 | 0 |
| 85 | MG | AS | 218 | 1/1 | 0.89 | 0.25 | 60,60,60,60 | 0 |
| 85 | MG | 4 | 216 | 1/1 | 0.89 | 0.62 | 55,55,55,55 | 0 |
| 85 | MG | 4 | 222 | 1/1 | 0.89 | 0.47 | 40,40,40,40 | 0 |
| 85 | MG | AR | 4083 | 1/1 | 0.89 | 0.16 | 57,57,57,57 | 0 |
| 85 | MG | AT | 222 | 1/1 | 0.89 | 0.72 | 48,48,48,48 | 0 |
| 84 | OHX | 1 | 3648 | 7/7 | 0.89 | 0.20 | 195,195,195,196 | 0 |
| 84 | OHX | A | 2007 | 7/7 | 0.89 | 0.19 | 220,222,222,223 | 0 |
| 85 | MG | 1 | 3741 | 1/1 | 0.89 | 0.34 | 43,43,43,43 | 0 |
| 84 | OHX | A | 2011 | 7/7 | 0.89 | 0.22 | 182,183,183,183 | 0 |
| 85 | MG | 1 | 4114 | 1/1 | 0.89 | 0.75 | 57,57,57,57 | 0 |
| 85 | MG | 1 | 3749 | 1/1 | 0.89 | 0.54 | 41,41,41,41 | 0 |
| 85 | MG | 1 | 3750 | 1/1 | 0.89 | 0.21 | 57,57,57,57 | 0 |
| 85 | MG | AR | 3927 | 1/1 | 0.89 | 0.48 | 36,36,36,36 | 0 |
| 85 | MG | AR | 3944 | 1/1 | 0.89 | 0.55 | 41,41,41,41 | 0 |
| 85 | MG | AR | 3951 | 1/1 | 0.89 | 0.12 | 39,39,39,39 | 0 |
| 85 | MG | sR | 2133 | 1/1 | 0.89 | 0.30 | 50,50,50,50 | 0 |
| 85 | MG | sR | 2136 | 1/1 | 0.89 | 0.33 | 71,71,71,71 | 0 |
| 85 | MG | CM | 203 | 1/1 | 0.89 | 0.14 | 60,60,60,60 | 0 |
| 85 | MG | AR | 4105 | 1/1 | 0.89 | 0.33 | 51,51,51,51 | 0 |
| 85 | MG | AR | 4107 | 1/1 | 0.89 | 0.28 | 38,38,38,38 | 0 |
| 84 | OHX | AR | 3736 | 7/7 | 0.89 | 0.32 | 154,155,155,156 | 0 |
| 85 | MG | 1 | 4019 | 1/1 | 0.89 | 0.45 | 53,53,53,53 | 0 |
| 85 | MG | sR | 2145 | 1/1 | 0.89 | 0.36 | 58,58,58,58 | 0 |
| 85 | MG | AR | 3963 | 1/1 | 0.89 | 0.14 | 34,34,34,34 | 0 |
| 85 | MG | sR | 2154 | 1/1 | 0.89 | 0.14 | 72,72,72,72 | 0 |
| 85 | MG | sR | 2155 | 1/1 | 0.89 | 0.22 | 67,67,67,67 | 0 |
| 85 | MG | AR | 3965 | 1/1 | 0.89 | 0.19 | 46,46,46,46 | 0 |
| 84 | OHX | AR | 3737 | 7/7 | 0.89 | 0.26 | 189,189,190,190 | 0 |
| 85 | MG | 1 | 3889 | 1/1 | 0.89 | 0.40 | 52,52,52,52 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | 1 | 4022 | 1/1 | 0.89 | 0.31 | 42,42,42,42 | 0 |
| 84 | OHX | AR | 3739 | 7/7 | 0.89 | 0.45 | 190,191,191,191 | 0 |
| 85 | MG | 1 | 4128 | 1/1 | 0.89 | 0.30 | 53,53,53,53 | 0 |
| 85 | MG | 1 | 4025 | 1/1 | 0.89 | 0.22 | 36,36,36,36 | 0 |
| 85 | MG | AR | 3978 | 1/1 | 0.89 | 0.21 | 55,55,55,55 | 0 |
| 85 | MG | AR | 4137 | 1/1 | 0.89 | 0.33 | 61,61,61,61 | 0 |
| 85 | MG | A | 2054 | 1/1 | 0.89 | 0.31 | 61,61,61,61 | 0 |
| 85 | MG | u | 201 | 1/1 | 0.89 | 0.19 | 62,62,62,62 | 0 |
| 85 | MG | AR | 3981 | 1/1 | 0.89 | 0.45 | 39,39,39,39 | 0 |
| 85 | MG | AR | 4141 | 1/1 | 0.89 | 0.50 | 81,81,81,81 | 0 |
| 85 | MG | 1 | 3758 | 1/1 | 0.89 | 0.31 | 41,41,41,41 | 0 |
| 85 | MG | AR | 4148 | 1/1 | 0.89 | 0.42 | 50,50,50,50 | 0 |
| 84 | OHX | A | 2030 | 7/7 | 0.89 | 0.33 | 163,164,165,165 | 0 |
| 85 | MG | 1 | 4140 | 1/1 | 0.89 | 0.44 | 56,56,56,56 | 0 |
| 85 | MG | 1 | 3764 | 1/1 | 0.89 | 0.53 | 47,47,47,47 | 0 |
| 85 | MG | 1 | 3938 | 1/1 | 0.89 | 0.45 | 52,52,52,52 | 0 |
| 85 | MG | c6 | 201 | 1/1 | 0.89 | 0.23 | 82,82,82,82 | 0 |
| 84 | OHX | AR | 3702 | 7/7 | 0.89 | 0.33 | 156,156,157,157 | 0 |
| 85 | MG | 1 | 3773 | 1/1 | 0.89 | 0.44 | 28,28,28,28 | 0 |
| 85 | MG | 1 | 3942 | 1/1 | 0.89 | 0.27 | 44,44,44,44 | 0 |
| 85 | MG | 1 | 4044 | 1/1 | 0.89 | 0.25 | 39,39,39,39 | 0 |
| 85 | MG | 1 | 3943 | 1/1 | 0.89 | 0.36 | 40,40,40,40 | 0 |
| 85 | MG | AR | 4013 | 1/1 | 0.89 | 0.60 | 52,52,52,52 | 0 |
| 84 | OHX | AR | 3708 | 7/7 | 0.89 | 0.34 | 181,182,182,182 | 0 |
| 85 | MG | AR | 3755 | 1/1 | 0.89 | 0.33 | 49,49,49,49 | 0 |
| 84 | OHX | sR | 2009 | 7/7 | 0.90 | 0.14 | 175,176,176,177 | 0 |
| 84 | OHX | sR | 2020 | 7/7 | 0.90 | 0.31 | 174,175,176,176 | 0 |
| 84 | OHX | AR | 3715 | 7/7 | 0.90 | 0.26 | 139,139,139,139 | 0 |
| 85 | MG | A | 2111 | 1/1 | 0.90 | 0.52 | 86,86,86,86 | 0 |
| 85 | MG | 1 | 3895 | 1/1 | 0.90 | 0.58 | 50,50,50,50 | 0 |
| 85 | MG | AR | 4040 | 1/1 | 0.90 | 0.19 | 53,53,53,53 | 0 |
| 85 | MG | 3 | 209 | 1/1 | 0.90 | 0.31 | 49,49,49,49 | 0 |
| 84 | OHX | sR | 2034 | 7/7 | 0.90 | 0.30 | 177,178,179,179 | 0 |
| 84 | OHX | 1 | 3693 | 7/7 | 0.90 | 0.38 | 183,184,184,184 | 0 |
| 85 | MG | A | 2128 | 1/1 | 0.90 | 0.35 | 63,63,63,63 | 0 |
| 85 | MG | AR | 4044 | 1/1 | 0.90 | 0.17 | 44,44,44,44 | 0 |
| 85 | MG | AR | 3832 | 1/1 | 0.90 | 0.17 | 53,53,53,53 | 0 |
| 84 | OHX | A | 1997 | 7/7 | 0.90 | 0.27 | 179,180,180,180 | 0 |
| 85 | MG | 1 | 3929 | 1/1 | 0.90 | 0.67 | 42,42,42,42 | 0 |
| 85 | MG | 1 | 4113 | 1/1 | 0.90 | 0.30 | 43,43,43,43 | 0 |
| 84 | OHX | AR | 3719 | 7/7 | 0.90 | 0.21 | 227,227,228,228 | 0 |
| 85 | MG | AR | 3843 | 1/1 | 0.90 | 0.39 | 41,41,41,41 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 84 | OHX | sR | 2044 | 7/7 | 0.90 | 0.27 | 194,194,195,195 | 0 |
| 85 | MG | A | 2140 | 1/1 | 0.90 | 0.49 | 57,57,57,57 | 0 |
| 84 | OHX | 1 | 3696 | 7/7 | 0.90 | 0.39 | 213,214,214,214 | 0 |
| 84 | OHX | A | 2012 | 7/7 | 0.90 | 0.26 | 162,162,163,163 | 0 |
| 85 | MG | AR | 3878 | 1/1 | 0.90 | 0.41 | 51,51,51,51 | 0 |
| 84 | OHX | sR | 2049 | 7/7 | 0.90 | 0.20 | 217,218,219,219 | 0 |
| 85 | MG | 1 | 3811 | 1/1 | 0.90 | 0.24 | 77,77,77,77 | 0 |
| 84 | OHX | AR | 3614 | 7/7 | 0.90 | 0.32 | 151,152,152,152 | 0 |
| 85 | MG | 1 | 3947 | 1/1 | 0.90 | 0.41 | 40,40,40,40 | 0 |
| 85 | MG | AR | 4070 | 1/1 | 0.90 | 0.51 | 63,63,63,63 | 0 |
| 85 | MG | sR | 2059 | 1/1 | 0.90 | 0.42 | 63,63,63,63 | 0 |
| 85 | MG | AR | 4073 | 1/1 | 0.90 | 0.14 | 62,62,62,62 | 0 |
| 85 | MG | sR | 2062 | 1/1 | 0.90 | 0.41 | 47,47,47,47 | 0 |
| 85 | MG | 1 | 4126 | 1/1 | 0.90 | 0.41 | 54,54,54,54 | 0 |
| 84 | OHX | A | 2022 | 7/7 | 0.90 | 0.29 | 194,195,195,196 | 0 |
| 85 | MG | 1 | 3821 | 1/1 | 0.90 | 0.25 | 27,27,27,27 | 0 |
| 85 | MG | 1 | 4034 | 1/1 | 0.90 | 0.22 | 34,34,34,34 | 0 |
| 84 | OHX | AR | 3681 | 7/7 | 0.90 | 0.26 | 165,165,166,166 | 0 |
| 85 | MG | AR | 4084 | 1/1 | 0.90 | 0.25 | 50,50,50,50 | 0 |
| 85 | MG | 1 | 4134 | 1/1 | 0.90 | 0.24 | 43,43,43,43 | 0 |
| 85 | MG | 1 | 4135 | 1/1 | 0.90 | 0.47 | 44,44,44,44 | 0 |
| 85 | MG | AR | 3924 | 1/1 | 0.90 | 0.36 | 35,35,35,35 | 0 |
| 85 | MG | AS | 220 | 1/1 | 0.90 | 0.24 | 70,70,70,70 | 0 |
| 85 | MG | AS | 227 | 1/1 | 0.90 | 0.30 | 57,57,57,57 | 0 |
| 84 | OHX | A | 2025 | 7/7 | 0.90 | 0.27 | 202,203,204,204 | 0 |
| 85 | MG | AR | 3940 | 1/1 | 0.90 | 0.34 | 28,28,28,28 | 0 |
| 85 | MG | 1 | 3825 | 1/1 | 0.90 | 0.25 | 75,75,75,75 | 0 |
| 85 | MG | 1 | 3958 | 1/1 | 0.90 | 0.39 | 71,71,71,71 | 0 |
| 85 | MG | v | 303 | 1/1 | 0.90 | 0.47 | 45,45,45,45 | 0 |
| 84 | OHX | 1 | 3631 | 7/7 | 0.90 | 0.23 | 170,170,171,172 | 0 |
| 84 | OHX | 1 | 3725 | 7/7 | 0.90 | 0.11 | 188,189,189,189 | 0 |
| 85 | MG | 1 | 3965 | 1/1 | 0.90 | 0.37 | 42,42,42,42 | 0 |
| 85 | MG | sR | 2105 | 1/1 | 0.90 | 0.46 | 56,56,56,56 | 0 |
| 84 | OHX | AR | 3727 | 7/7 | 0.90 | 0.31 | 174,174,174,175 | 0 |
| 84 | OHX | 1 | 3629 | 7/7 | 0.90 | 0.19 | 163,163,163,163 | 0 |
| 85 | MG | AR | 4111 | 1/1 | 0.90 | 0.09 | 41,41,41,41 | 0 |
| 85 | MG | 1 | 4159 | 1/1 | 0.90 | 0.34 | 54,54,54,54 | 0 |
| 85 | MG | 1 | 3969 | 1/1 | 0.90 | 0.24 | 66,66,66,66 | 0 |
| 85 | MG | AR | 4116 | 1/1 | 0.90 | 0.47 | 65,65,65,65 | 0 |
| 85 | MG | 1 | 3843 | 1/1 | 0.90 | 0.40 | 34,34,34,34 | 0 |
| 85 | MG | AR | 4120 | 1/1 | 0.90 | 0.27 | 45,45,45,45 | 0 |
| 85 | MG | 1 | 4060 | 1/1 | 0.90 | 0.23 | 47,47,47,47 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | CQ | 201 | 1/1 | 0.90 | 0.34 | 48,48,48,48 | 0 |
| 84 | OHX | AR | 3701 | 7/7 | 0.90 | 0.24 | 168,168,169,169 | 0 |
| 85 | MG | 1 | 4164 | 1/1 | 0.90 | 0.38 | 34,34,34,34 | 0 |
| 84 | OHX | AT | 217 | 7/7 | 0.90 | 0.28 | 153,153,153,153 | 0 |
| 84 | OHX | 1 | 3678 | 7/7 | 0.90 | 0.23 | 189,189,190,190 | 0 |
| 84 | OHX | AR | 3659 | 7/7 | 0.90 | 0.31 | 144,144,145,145 | 0 |
| 85 | MG | DC | 201 | 1/1 | 0.90 | 0.47 | 44,44,44,44 | 0 |
| 84 | OHX | AR | 3734 | 7/7 | 0.90 | 0.17 | 240,241,242,242 | 0 |
| 85 | MG | sR | 2143 | 1/1 | 0.90 | 0.14 | 51,51,51,51 | 0 |
| 85 | MG | AR | 3988 | 1/1 | 0.90 | 0.31 | 54,54,54,54 | 0 |
| 85 | MG | 1 | 4072 | 1/1 | 0.90 | 0.23 | 44,44,44,44 | 0 |
| 85 | MG | sR | 2153 | 1/1 | 0.90 | 0.33 | 63,63,63,63 | 0 |
| 85 | MG | AR | 3992 | 1/1 | 0.90 | 0.22 | 50,50,50,50 | 0 |
| 85 | MG | AR | 3993 | 1/1 | 0.90 | 0.20 | 41,41,41,41 | 0 |
| 85 | MG | AR | 3994 | 1/1 | 0.90 | 0.57 | 49,49,49,49 | 0 |
| 85 | MG | 1 | 3867 | 1/1 | 0.90 | 0.60 | 58,58,58,58 | 0 |
| 85 | MG | AR | 3771 | 1/1 | 0.90 | 0.47 | 49,49,49,49 | 0 |
| 85 | MG | 1 | 4179 | 1/1 | 0.90 | 0.19 | 52,52,52,52 | 0 |
| 85 | MG | 1 | 4074 | 1/1 | 0.90 | 0.30 | 53,53,53,53 | 0 |
| 84 | OHX | 1 | 3703 | 7/7 | 0.90 | 0.36 | 209,209,210,210 | 0 |
| 85 | MG | sR | 2169 | 1/1 | 0.90 | 0.70 | 55,55,55,55 | 0 |
| 85 | MG | A | 2063 | 1/1 | 0.90 | 0.44 | 44,44,44,44 | 0 |
| 85 | MG | AR | 4011 | 1/1 | 0.90 | 0.41 | 30,30,30,30 | 0 |
| 85 | MG | AR | 4160 | 1/1 | 0.90 | 0.34 | 52,52,52,52 | 0 |
| 85 | MG | 1 | 3874 | 1/1 | 0.90 | 0.43 | 36,36,36,36 | 0 |
| 84 | OHX | sR | 1969 | 7/7 | 0.90 | 0.17 | 155,155,156,156 | 0 |
| 85 | MG | AR | 3780 | 1/1 | 0.90 | 0.35 | 76,76,76,76 | 0 |
| 85 | MG | A | 2080 | 1/1 | 0.90 | 0.44 | 59,59,59,59 | 0 |
| 85 | MG | sR | 2184 | 1/1 | 0.90 | 0.25 | 55,55,55,55 | 0 |
| 84 | OHX | 1 | 3654 | 7/7 | 0.90 | 0.22 | 159,159,159,159 | 0 |
| 85 | MG | AR | 3785 | 1/1 | 0.90 | 0.29 | 60,60,60,60 | 0 |
| 85 | MG | 1 | 3991 | 1/1 | 0.90 | 0.62 | 44,44,44,44 | 0 |
| 85 | MG | AR | 3794 | 1/1 | 0.90 | 0.40 | 43,43,43,43 | 0 |
| 85 | MG | AR | 3795 | 1/1 | 0.90 | 0.24 | 39,39,39,39 | 0 |
| 84 | OHX | sR | 1998 | 7/7 | 0.90 | 0.21 | 190,191,192,192 | 0 |
| 85 | MG | 1 | 3879 | 1/1 | 0.90 | 0.46 | 43,43,43,43 | 0 |
| 85 | MG | 1 | 4096 | 1/1 | 0.90 | 0.34 | 45,45,45,45 | 0 |
| 85 | MG | AR | 4174 | 1/1 | 0.90 | 0.21 | 60,60,60,60 | 0 |
| 85 | MG | AR | 3809 | 1/1 | 0.90 | 0.49 | 43,43,43,43 | 0 |
| 85 | MG | AR | 4177 | 1/1 | 0.90 | 0.19 | 45,45,45,45 | 0 |
| 84 | OHX | DL | 101 | 7/7 | 0.90 | 0.34 | 167,167,167,167 | 0 |
| 85 | MG | AR | 3813 | 1/1 | 0.90 | 0.22 | 60,60,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | d9 | 102 | 1/1 | 0.90 | 0.13 | 94,94,94,94 | 0 |
| 85 | MG | AR | 4032 | 1/1 | 0.90 | 0.34 | 40,40,40,40 | 0 |
| 85 | MG | 1 | 4002 | 1/1 | 0.90 | 0.38 | 38,38,38,38 | 0 |
| 84 | OHX | sR | 2036 | 7/7 | 0.91 | 0.34 | 173,173,174,175 | 0 |
| 85 | MG | 1 | 4057 | 1/1 | 0.91 | 0.31 | 68,68,68,68 | 0 |
| 85 | MG | AR | 4152 | 1/1 | 0.91 | 0.36 | 69,69,69,69 | 0 |
| 85 | MG | AR | 4154 | 1/1 | 0.91 | 0.34 | 47,47,47,47 | 0 |
| 84 | OHX | 1 | 3606 | 7/7 | 0.91 | 0.35 | 141,142,142,143 | 0 |
| 85 | MG | AR | 4001 | 1/1 | 0.91 | 0.69 | 65,65,65,65 | 0 |
| 84 | OHX | A | 1981 | 7/7 | 0.91 | 0.11 | 215,217,217,217 | 0 |
| 85 | MG | AR | 4159 | 1/1 | 0.91 | 0.63 | 51,51,51,51 | 0 |
| 84 | OHX | A | 1993 | 7/7 | 0.91 | 0.42 | 172,173,174,174 | 0 |
| 85 | MG | A | 2095 | 1/1 | 0.91 | 0.37 | 79,79,79,79 | 0 |
| 85 | MG | 1 | 4166 | 1/1 | 0.91 | 0.23 | 70,70,70,70 | 0 |
| 84 | OHX | AR | 3511 | 7/7 | 0.91 | 0.21 | 126,127,127,127 | 0 |
| 85 | MG | A | 2101 | 1/1 | 0.91 | 0.64 | 63,63,63,63 | 0 |
| 85 | MG | AR | 4009 | 1/1 | 0.91 | 0.57 | 35,35,35,35 | 0 |
| 85 | MG | AR | 4010 | 1/1 | 0.91 | 0.38 | 62,62,62,62 | 0 |
| 84 | OHX | 1 | 3647 | 7/7 | 0.91 | 0.39 | 147,148,148,148 | 0 |
| 84 | OHX | 1 | 3555 | 7/7 | 0.91 | 0.19 | 153,153,154,154 | 0 |
| 84 | OHX | AR | 3692 | 7/7 | 0.91 | 0.49 | 146,146,146,146 | 0 |
| 85 | MG | 1 | 4067 | 1/1 | 0.91 | 0.21 | 64,64,64,64 | 0 |
| 85 | MG | AR | 4017 | 1/1 | 0.91 | 0.35 | 31,31,31,31 | 0 |
| 85 | MG | AR | 3781 | 1/1 | 0.91 | 0.26 | 72,72,72,72 | 0 |
| 85 | MG | A | 2112 | 1/1 | 0.91 | 0.30 | 91,91,91,91 | 0 |
| 84 | OHX | 1 | 3564 | 7/7 | 0.91 | 0.21 | 142,142,143,143 | 0 |
| 85 | MG | A | 2114 | 1/1 | 0.91 | 0.31 | 55,55,55,55 | 0 |
| 84 | OHX | AR | 3604 | 7/7 | 0.91 | 0.19 | 156,157,157,157 | 0 |
| 85 | MG | A | 2117 | 1/1 | 0.91 | 0.53 | 69,69,69,69 | 0 |
| 84 | OHX | A | 2023 | 7/7 | 0.91 | 0.28 | 178,179,180,180 | 0 |
| 84 | OHX | AR | 3606 | 7/7 | 0.91 | 0.30 | 145,146,146,146 | 0 |
| 84 | OHX | AR | 3741 | 7/7 | 0.91 | 0.26 | 172,173,173,173 | 0 |
| 85 | MG | 1 | 4079 | 1/1 | 0.91 | 0.21 | 55,55,55,55 | 0 |
| 84 | OHX | d9 | 101 | 7/7 | 0.91 | 0.39 | 182,183,183,184 | 0 |
| 85 | MG | 1 | 4082 | 1/1 | 0.91 | 0.41 | 58,58,58,58 | 0 |
| 84 | OHX | A | 2026 | 7/7 | 0.91 | 0.38 | 150,150,151,151 | 0 |
| 84 | OHX | A | 2028 | 7/7 | 0.91 | 0.21 | 186,187,187,188 | 0 |
| 85 | MG | AR | 4188 | 1/1 | 0.91 | 0.15 | 46,46,46,46 | 0 |
| 85 | MG | 1 | 4091 | 1/1 | 0.91 | 0.29 | 48,48,48,48 | 0 |
| 85 | MG | AR | 4033 | 1/1 | 0.91 | 0.38 | 44,44,44,44 | 0 |
| 84 | OHX | 1 | 3702 | 7/7 | 0.91 | 0.48 | 192,192,193,193 | 0 |
| 85 | MG | A | 2139 | 1/1 | 0.91 | 0.20 | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | 1 | 3992 | 1/1 | 0.91 | 0.60 | 56,56,56,56 | 0 |
| 85 | MG | 1 | 4196 | 1/1 | 0.91 | 0.21 | 68,68,68,68 | 0 |
| 84 | OHX | 1 | 3656 | 7/7 | 0.91 | 0.32 | 137,137,137,137 | 0 |
| 85 | MG | 1 | 3997 | 1/1 | 0.91 | 0.15 | 52,52,52,52 | 0 |
| 85 | MG | 1 | 4201 | 1/1 | 0.91 | 0.71 | 47,47,47,47 | 0 |
| 85 | MG | 1 | 4204 | 1/1 | 0.91 | 0.38 | 42,42,42,42 | 0 |
| 85 | MG | 1 | 4209 | 1/1 | 0.91 | 0.23 | 42,42,42,42 | 0 |
| 84 | OHX | AR | 3621 | 7/7 | 0.91 | 0.31 | 159,159,160,160 | 0 |
| 85 | MG | AR | 4213 | 1/1 | 0.91 | 0.18 | 52,52,52,52 | 0 |
| 85 | MG | AR | 3833 | 1/1 | 0.91 | 0.32 | 56,56,56,56 | 0 |
| 84 | OHX | AR | 3745 | 7/7 | 0.91 | 0.23 | 208,208,209,209 | 0 |
| 85 | MG | 1 | 3751 | 1/1 | 0.91 | 0.32 | 74,74,74,74 | 0 |
| 85 | MG | 3 | 213 | 1/1 | 0.91 | 0.50 | 32,32,32,32 | 0 |
| 84 | OHX | 1 | 3665 | 7/7 | 0.91 | 0.38 | 150,150,151,151 | 0 |
| 85 | MG | sR | 2067 | 1/1 | 0.91 | 0.33 | 56,56,56,56 | 0 |
| 84 | OHX | AR | 3645 | 7/7 | 0.91 | 0.20 | 165,165,166,166 | 0 |
| 85 | MG | AR | 3847 | 1/1 | 0.91 | 0.50 | 52,52,52,52 | 0 |
| 84 | OHX | 1 | 3618 | 7/7 | 0.91 | 0.23 | 161,161,161,162 | 0 |
| 85 | MG | AR | 3865 | 1/1 | 0.91 | 0.27 | 39,39,39,39 | 0 |
| 85 | MG | sR | 2072 | 1/1 | 0.91 | 0.87 | 70,70,70,70 | 0 |
| 84 | OHX | AR | 3650 | 7/7 | 0.91 | 0.24 | 157,158,158,159 | 0 |
| 85 | MG | AR | 4058 | 1/1 | 0.91 | 0.25 | 48,48,48,48 | 0 |
| 85 | MG | 1 | 3760 | 1/1 | 0.91 | 0.51 | 49,49,49,49 | 0 |
| 85 | MG | 4 | 217 | 1/1 | 0.91 | 0.55 | 47,47,47,47 | 0 |
| 85 | MG | AR | 4062 | 1/1 | 0.91 | 0.20 | 64,64,64,64 | 0 |
| 85 | MG | AR | 3882 | 1/1 | 0.91 | 0.45 | 50,50,50,50 | 0 |
| 85 | MG | 4 | 220 | 1/1 | 0.91 | 0.52 | 54,54,54,54 | 0 |
| 85 | MG | AR | 4068 | 1/1 | 0.91 | 0.43 | 57,57,57,57 | 0 |
| 85 | MG | AR | 3889 | 1/1 | 0.91 | 0.48 | 36,36,36,36 | 0 |
| 85 | MG | sR | 2091 | 1/1 | 0.91 | 0.36 | 56,56,56,56 | 0 |
| 84 | OHX | AR | 3722 | 7/7 | 0.91 | 0.23 | 188,188,188,189 | 0 |
| 85 | MG | AR | 4071 | 1/1 | 0.91 | 0.25 | 46,46,46,46 | 0 |
| 85 | MG | AR | 3897 | 1/1 | 0.91 | 0.57 | 55,55,55,55 | 0 |
| 84 | OHX | H | 301 | 7/7 | 0.91 | 0.35 | 182,183,184,184 | 0 |
| 85 | MG | AS | 221 | 1/1 | 0.91 | 0.17 | 50,50,50,50 | 0 |
| 85 | MG | AR | 4076 | 1/1 | 0.91 | 0.20 | 43,43,43,43 | 0 |
| 85 | MG | 1 | 4018 | 1/1 | 0.91 | 0.22 | 43,43,43,43 | 0 |
| 85 | MG | AT | 201 | 1/1 | 0.91 | 0.29 | 57,57,57,57 | 0 |
| 85 | MG | AR | 4080 | 1/1 | 0.91 | 0.46 | 43,43,43,43 | 0 |
| 85 | MG | 1 | 3907 | 1/1 | 0.91 | 0.47 | 30,30,30,30 | 0 |
| 84 | OHX | 1 | 3619 | 7/7 | 0.91 | 0.20 | 179,180,180,181 | 0 |
| 84 | OHX | 1 | 3622 | 7/7 | 0.91 | 0.21 | 151,151,152,152 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | 1 | 3774 | 1/1 | 0.91 | 0.27 | 72,72,72,72 | 0 |
| 85 | MG | 1 | 4023 | 1/1 | 0.91 | 0.83 | 58,58,58,58 | 0 |
| 85 | MG | sR | 2131 | 1/1 | 0.91 | 0.51 | 53,53,53,53 | 0 |
| 84 | OHX | 1 | 3731 | 7/7 | 0.91 | 0.20 | 165,166,167,168 | 0 |
| 85 | MG | CD | 302 | 1/1 | 0.91 | 0.47 | 46,46,46,46 | 0 |
| 85 | MG | sR | 2134 | 1/1 | 0.91 | 0.32 | 58,58,58,58 | 0 |
| 84 | OHX | CG | 301 | 7/7 | 0.91 | 0.19 | 174,175,176,176 | 0 |
| 84 | OHX | 1 | 3623 | 7/7 | 0.91 | 0.23 | 148,148,148,148 | 0 |
| 84 | OHX | sR | 2007 | 7/7 | 0.91 | 0.20 | 185,186,187,187 | 0 |
| 84 | OHX | 1 | 3692 | 7/7 | 0.91 | 0.50 | 183,183,184,184 | 0 |
| 84 | OHX | sR | 2019 | 7/7 | 0.91 | 0.19 | 222,223,224,225 | 0 |
| 85 | MG | AR | 4095 | 1/1 | 0.91 | 0.39 | 46,46,46,46 | 0 |
| 85 | MG | AR | 4097 | 1/1 | 0.91 | 0.26 | 37,37,37,37 | 0 |
| 85 | MG | sR | 2144 | 1/1 | 0.91 | 0.93 | 85,85,85,85 | 0 |
| 85 | MG | 1 | 3788 | 1/1 | 0.91 | 0.39 | 26,26,26,26 | 0 |
| 85 | MG | sR | 2146 | 1/1 | 0.91 | 0.22 | 40,40,40,40 | 0 |
| 85 | MG | t | 202 | 1/1 | 0.91 | 0.39 | 86,86,86,86 | 0 |
| 85 | MG | AR | 3954 | 1/1 | 0.91 | 0.50 | 48,48,48,48 | 0 |
| 85 | MG | AR | 3955 | 1/1 | 0.91 | 0.13 | 36,36,36,36 | 0 |
| 85 | MG | 1 | 3946 | 1/1 | 0.91 | 0.56 | 44,44,44,44 | 0 |
| 85 | MG | AR | 4109 | 1/1 | 0.91 | 0.53 | 50,50,50,50 | 0 |
| 85 | MG | CU | 201 | 1/1 | 0.91 | 0.36 | 48,48,48,48 | 0 |
| 84 | OHX | AR | 3728 | 7/7 | 0.91 | 0.45 | 172,172,173,173 | 0 |
| 85 | MG | 1 | 4136 | 1/1 | 0.91 | 0.29 | 58,58,58,58 | 0 |
| 85 | MG | 1 | 3794 | 1/1 | 0.91 | 0.42 | 23,23,23,23 | 0 |
| 85 | MG | DC | 203 | 1/1 | 0.91 | 0.32 | 57,57,57,57 | 0 |
| 85 | MG | sR | 2165 | 1/1 | 0.91 | 0.65 | 59,59,59,59 | 0 |
| 85 | MG | 1 | 4039 | 1/1 | 0.91 | 0.39 | 57,57,57,57 | 0 |
| 85 | MG | AR | 3969 | 1/1 | 0.91 | 0.71 | 57,57,57,57 | 0 |
| 85 | MG | AR | 3971 | 1/1 | 0.91 | 0.28 | 42,42,42,42 | 0 |
| 85 | MG | DH | 202 | 1/1 | 0.91 | 0.23 | 51,51,51,51 | 0 |
| 85 | MG | DR | 503 | 1/1 | 0.91 | 0.33 | 80,80,80,80 | 0 |
| 85 | MG | 1 | 4141 | 1/1 | 0.91 | 0.42 | 53,53,53,53 | 0 |
| 85 | MG | A | 2047 | 1/1 | 0.91 | 0.69 | 55,55,55,55 | 0 |
| 85 | MG | A | 2048 | 1/1 | 0.91 | 0.28 | 45,45,45,45 | 0 |
| 85 | MG | AR | 3973 | 1/1 | 0.91 | 0.34 | 44,44,44,44 | 0 |
| 85 | MG | 1 | 4143 | 1/1 | 0.91 | 0.36 | 47,47,47,47 | 0 |
| 85 | MG | 1 | 4041 | 1/1 | 0.91 | 0.38 | 43,43,43,43 | 0 |
| 84 | OHX | 1 | 3717 | 7/7 | 0.91 | 0.33 | 188,189,189,189 | 0 |
| 84 | OHX | sR | 2023 | 7/7 | 0.91 | 0.33 | 153,154,155,155 | 0 |
| 85 | MG | A | 2057 | 1/1 | 0.91 | 0.50 | 58,58,58,58 | 0 |
| 84 | OHX | sR | 2030 | 7/7 | 0.91 | 0.28 | 190,190,191,192 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | AR | 4133 | 1/1 | 0.91 | 0.14 | 97,97,97,97 | 0 |
| 85 | MG | 1 | 4153 | 1/1 | 0.91 | 0.30 | 52,52,52,52 | 0 |
| 85 | MG | 1 | 3956 | 1/1 | 0.91 | 0.44 | 53,53,53,53 | 0 |
| 85 | MG | AR | 3752 | 1/1 | 0.91 | 0.21 | 38,38,38,38 | 0 |
| 84 | OHX | sR | 2031 | 7/7 | 0.91 | 0.25 | 134,134,135,135 | 0 |
| 85 | MG | AR | 3754 | 1/1 | 0.91 | 0.29 | 23,23,23,23 | 0 |
| 85 | MG | A | 2071 | 1/1 | 0.91 | 0.34 | 53,53,53,53 | 0 |
| 85 | MG | A | 2072 | 1/1 | 0.91 | 0.29 | 60,60,60,60 | 0 |
| 85 | MG | 1 | 3813 | 1/1 | 0.91 | 0.53 | 36,36,36,36 | 0 |
| 84 | OHX | 1 | 3598 | 7/7 | 0.91 | 0.39 | 180,180,180,180 | 0 |
| 85 | MG | A | 2122 | 1/1 | 0.92 | 0.17 | 87,87,87,87 | 0 |
| 85 | MG | AR | 4232 | 1/1 | 0.92 | 0.18 | 41,41,41,41 | 0 |
| 85 | MG | A | 2125 | 1/1 | 0.92 | 0.60 | 52,52,52,52 | 0 |
| 84 | OHX | A | 1966 | 7/7 | 0.92 | 0.17 | 146,147,147,148 | 0 |
| 85 | MG | AR | 3962 | 1/1 | 0.92 | 0.30 | 46,46,46,46 | 0 |
| 84 | OHX | AR | 3707 | 7/7 | 0.92 | 0.44 | 177,177,177,178 | 0 |
| 85 | MG | A | 2130 | 1/1 | 0.92 | 0.36 | 58,58,58,58 | 0 |
| 84 | OHX | A | 1977 | 7/7 | 0.92 | 0.27 | 175,176,177,177 | 0 |
| 84 | OHX | 1 | 3560 | 7/7 | 0.92 | 0.16 | 169,169,170,170 | 0 |
| 85 | MG | AR | 3767 | 1/1 | 0.92 | 0.20 | 65,65,65,65 | 0 |
| 85 | MG | AR | 4240 | 1/1 | 0.92 | 0.79 | 66,66,66,66 | 0 |
| 84 | OHX | A | 1985 | 7/7 | 0.92 | 0.22 | 146,147,148,148 | 0 |
| 85 | MG | AR | 3769 | 1/1 | 0.92 | 0.16 | 39,39,39,39 | 0 |
| 84 | OHX | sR | 2014 | 7/7 | 0.92 | 0.33 | 141,141,142,142 | 0 |
| 84 | OHX | AR | 3710 | 7/7 | 0.92 | 0.45 | 180,180,181,181 | 0 |
| 84 | OHX | 1 | 3657 | 7/7 | 0.92 | 0.20 | 166,167,167,167 | 0 |
| 85 | MG | A | 2144 | 1/1 | 0.92 | 0.36 | 61,61,61,61 | 0 |
| 85 | MG | AS | 213 | 1/1 | 0.92 | 0.51 | 31,31,31,31 | 0 |
| 84 | OHX | 1 | 3660 | 7/7 | 0.92 | 0.42 | 177,177,178,178 | 0 |
| 85 | MG | A | 2149 | 1/1 | 0.92 | 0.20 | 73,73,73,73 | 0 |
| 85 | MG | 1 | 3891 | 1/1 | 0.92 | 0.41 | 36,36,36,36 | 0 |
| 85 | MG | D | 301 | 1/1 | 0.92 | 0.64 | 72,72,72,72 | 0 |
| 85 | MG | AS | 219 | 1/1 | 0.92 | 0.39 | 52,52,52,52 | 0 |
| 85 | MG | AR | 4098 | 1/1 | 0.92 | 0.25 | 65,65,65,65 | 0 |
| 84 | OHX | AR | 3714 | 7/7 | 0.92 | 0.26 | 169,170,170,170 | 0 |
| 85 | MG | AR | 4101 | 1/1 | 0.92 | 0.14 | 52,52,52,52 | 0 |
| 85 | MG | AR | 3979 | 1/1 | 0.92 | 0.20 | 56,56,56,56 | 0 |
| 84 | OHX | sR | 2027 | 7/7 | 0.92 | 0.24 | 177,177,178,178 | 0 |
| 85 | MG | 1 | 3783 | 1/1 | 0.92 | 0.29 | 30,30,30,30 | 0 |
| 85 | MG | 1 | 4014 | 1/1 | 0.92 | 0.48 | 63,63,63,63 | 0 |
| 85 | MG | 1 | 3912 | 1/1 | 0.92 | 0.30 | 39,39,39,39 | 0 |
| 85 | MG | AR | 3984 | 1/1 | 0.92 | 0.27 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 84 | OHX | AR | 3658 | 7/7 | 0.92 | 0.34 | 146,146,146,146 | 0 |
| 84 | OHX | 1 | 3663 | 7/7 | 0.92 | 0.22 | 169,169,170,170 | 0 |
| 84 | OHX | A | 2017 | 7/7 | 0.92 | 0.26 | 186,187,188,188 | 0 |
| 85 | MG | 1 | 4215 | 1/1 | 0.92 | 0.48 | 40,40,40,40 | 0 |
| 84 | OHX | A | 2018 | 7/7 | 0.92 | 0.31 | 190,191,191,192 | 0 |
| 84 | OHX | sR | 2038 | 7/7 | 0.92 | 0.39 | 167,167,168,169 | 0 |
| 85 | MG | AR | 3995 | 1/1 | 0.92 | 0.23 | 42,42,42,42 | 0 |
| 85 | MG | AR | 3804 | 1/1 | 0.92 | 0.51 | 30,30,30,30 | 0 |
| 85 | MG | 1 | 3789 | 1/1 | 0.92 | 0.34 | 36,36,36,36 | 0 |
| 84 | OHX | sR | 2039 | 7/7 | 0.92 | 0.41 | 197,198,198,198 | 0 |
| 84 | OHX | A | 2021 | 7/7 | 0.92 | 0.41 | 158,159,160,160 | 0 |
| 85 | MG | 1 | 3795 | 1/1 | 0.92 | 0.35 | 50,50,50,50 | 0 |
| 85 | MG | 1 | 3796 | 1/1 | 0.92 | 0.47 | 59,59,59,59 | 0 |
| 84 | OHX | AR | 3533 | 7/7 | 0.92 | 0.22 | 114,114,114,114 | 0 |
| 85 | MG | CQ | 202 | 1/1 | 0.92 | 0.45 | 40,40,40,40 | 0 |
| 84 | OHX | 1 | 3489 | 7/7 | 0.92 | 0.22 | 107,108,108,108 | 0 |
| 84 | OHX | 1 | 3668 | 7/7 | 0.92 | 0.26 | 120,121,121,121 | 0 |
| 85 | MG | AR | 3820 | 1/1 | 0.92 | 0.26 | 40,40,40,40 | 0 |
| 85 | MG | AR | 3822 | 1/1 | 0.92 | 0.66 | 55,55,55,55 | 0 |
| 85 | MG | 1 | 3810 | 1/1 | 0.92 | 0.49 | 45,45,45,45 | 0 |
| 85 | MG | 1 | 3950 | 1/1 | 0.92 | 0.40 | 51,51,51,51 | 0 |
| 84 | OHX | 1 | 3646 | 7/7 | 0.92 | 0.29 | 168,169,169,169 | 0 |
| 85 | MG | 1 | 3953 | 1/1 | 0.92 | 0.07 | 63,63,63,63 | 0 |
| 84 | OHX | 1 | 3608 | 7/7 | 0.92 | 0.26 | 173,173,173,173 | 0 |
| 84 | OHX | sR | 2048 | 7/7 | 0.92 | 0.27 | 188,189,190,190 | 0 |
| 84 | OHX | AR | 3680 | 7/7 | 0.92 | 0.38 | 170,170,171,171 | 0 |
| 85 | MG | AR | 3836 | 1/1 | 0.92 | 0.26 | 52,52,52,52 | 0 |
| 85 | MG | DR | 502 | 1/1 | 0.92 | 0.18 | 61,61,61,61 | 0 |
| 85 | MG | 4 | 233 | 1/1 | 0.92 | 0.34 | 44,44,44,44 | 0 |
| 84 | OHX | AT | 216 | 7/7 | 0.92 | 0.39 | 154,155,155,155 | 0 |
| 85 | MG | 1 | 3959 | 1/1 | 0.92 | 0.27 | 29,29,29,29 | 0 |
| 84 | OHX | 1 | 3557 | 7/7 | 0.92 | 0.20 | 145,145,145,145 | 0 |
| 84 | OHX | AR | 3609 | 7/7 | 0.92 | 0.15 | 171,171,172,172 | 0 |
| 85 | MG | AR | 3852 | 1/1 | 0.92 | 0.31 | 45,45,45,45 | 0 |
| 85 | MG | AR | 3854 | 1/1 | 0.92 | 0.58 | 39,39,39,39 | 0 |
| 85 | MG | AR | 3862 | 1/1 | 0.92 | 0.19 | 26,26,26,26 | 0 |
| 85 | MG | 1 | 4144 | 1/1 | 0.92 | 0.51 | 34,34,34,34 | 0 |
| 85 | MG | AR | 3868 | 1/1 | 0.92 | 0.65 | 28,28,28,28 | 0 |
| 84 | OHX | A | 2035 | 7/7 | 0.92 | 0.36 | 148,149,150,150 | 0 |
| 85 | MG | 1 | 4053 | 1/1 | 0.92 | 0.26 | 55,55,55,55 | 0 |
| 85 | MG | A | 2062 | 1/1 | 0.92 | 0.58 | 58,58,58,58 | 0 |
| 85 | MG | 1 | 4150 | 1/1 | 0.92 | 0.84 | 36,36,36,36 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | o | 301 | 1/1 | 0.92 | 0.20 | 44,44,44,44 | 0 |
| 85 | MG | A | 2066 | 1/1 | 0.92 | 0.68 | 76,76,76,76 | 0 |
| 85 | MG | A | 2067 | 1/1 | 0.92 | 0.86 | 73,73,73,73 | 0 |
| 85 | MG | AR | 3883 | 1/1 | 0.92 | 0.35 | 47,47,47,47 | 0 |
| 84 | OHX | 1 | 3679 | 7/7 | 0.92 | 0.38 | 165,166,166,166 | 0 |
| 85 | MG | AR | 3885 | 1/1 | 0.92 | 0.56 | 41,41,41,41 | 0 |
| 85 | MG | AR | 3888 | 1/1 | 0.92 | 0.61 | 37,37,37,37 | 0 |
| 84 | OHX | A | 2037 | 7/7 | 0.92 | 0.34 | 188,189,189,189 | 0 |
| 85 | MG | 1 | 3968 | 1/1 | 0.92 | 0.18 | 48,48,48,48 | 0 |
| 85 | MG | AR | 4050 | 1/1 | 0.92 | 0.25 | 48,48,48,48 | 0 |
| 84 | OHX | 1 | 3681 | 7/7 | 0.92 | 0.24 | 160,161,162,162 | 0 |
| 85 | MG | 1 | 3737 | 1/1 | 0.92 | 0.27 | 32,32,32,32 | 0 |
| 84 | OHX | 1 | 3649 | 7/7 | 0.92 | 0.26 | 154,155,156,156 | 0 |
| 85 | MG | AR | 3904 | 1/1 | 0.92 | 0.55 | 29,29,29,29 | 0 |
| 85 | MG | 1 | 3972 | 1/1 | 0.92 | 0.19 | 42,42,42,42 | 0 |
| 85 | MG | 1 | 3973 | 1/1 | 0.92 | 0.19 | 55,55,55,55 | 0 |
| 84 | OHX | CL | 302 | 7/7 | 0.92 | 0.16 | 142,142,143,143 | 0 |
| 84 | OHX | AR | 3697 | 7/7 | 0.92 | 0.44 | 157,158,158,159 | 0 |
| 85 | MG | 1 | 3747 | 1/1 | 0.92 | 0.43 | 31,31,31,31 | 0 |
| 85 | MG | 1 | 4069 | 1/1 | 0.92 | 0.40 | 95,95,95,95 | 0 |
| 85 | MG | AR | 4206 | 1/1 | 0.92 | 0.35 | 44,44,44,44 | 0 |
| 85 | MG | AB | 202 | 1/1 | 0.92 | 0.26 | 62,62,62,62 | 0 |
| 85 | MG | 1 | 3980 | 1/1 | 0.92 | 0.37 | 37,37,37,37 | 0 |
| 84 | OHX | AR | 3699 | 7/7 | 0.92 | 0.28 | 202,202,203,203 | 0 |
| 85 | MG | AR | 3930 | 1/1 | 0.92 | 0.36 | 38,38,38,38 | 0 |
| 85 | MG | AR | 3931 | 1/1 | 0.92 | 0.33 | 30,30,30,30 | 0 |
| 84 | OHX | 1 | 3652 | 7/7 | 0.92 | 0.42 | 154,155,155,155 | 0 |
| 85 | MG | s1 | 302 | 1/1 | 0.92 | 0.13 | 63,63,63,63 | 0 |
| 85 | MG | AR | 4072 | 1/1 | 0.92 | 0.17 | 73,73,73,73 | 0 |
| 85 | MG | c1 | 201 | 1/1 | 0.92 | 0.47 | 69,69,69,69 | 0 |
| 85 | MG | AR | 4217 | 1/1 | 0.92 | 0.56 | 43,43,43,43 | 0 |
| 85 | MG | AR | 4218 | 1/1 | 0.92 | 0.40 | 60,60,60,60 | 0 |
| 84 | OHX | 1 | 3625 | 7/7 | 0.92 | 0.17 | 156,157,158,158 | 0 |
| 85 | MG | AR | 4074 | 1/1 | 0.92 | 0.27 | 53,53,53,53 | 0 |
| 84 | OHX | A | 1959 | 7/7 | 0.92 | 0.16 | 165,166,167,167 | 0 |
| 85 | MG | AR | 4225 | 1/1 | 0.92 | 0.10 | 82,82,82,82 | 0 |
| 85 | MG | 1 | 4077 | 1/1 | 0.92 | 0.21 | 58,58,58,58 | 0 |
| 85 | MG | 1 | 3873 | 1/1 | 0.92 | 0.57 | 33,33,33,33 | 0 |
| 85 | MG | AR | 3756 | 1/1 | 0.92 | 0.32 | 48,48,48,48 | 0 |
| 85 | MG | A | 2121 | 1/1 | 0.92 | 0.25 | 73,73,73,73 | 0 |
| 84 | OHX | s4 | 301 | 7/7 | 0.93 | 0.18 | 178,179,179,180 | 0 |
| 84 | OHX | A | 2031 | 7/7 | 0.93 | 0.24 | 199,200,201,202 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 84 | OHX | A | 2032 | 7/7 | 0.93 | 0.21 | 185,186,186,187 | 0 |
| 85 | MG | 1 | 3732 | 1/1 | 0.93 | 0.47 | 39,39,39,39 | 0 |
| 84 | OHX | A | 2033 | 7/7 | 0.93 | 0.22 | 178,179,179,179 | 0 |
| 85 | MG | AR | 4005 | 1/1 | 0.93 | 0.38 | 68,68,68,68 | 0 |
| 84 | OHX | CE | 402 | 7/7 | 0.93 | 0.40 | 187,187,188,188 | 0 |
| 85 | MG | A | 2100 | 1/1 | 0.93 | 0.60 | 54,54,54,54 | 0 |
| 84 | OHX | 1 | 3630 | 7/7 | 0.93 | 0.28 | 149,149,150,150 | 0 |
| 84 | OHX | 1 | 3589 | 7/7 | 0.93 | 0.17 | 151,151,152,152 | 0 |
| 85 | MG | 1 | 3742 | 1/1 | 0.93 | 0.46 | 39,39,39,39 | 0 |
| 85 | MG | 1 | 3745 | 1/1 | 0.93 | 0.42 | 32,32,32,32 | 0 |
| 84 | OHX | 1 | 3712 | 7/7 | 0.93 | 0.38 | 176,177,177,177 | 0 |
| 85 | MG | AR | 3792 | 1/1 | 0.93 | 0.29 | 33,33,33,33 | 0 |
| 85 | MG | 1 | 3894 | 1/1 | 0.93 | 0.33 | 45,45,45,45 | 0 |
| 84 | OHX | CK | 201 | 7/7 | 0.93 | 0.21 | 150,151,151,151 | 0 |
| 84 | OHX | AR | 3679 | 7/7 | 0.93 | 0.19 | 147,148,148,148 | 0 |
| 85 | MG | 1 | 4040 | 1/1 | 0.93 | 0.75 | 61,61,61,61 | 0 |
| 85 | MG | AR | 4021 | 1/1 | 0.93 | 0.46 | 53,53,53,53 | 0 |
| 85 | MG | AR | 3802 | 1/1 | 0.93 | 0.22 | 51,51,51,51 | 0 |
| 84 | OHX | 1 | 3694 | 7/7 | 0.93 | 0.23 | 160,161,161,161 | 0 |
| 85 | MG | 1 | 4043 | 1/1 | 0.93 | 0.31 | 39,39,39,39 | 0 |
| 85 | MG | AR | 3808 | 1/1 | 0.93 | 0.30 | 33,33,33,33 | 0 |
| 84 | OHX | 1 | 3715 | 7/7 | 0.93 | 0.24 | 173,173,174,174 | 0 |
| 84 | OHX | CS | 201 | 1/7 | 0.93 | 0.09 | 173,173,173,173 | 0 |
| 84 | OHX | AR | 3683 | 7/7 | 0.93 | 0.35 | 136,136,136,137 | 0 |
| 85 | MG | 1 | 3923 | 1/1 | 0.93 | 0.36 | 42,42,42,42 | 0 |
| 85 | MG | A | 2126 | 1/1 | 0.93 | 0.34 | 77,77,77,77 | 0 |
| 85 | MG | 1 | 4049 | 1/1 | 0.93 | 0.20 | 38,38,38,38 | 0 |
| 85 | MG | AR | 3816 | 1/1 | 0.93 | 0.28 | 37,37,37,37 | 0 |
| 85 | MG | 1 | 3756 | 1/1 | 0.93 | 0.27 | 32,32,32,32 | 0 |
| 84 | OHX | sR | 1932 | 7/7 | 0.93 | 0.21 | 125,125,126,126 | 0 |
| 85 | MG | AR | 4212 | 1/1 | 0.93 | 0.24 | 36,36,36,36 | 0 |
| 84 | OHX | sR | 1950 | 7/7 | 0.93 | 0.17 | 145,145,146,147 | 0 |
| 84 | OHX | AR | 3684 | 7/7 | 0.93 | 0.39 | 171,171,172,172 | 0 |
| 85 | MG | 1 | 4188 | 1/1 | 0.93 | 0.20 | 54,54,54,54 | 0 |
| 85 | MG | AR | 4216 | 1/1 | 0.93 | 0.17 | 29,29,29,29 | 0 |
| 84 | OHX | A | 1958 | 7/7 | 0.93 | 0.17 | 191,191,193,193 | 0 |
| 85 | MG | AR | 3827 | 1/1 | 0.93 | 0.52 | 56,56,56,56 | 0 |
| 84 | OHX | 3 | 205 | 7/7 | 0.93 | 0.15 | 133,134,135,135 | 0 |
| 85 | MG | 1 | 4193 | 1/1 | 0.93 | 0.58 | 45,45,45,45 | 0 |
| 85 | MG | A | 2142 | 1/1 | 0.93 | 0.15 | 70,70,70,70 | 0 |
| 85 | MG | AR | 4223 | 1/1 | 0.93 | 0.58 | 57,57,57,57 | 0 |
| 85 | MG | 1 | 3765 | 1/1 | 0.93 | 0.22 | 33,33,33,33 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | 1 | 4059 | 1/1 | 0.93 | 0.23 | 40,40,40,40 | 0 |
| 85 | MG | A | 2148 | 1/1 | 0.93 | 0.33 | 86,86,86,86 | 0 |
| 84 | OHX | A | 1964 | 7/7 | 0.93 | 0.28 | 139,139,140,140 | 0 |
| 85 | MG | 1 | 4198 | 1/1 | 0.93 | 0.57 | 32,32,32,32 | 0 |
| 84 | OHX | sR | 2002 | 7/7 | 0.93 | 0.37 | 139,140,141,141 | 0 |
| 84 | OHX | AR | 3731 | 7/7 | 0.93 | 0.34 | 162,163,163,164 | 0 |
| 84 | OHX | 1 | 3695 | 7/7 | 0.93 | 0.48 | 190,190,190,190 | 0 |
| 85 | MG | 1 | 3776 | 1/1 | 0.93 | 0.44 | 34,34,34,34 | 0 |
| 85 | MG | AR | 3845 | 1/1 | 0.93 | 0.29 | 31,31,31,31 | 0 |
| 85 | MG | 1 | 4208 | 1/1 | 0.93 | 0.24 | 26,26,26,26 | 0 |
| 85 | MG | 1 | 3777 | 1/1 | 0.93 | 0.08 | 38,38,38,38 | 0 |
| 85 | MG | 1 | 4212 | 1/1 | 0.93 | 0.19 | 25,25,25,25 | 0 |
| 85 | MG | 1 | 3951 | 1/1 | 0.93 | 0.27 | 52,52,52,52 | 0 |
| 85 | MG | sR | 2063 | 1/1 | 0.93 | 0.39 | 81,81,81,81 | 0 |
| 85 | MG | AR | 3857 | 1/1 | 0.93 | 0.67 | 36,36,36,36 | 0 |
| 85 | MG | 1 | 3778 | 1/1 | 0.93 | 0.32 | 43,43,43,43 | 0 |
| 84 | OHX | sR | 2008 | 7/7 | 0.93 | 0.17 | 175,175,176,177 | 0 |
| 85 | MG | 1 | 3781 | 1/1 | 0.93 | 0.26 | 43,43,43,43 | 0 |
| 85 | MG | 1 | 3955 | 1/1 | 0.93 | 0.26 | 44,44,44,44 | 0 |
| 85 | MG | AR | 3875 | 1/1 | 0.93 | 0.54 | 29,29,29,29 | 0 |
| 84 | OHX | A | 1974 | 7/7 | 0.93 | 0.13 | 168,169,170,170 | 0 |
| 84 | OHX | sR | 2012 | 7/7 | 0.93 | 0.25 | 167,168,168,169 | 0 |
| 84 | OHX | AR | 3628 | 7/7 | 0.93 | 0.23 | 163,164,164,164 | 0 |
| 84 | OHX | sR | 2016 | 7/7 | 0.93 | 0.30 | 158,158,159,159 | 0 |
| 84 | OHX | 4 | 213 | 7/7 | 0.93 | 0.26 | 142,142,143,143 | 0 |
| 85 | MG | AS | 225 | 1/1 | 0.93 | 0.17 | 54,54,54,54 | 0 |
| 84 | OHX | AR | 3640 | 7/7 | 0.93 | 0.28 | 136,136,136,136 | 0 |
| 85 | MG | AR | 3887 | 1/1 | 0.93 | 0.44 | 44,44,44,44 | 0 |
| 84 | OHX | 1 | 3674 | 7/7 | 0.93 | 0.44 | 151,151,151,151 | 0 |
| 84 | OHX | AR | 3700 | 7/7 | 0.93 | 0.38 | 183,183,184,184 | 0 |
| 85 | MG | AR | 3891 | 1/1 | 0.93 | 0.54 | 27,27,27,27 | 0 |
| 85 | MG | sR | 2090 | 1/1 | 0.93 | 0.61 | 44,44,44,44 | 0 |
| 84 | OHX | sR | 2024 | 7/7 | 0.93 | 0.28 | 188,189,190,191 | 0 |
| 85 | MG | 4 | 228 | 1/1 | 0.93 | 0.18 | 52,52,52,52 | 0 |
| 84 | OHX | sR | 2025 | 7/7 | 0.93 | 0.29 | 173,173,174,175 | 0 |
| 85 | MG | AR | 3901 | 1/1 | 0.93 | 0.59 | 37,37,37,37 | 0 |
| 85 | MG | sR | 2100 | 1/1 | 0.93 | 0.49 | 35,35,35,35 | 0 |
| 85 | MG | sR | 2101 | 1/1 | 0.93 | 0.55 | 55,55,55,55 | 0 |
| 85 | MG | AT | 226 | 1/1 | 0.93 | 0.17 | 67,67,67,67 | 0 |
| 85 | MG | sR | 2103 | 1/1 | 0.93 | 0.42 | 57,57,57,57 | 0 |
| 85 | MG | sR | 2104 | 1/1 | 0.93 | 0.22 | 68,68,68,68 | 0 |
| 84 | OHX | A | 2001 | 7/7 | 0.93 | 0.20 | 169,170,171,171 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | sR | 2107 | 1/1 | 0.93 | 0.56 | 40,40,40,40 | 0 |
| 85 | MG | AT | 229 | 1/1 | 0.93 | 0.49 | 65,65,65,65 | 0 |
| 85 | MG | sR | 2114 | 1/1 | 0.93 | 0.31 | 77,77,77,77 | 0 |
| 85 | MG | CD | 301 | 1/1 | 0.93 | 0.77 | 52,52,52,52 | 0 |
| 85 | MG | AR | 3903 | 1/1 | 0.93 | 0.82 | 42,42,42,42 | 0 |
| 85 | MG | 1 | 3798 | 1/1 | 0.93 | 0.14 | 44,44,44,44 | 0 |
| 85 | MG | 1 | 3799 | 1/1 | 0.93 | 0.15 | 37,37,37,37 | 0 |
| 84 | OHX | sR | 2029 | 7/7 | 0.93 | 0.34 | 157,157,157,158 | 0 |
| 85 | MG | 1 | 3803 | 1/1 | 0.93 | 0.51 | 46,46,46,46 | 0 |
| 85 | MG | 1 | 4101 | 1/1 | 0.93 | 0.31 | 27,27,27,27 | 0 |
| 84 | OHX | A | 2002 | 7/7 | 0.93 | 0.19 | 177,179,179,179 | 0 |
| 85 | MG | sR | 2129 | 1/1 | 0.93 | 0.32 | 36,36,36,36 | 0 |
| 84 | OHX | A | 2005 | 7/7 | 0.93 | 0.33 | 157,157,158,158 | 0 |
| 84 | OHX | sR | 2032 | 7/7 | 0.93 | 0.28 | 149,150,150,151 | 0 |
| 85 | MG | AR | 4099 | 1/1 | 0.93 | 0.27 | 41,41,41,41 | 0 |
| 84 | OHX | sR | 2033 | 7/7 | 0.93 | 0.45 | 154,155,155,156 | 0 |
| 84 | OHX | 1 | 3675 | 7/7 | 0.93 | 0.37 | 169,169,170,170 | 0 |
| 85 | MG | CQ | 203 | 1/1 | 0.93 | 0.23 | 55,55,55,55 | 0 |
| 84 | OHX | sR | 2035 | 7/7 | 0.93 | 0.19 | 179,179,181,181 | 0 |
| 84 | OHX | A | 2009 | 7/7 | 0.93 | 0.35 | 156,157,157,158 | 0 |
| 85 | MG | CR | 204 | 1/1 | 0.93 | 0.31 | 59,59,59,59 | 0 |
| 85 | MG | AR | 3939 | 1/1 | 0.93 | 0.42 | 30,30,30,30 | 0 |
| 85 | MG | 1 | 4112 | 1/1 | 0.93 | 0.17 | 52,52,52,52 | 0 |
| 85 | MG | AR | 4108 | 1/1 | 0.93 | 0.42 | 52,52,52,52 | 0 |
| 84 | OHX | sR | 2037 | 7/7 | 0.93 | 0.35 | 174,174,175,175 | 0 |
| 85 | MG | AR | 3949 | 1/1 | 0.93 | 0.12 | 31,31,31,31 | 0 |
| 85 | MG | sR | 2148 | 1/1 | 0.93 | 0.20 | 58,58,58,58 | 0 |
| 85 | MG | DC | 202 | 1/1 | 0.93 | 0.38 | 27,27,27,27 | 0 |
| 84 | OHX | 1 | 3676 | 7/7 | 0.93 | 0.23 | 134,134,135,135 | 0 |
| 84 | OHX | 1 | 3638 | 7/7 | 0.93 | 0.16 | 167,167,168,168 | 0 |
| 84 | OHX | 1 | 3628 | 7/7 | 0.93 | 0.19 | 163,164,164,164 | 0 |
| 85 | MG | 1 | 3827 | 1/1 | 0.93 | 0.46 | 49,49,49,49 | 0 |
| 85 | MG | 1 | 3993 | 1/1 | 0.93 | 0.96 | 52,52,52,52 | 0 |
| 85 | MG | DO | 202 | 1/1 | 0.93 | 0.15 | 45,45,45,45 | 0 |
| 85 | MG | AR | 4119 | 1/1 | 0.93 | 0.18 | 47,47,47,47 | 0 |
| 84 | OHX | AR | 3709 | 7/7 | 0.93 | 0.36 | 174,174,174,174 | 0 |
| 85 | MG | sR | 2163 | 1/1 | 0.93 | 0.33 | 62,62,62,62 | 0 |
| 85 | MG | 1 | 3830 | 1/1 | 0.93 | 0.38 | 32,32,32,32 | 0 |
| 84 | OHX | AR | 3655 | 7/7 | 0.93 | 0.31 | 177,177,177,177 | 0 |
| 85 | MG | sR | 2167 | 1/1 | 0.93 | 0.43 | 47,47,47,47 | 0 |
| 84 | OHX | sR | 2043 | 7/7 | 0.93 | 0.26 | 197,198,198,199 | 0 |
| 85 | MG | AR | 4128 | 1/1 | 0.93 | 0.39 | 46,46,46,46 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | 6 | 201 | 1/1 | 0.93 | 0.44 | 27,27,27,27 | 0 |
| 85 | MG | sR | 2173 | 1/1 | 0.93 | 0.21 | 77,77,77,77 | 0 |
| 84 | OHX | 1 | 3666 | 7/7 | 0.93 | 0.22 | 134,134,134,135 | 0 |
| 85 | MG | AR | 3970 | 1/1 | 0.93 | 0.15 | 97,97,97,97 | 0 |
| 84 | OHX | AR | 3712 | 7/7 | 0.93 | 0.20 | 171,171,172,172 | 0 |
| 85 | MG | 1 | 3844 | 1/1 | 0.93 | 0.67 | 35,35,35,35 | 0 |
| 85 | MG | AR | 4136 | 1/1 | 0.93 | 0.26 | 64,64,64,64 | 0 |
| 85 | MG | 1 | 4131 | 1/1 | 0.93 | 0.22 | 52,52,52,52 | 0 |
| 85 | MG | AR | 3748 | 1/1 | 0.93 | 0.29 | 28,28,28,28 | 0 |
| 85 | MG | AR | 3749 | 1/1 | 0.93 | 0.40 | 49,49,49,49 | 0 |
| 85 | MG | 1 | 3846 | 1/1 | 0.93 | 0.45 | 33,33,33,33 | 0 |
| 85 | MG | A | 2065 | 1/1 | 0.93 | 0.62 | 49,49,49,49 | 0 |
| 85 | MG | 1 | 4006 | 1/1 | 0.93 | 0.77 | 70,70,70,70 | 0 |
| 85 | MG | 1 | 4007 | 1/1 | 0.93 | 0.33 | 59,59,59,59 | 0 |
| 85 | MG | 1 | 4008 | 1/1 | 0.93 | 0.29 | 22,22,22,22 | 0 |
| 84 | OHX | AR | 3532 | 7/7 | 0.93 | 0.19 | 129,129,130,130 | 0 |
| 84 | OHX | AR | 3662 | 7/7 | 0.93 | 0.27 | 164,164,165,165 | 0 |
| 85 | MG | c7 | 201 | 1/1 | 0.93 | 0.52 | 71,71,71,71 | 0 |
| 85 | MG | 1 | 4013 | 1/1 | 0.93 | 0.26 | 37,37,37,37 | 0 |
| 84 | OHX | AR | 3664 | 7/7 | 0.93 | 0.29 | 143,144,144,144 | 0 |
| 84 | OHX | AR | 3717 | 7/7 | 0.93 | 0.29 | 201,201,202,202 | 0 |
| 85 | MG | AR | 3765 | 1/1 | 0.93 | 0.40 | 31,31,31,31 | 0 |
| 85 | MG | 1 | 3864 | 1/1 | 0.93 | 0.31 | 32,32,32,32 | 0 |
| 85 | MG | AR | 3991 | 1/1 | 0.93 | 0.20 | 38,38,38,38 | 0 |
| 84 | OHX | AR | 3666 | 7/7 | 0.93 | 0.31 | 146,146,147,147 | 0 |
| 84 | OHX | 1 | 3568 | 7/7 | 0.93 | 0.15 | 152,153,153,154 | 0 |
| 84 | OHX | 1 | 3690 | 7/7 | 0.93 | 0.35 | 173,173,174,174 | 0 |
| 85 | MG | 1 | 4203 | 1/1 | 0.94 | 0.60 | 45,45,45,45 | 0 |
| 84 | OHX | AR | 3620 | 7/7 | 0.94 | 0.24 | 133,133,133,134 | 0 |
| 85 | MG | 1 | 3876 | 1/1 | 0.94 | 0.48 | 61,61,61,61 | 0 |
| 84 | OHX | 1 | 3667 | 7/7 | 0.94 | 0.25 | 142,142,142,143 | 0 |
| 84 | OHX | AR | 3623 | 7/7 | 0.94 | 0.28 | 147,148,148,148 | 0 |
| 84 | OHX | AR | 3626 | 7/7 | 0.94 | 0.28 | 172,173,173,174 | 0 |
| 85 | MG | AR | 3890 | 1/1 | 0.94 | 0.47 | 25,25,25,25 | 0 |
| 84 | OHX | sR | 2045 | 7/7 | 0.94 | 0.38 | 163,164,164,165 | 0 |
| 84 | OHX | AR | 3716 | 7/7 | 0.94 | 0.21 | 162,162,163,163 | 0 |
| 85 | MG | AR | 3894 | 1/1 | 0.94 | 0.35 | 61,61,61,61 | 0 |
| 85 | MG | 1 | 3885 | 1/1 | 0.94 | 0.52 | 36,36,36,36 | 0 |
| 85 | MG | A | 2074 | 1/1 | 0.94 | 0.52 | 44,44,44,44 | 0 |
| 85 | MG | A | 2075 | 1/1 | 0.94 | 0.45 | 61,61,61,61 | 0 |
| 84 | OHX | AR | 3627 | 7/7 | 0.94 | 0.34 | 164,164,165,165 | 0 |
| 85 | MG | A | 2077 | 1/1 | 0.94 | 0.39 | 53,53,53,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | 3 | 214 | 1/1 | 0.94 | 0.48 | 30,30,30,30 | 0 |
| 85 | MG | 3 | 215 | 1/1 | 0.94 | 0.37 | 53,53,53,53 | 0 |
| 84 | OHX | 1 | 3645 | 7/7 | 0.94 | 0.29 | 162,162,163,163 | 0 |
| 84 | OHX | A | 2010 | 7/7 | 0.94 | 0.19 | 171,173,173,174 | 0 |
| 84 | OHX | AR | 3633 | 7/7 | 0.94 | 0.26 | 151,151,151,151 | 0 |
| 85 | MG | AR | 3907 | 1/1 | 0.94 | 0.59 | 30,30,30,30 | 0 |
| 84 | OHX | 1 | 3670 | 7/7 | 0.94 | 0.31 | 151,152,152,152 | 0 |
| 85 | MG | AR | 4127 | 1/1 | 0.94 | 0.28 | 43,43,43,43 | 0 |
| 84 | OHX | A | 2013 | 7/7 | 0.94 | 0.27 | 154,155,155,155 | 0 |
| 85 | MG | A | 2090 | 1/1 | 0.94 | 0.39 | 55,55,55,55 | 0 |
| 85 | MG | 1 | 3904 | 1/1 | 0.94 | 0.52 | 32,32,32,32 | 0 |
| 84 | OHX | AR | 3639 | 7/7 | 0.94 | 0.17 | 153,154,154,154 | 0 |
| 85 | MG | 4 | 221 | 1/1 | 0.94 | 0.42 | 36,36,36,36 | 0 |
| 85 | MG | 1 | 3911 | 1/1 | 0.94 | 0.38 | 44,44,44,44 | 0 |
| 85 | MG | 4 | 225 | 1/1 | 0.94 | 0.23 | 59,59,59,59 | 0 |
| 85 | MG | AR | 3926 | 1/1 | 0.94 | 0.36 | 47,47,47,47 | 0 |
| 84 | OHX | 1 | 3545 | 7/7 | 0.94 | 0.15 | 142,143,143,143 | 0 |
| 85 | MG | 4 | 227 | 1/1 | 0.94 | 0.45 | 39,39,39,39 | 0 |
| 84 | OHX | s8 | 301 | 7/7 | 0.94 | 0.32 | 194,195,195,196 | 0 |
| 85 | MG | AR | 3932 | 1/1 | 0.94 | 0.45 | 34,34,34,34 | 0 |
| 85 | MG | AR | 4143 | 1/1 | 0.94 | 0.21 | 55,55,55,55 | 0 |
| 84 | OHX | AR | 3641 | 7/7 | 0.94 | 0.20 | 164,164,165,165 | 0 |
| 85 | MG | 1 | 4070 | 1/1 | 0.94 | 0.28 | 47,47,47,47 | 0 |
| 85 | MG | AR | 3941 | 1/1 | 0.94 | 0.59 | 47,47,47,47 | 0 |
| 85 | MG | AR | 3943 | 1/1 | 0.94 | 0.47 | 30,30,30,30 | 0 |
| 85 | MG | 1 | 4071 | 1/1 | 0.94 | 0.25 | 37,37,37,37 | 0 |
| 85 | MG | AR | 3947 | 1/1 | 0.94 | 0.55 | 34,34,34,34 | 0 |
| 84 | OHX | A | 2019 | 7/7 | 0.94 | 0.21 | 210,210,212,212 | 0 |
| 85 | MG | AR | 3950 | 1/1 | 0.94 | 0.11 | 39,39,39,39 | 0 |
| 85 | MG | A | 2118 | 1/1 | 0.94 | 0.13 | 67,67,67,67 | 0 |
| 85 | MG | 1 | 3924 | 1/1 | 0.94 | 0.42 | 49,49,49,49 | 0 |
| 85 | MG | A | 2120 | 1/1 | 0.94 | 0.38 | 49,49,49,49 | 0 |
| 85 | MG | 4 | 234 | 1/1 | 0.94 | 0.66 | 52,52,52,52 | 0 |
| 85 | MG | 1 | 3928 | 1/1 | 0.94 | 0.55 | 23,23,23,23 | 0 |
| 84 | OHX | A | 2020 | 7/7 | 0.94 | 0.15 | 156,157,157,157 | 0 |
| 84 | OHX | AR | 3642 | 7/7 | 0.94 | 0.51 | 153,154,154,154 | 0 |
| 85 | MG | AR | 3958 | 1/1 | 0.94 | 0.40 | 24,24,24,24 | 0 |
| 85 | MG | AR | 3960 | 1/1 | 0.94 | 0.37 | 34,34,34,34 | 0 |
| 85 | MG | 1 | 3734 | 1/1 | 0.94 | 0.40 | 37,37,37,37 | 0 |
| 84 | OHX | AR | 3643 | 7/7 | 0.94 | 0.33 | 158,159,159,159 | 0 |
| 85 | MG | 1 | 4080 | 1/1 | 0.94 | 0.19 | 30,30,30,30 | 0 |
| 84 | OHX | 1 | 3672 | 7/7 | 0.94 | 0.31 | 154,155,155,156 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 84 | OHX | 1 | 3706 | 7/7 | 0.94 | 0.25 | 194,194,195,195 | 0 |
| 84 | OHX | AR | 3647 | 7/7 | 0.94 | 0.34 | 156,156,157,157 | 0 |
| 85 | MG | 1 | 4084 | 1/1 | 0.94 | 0.29 | 52,52,52,52 | 0 |
| 85 | MG | 1 | 4087 | 1/1 | 0.94 | 0.25 | 40,40,40,40 | 0 |
| 84 | OHX | 1 | 3707 | 7/7 | 0.94 | 0.41 | 174,175,175,175 | 0 |
| 84 | OHX | 1 | 3593 | 7/7 | 0.94 | 0.31 | 147,147,148,148 | 0 |
| 84 | OHX | 1 | 3463 | 7/7 | 0.94 | 0.21 | 104,104,105,105 | 0 |
| 84 | OHX | 1 | 3604 | 7/7 | 0.94 | 0.24 | 145,146,146,146 | 0 |
| 84 | OHX | AR | 3657 | 7/7 | 0.94 | 0.21 | 165,165,166,166 | 0 |
| 84 | OHX | 1 | 3486 | 7/7 | 0.94 | 0.17 | 120,121,121,121 | 0 |
| 84 | OHX | x | 202 | 7/7 | 0.94 | 0.33 | 176,176,176,176 | 0 |
| 84 | OHX | 1 | 3626 | 7/7 | 0.94 | 0.25 | 182,182,183,183 | 0 |
| 84 | OHX | AR | 3663 | 7/7 | 0.94 | 0.28 | 161,161,162,162 | 0 |
| 84 | OHX | AK | 102 | 7/7 | 0.94 | 0.14 | 114,114,114,114 | 0 |
| 84 | OHX | AR | 3665 | 7/7 | 0.94 | 0.29 | 161,162,162,162 | 0 |
| 85 | MG | 1 | 4105 | 1/1 | 0.94 | 0.28 | 41,41,41,41 | 0 |
| 85 | MG | AB | 203 | 1/1 | 0.94 | 0.56 | 44,44,44,44 | 0 |
| 85 | MG | AR | 3986 | 1/1 | 0.94 | 0.07 | 63,63,63,63 | 0 |
| 84 | OHX | AR | 3499 | 7/7 | 0.94 | 0.17 | 127,128,128,128 | 0 |
| 85 | MG | AH | 201 | 1/1 | 0.94 | 0.17 | 47,47,47,47 | 0 |
| 85 | MG | AK | 104 | 1/1 | 0.94 | 0.83 | 59,59,59,59 | 0 |
| 85 | MG | sR | 2054 | 1/1 | 0.94 | 0.39 | 57,57,57,57 | 0 |
| 85 | MG | sR | 2055 | 1/1 | 0.94 | 0.75 | 54,54,54,54 | 0 |
| 85 | MG | sR | 2056 | 1/1 | 0.94 | 0.26 | 67,67,67,67 | 0 |
| 84 | OHX | AR | 3508 | 7/7 | 0.94 | 0.15 | 117,118,119,119 | 0 |
| 85 | MG | 1 | 3763 | 1/1 | 0.94 | 0.43 | 46,46,46,46 | 0 |
| 84 | OHX | 1 | 3655 | 7/7 | 0.94 | 0.17 | 165,165,166,166 | 0 |
| 84 | OHX | 1 | 3446 | 7/7 | 0.94 | 0.25 | 99,99,100,100 | 0 |
| 85 | MG | 1 | 3766 | 1/1 | 0.94 | 0.49 | 44,44,44,44 | 0 |
| 85 | MG | AR | 4000 | 1/1 | 0.94 | 0.11 | 64,64,64,64 | 0 |
| 84 | OHX | AR | 3675 | 7/7 | 0.94 | 0.12 | 200,201,201,201 | 0 |
| 84 | OHX | AR | 3526 | 7/7 | 0.94 | 0.28 | 124,125,125,126 | 0 |
| 84 | OHX | O | 201 | 7/7 | 0.94 | 0.15 | 198,199,199,199 | 0 |
| 84 | OHX | sR | 1919 | 7/7 | 0.94 | 0.18 | 107,107,108,108 | 0 |
| 84 | OHX | 1 | 3502 | 7/7 | 0.94 | 0.18 | 123,123,124,124 | 0 |
| 85 | MG | AR | 3758 | 1/1 | 0.94 | 0.46 | 42,42,42,42 | 0 |
| 84 | OHX | sR | 1940 | 7/7 | 0.94 | 0.13 | 162,163,164,164 | 0 |
| 84 | OHX | 1 | 3659 | 7/7 | 0.94 | 0.28 | 169,169,169,169 | 0 |
| 85 | MG | sR | 2078 | 1/1 | 0.94 | 0.54 | 48,48,48,48 | 0 |
| 85 | MG | 1 | 3779 | 1/1 | 0.94 | 0.38 | 39,39,39,39 | 0 |
| 84 | OHX | AR | 3541 | 7/7 | 0.94 | 0.17 | 148,148,149,149 | 0 |
| 85 | MG | sR | 2081 | 1/1 | 0.94 | 0.34 | 59,59,59,59 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | 1 | 3976 | 1/1 | 0.94 | 0.43 | 52,52,52,52 | 0 |
| 84 | OHX | sR | 1961 | 7/7 | 0.94 | 0.16 | 135,136,136,137 | 0 |
| 85 | MG | AR | 4015 | 1/1 | 0.94 | 0.59 | 49,49,49,49 | 0 |
| 84 | OHX | sR | 1966 | 7/7 | 0.94 | 0.16 | 146,146,147,147 | 0 |
| 84 | OHX | AT | 214 | 7/7 | 0.94 | 0.24 | 153,153,153,153 | 0 |
| 85 | MG | sR | 2088 | 1/1 | 0.94 | 0.45 | 74,74,74,74 | 0 |
| 84 | OHX | sR | 1971 | 7/7 | 0.94 | 0.19 | 151,151,152,152 | 0 |
| 85 | MG | AR | 4020 | 1/1 | 0.94 | 0.37 | 43,43,43,43 | 0 |
| 84 | OHX | sR | 1976 | 7/7 | 0.94 | 0.15 | 170,171,172,172 | 0 |
| 84 | OHX | sR | 1978 | 7/7 | 0.94 | 0.21 | 126,126,127,127 | 0 |
| 85 | MG | 1 | 3983 | 1/1 | 0.94 | 0.26 | 47,47,47,47 | 0 |
| 85 | MG | sR | 2097 | 1/1 | 0.94 | 0.49 | 48,48,48,48 | 0 |
| 84 | OHX | sR | 1979 | 7/7 | 0.94 | 0.26 | 160,160,161,161 | 0 |
| 84 | OHX | sR | 1981 | 7/7 | 0.94 | 0.33 | 127,128,129,129 | 0 |
| 84 | OHX | AT | 215 | 7/7 | 0.94 | 0.21 | 157,157,157,158 | 0 |
| 84 | OHX | sR | 1996 | 7/7 | 0.94 | 0.17 | 184,184,185,186 | 0 |
| 85 | MG | AR | 3784 | 1/1 | 0.94 | 0.43 | 41,41,41,41 | 0 |
| 84 | OHX | AR | 3548 | 7/7 | 0.94 | 0.22 | 142,142,142,143 | 0 |
| 84 | OHX | sR | 2000 | 7/7 | 0.94 | 0.22 | 162,163,163,164 | 0 |
| 85 | MG | AR | 3791 | 1/1 | 0.94 | 0.33 | 21,21,21,21 | 0 |
| 84 | OHX | sR | 2001 | 7/7 | 0.94 | 0.14 | 160,160,161,161 | 0 |
| 85 | MG | sR | 2115 | 1/1 | 0.94 | 0.28 | 59,59,59,59 | 0 |
| 85 | MG | 1 | 4148 | 1/1 | 0.94 | 0.19 | 53,53,53,53 | 0 |
| 84 | OHX | AR | 3682 | 7/7 | 0.94 | 0.26 | 153,154,154,154 | 0 |
| 85 | MG | 1 | 3801 | 1/1 | 0.94 | 0.37 | 49,49,49,49 | 0 |
| 85 | MG | sR | 2120 | 1/1 | 0.94 | 0.40 | 70,70,70,70 | 0 |
| 85 | MG | AS | 223 | 1/1 | 0.94 | 0.30 | 75,75,75,75 | 0 |
| 85 | MG | 1 | 3999 | 1/1 | 0.94 | 0.43 | 47,47,47,47 | 0 |
| 84 | OHX | AR | 3560 | 7/7 | 0.94 | 0.23 | 122,122,122,122 | 0 |
| 84 | OHX | sR | 2005 | 7/7 | 0.94 | 0.28 | 176,176,177,178 | 0 |
| 85 | MG | sR | 2125 | 1/1 | 0.94 | 0.21 | 52,52,52,52 | 0 |
| 84 | OHX | sR | 2006 | 7/7 | 0.94 | 0.25 | 148,149,150,150 | 0 |
| 84 | OHX | 1 | 3611 | 7/7 | 0.94 | 0.25 | 141,141,141,141 | 0 |
| 85 | MG | sR | 2130 | 1/1 | 0.94 | 0.12 | 83,83,83,83 | 0 |
| 85 | MG | 1 | 3809 | 1/1 | 0.94 | 0.48 | 49,49,49,49 | 0 |
| 85 | MG | AR | 3811 | 1/1 | 0.94 | 0.41 | 53,53,53,53 | 0 |
| 84 | OHX | AR | 3685 | 7/7 | 0.94 | 0.25 | 182,182,183,183 | 0 |
| 84 | OHX | AR | 3570 | 7/7 | 0.94 | 0.15 | 169,170,170,171 | 0 |
| 85 | MG | sR | 2135 | 1/1 | 0.94 | 0.12 | 82,82,82,82 | 0 |
| 84 | OHX | AR | 3590 | 7/7 | 0.94 | 0.12 | 153,154,155,155 | 0 |
| 85 | MG | 1 | 3814 | 1/1 | 0.94 | 0.22 | 21,21,21,21 | 0 |
| 84 | OHX | AR | 3690 | 7/7 | 0.94 | 0.40 | 145,146,146,146 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | sR | 2139 | 1/1 | 0.94 | 0.19 | 54,54,54,54 | 0 |
| 85 | MG | AT | 228 | 1/1 | 0.94 | 0.35 | 43,43,43,43 | 0 |
| 84 | OHX | AR | 3691 | 7/7 | 0.94 | 0.26 | 149,149,150,150 | 0 |
| 85 | MG | AT | 230 | 1/1 | 0.94 | 0.79 | 49,49,49,49 | 0 |
| 84 | OHX | sR | 2017 | 7/7 | 0.94 | 0.28 | 150,150,151,151 | 0 |
| 85 | MG | AR | 4054 | 1/1 | 0.94 | 0.34 | 35,35,35,35 | 0 |
| 84 | OHX | AR | 3595 | 7/7 | 0.94 | 0.38 | 135,135,136,136 | 0 |
| 85 | MG | 1 | 4168 | 1/1 | 0.94 | 0.27 | 34,34,34,34 | 0 |
| 85 | MG | AR | 3821 | 1/1 | 0.94 | 0.38 | 51,51,51,51 | 0 |
| 85 | MG | 1 | 3823 | 1/1 | 0.94 | 0.46 | 29,29,29,29 | 0 |
| 85 | MG | AR | 3824 | 1/1 | 0.94 | 0.23 | 24,24,24,24 | 0 |
| 85 | MG | AR | 4060 | 1/1 | 0.94 | 0.36 | 47,47,47,47 | 0 |
| 84 | OHX | AR | 3601 | 7/7 | 0.94 | 0.18 | 150,150,151,151 | 0 |
| 85 | MG | sR | 2156 | 1/1 | 0.94 | 0.27 | 62,62,62,62 | 0 |
| 85 | MG | 1 | 4017 | 1/1 | 0.94 | 0.34 | 41,41,41,41 | 0 |
| 85 | MG | AR | 4063 | 1/1 | 0.94 | 0.41 | 49,49,49,49 | 0 |
| 85 | MG | CP | 505 | 1/1 | 0.94 | 0.85 | 106,106,106,106 | 0 |
| 85 | MG | 1 | 4177 | 1/1 | 0.94 | 0.48 | 80,80,80,80 | 0 |
| 84 | OHX | sR | 2021 | 7/7 | 0.94 | 0.13 | 162,162,163,164 | 0 |
| 84 | OHX | AR | 3695 | 7/7 | 0.94 | 0.24 | 160,161,161,162 | 0 |
| 84 | OHX | 1 | 3662 | 7/7 | 0.94 | 0.27 | 187,188,188,189 | 0 |
| 84 | OHX | A | 1915 | 7/7 | 0.94 | 0.17 | 133,134,135,135 | 0 |
| 84 | OHX | A | 1918 | 7/7 | 0.94 | 0.18 | 108,109,109,109 | 0 |
| 85 | MG | sR | 2168 | 1/1 | 0.94 | 0.34 | 47,47,47,47 | 0 |
| 85 | MG | CR | 205 | 1/1 | 0.94 | 0.37 | 44,44,44,44 | 0 |
| 84 | OHX | sR | 2026 | 7/7 | 0.94 | 0.47 | 143,144,144,144 | 0 |
| 84 | OHX | 1 | 3616 | 7/7 | 0.94 | 0.36 | 146,147,147,148 | 0 |
| 85 | MG | CX | 203 | 1/1 | 0.94 | 0.43 | 30,30,30,30 | 0 |
| 84 | OHX | sR | 2028 | 7/7 | 0.94 | 0.35 | 184,184,185,185 | 0 |
| 85 | MG | CX | 205 | 1/1 | 0.94 | 0.19 | 48,48,48,48 | 0 |
| 84 | OHX | A | 1953 | 7/7 | 0.94 | 0.27 | 164,165,166,166 | 0 |
| 85 | MG | AR | 3844 | 1/1 | 0.94 | 0.39 | 28,28,28,28 | 0 |
| 85 | MG | AR | 4077 | 1/1 | 0.94 | 0.28 | 43,43,43,43 | 0 |
| 84 | OHX | AR | 3605 | 7/7 | 0.94 | 0.24 | 145,146,146,146 | 0 |
| 84 | OHX | 1 | 3722 | 7/7 | 0.94 | 0.26 | 176,176,177,177 | 0 |
| 85 | MG | 1 | 4190 | 1/1 | 0.94 | 0.33 | 18,18,18,18 | 0 |
| 84 | OHX | 1 | 3664 | 7/7 | 0.94 | 0.28 | 188,189,190,190 | 0 |
| 85 | MG | AR | 3853 | 1/1 | 0.94 | 0.27 | 43,43,43,43 | 0 |
| 85 | MG | sR | 2190 | 1/1 | 0.94 | 0.38 | 57,57,57,57 | 0 |
| 85 | MG | 1 | 3853 | 1/1 | 0.94 | 0.61 | 34,34,34,34 | 0 |
| 84 | OHX | AR | 3705 | 7/7 | 0.94 | 0.43 | 142,142,142,143 | 0 |
| 85 | MG | AR | 4086 | 1/1 | 0.94 | 0.36 | 41,41,41,41 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | AR | 3859 | 1/1 | 0.94 | 0.40 | 39,39,39,39 | 0 |
| 84 | OHX | 1 | 3635 | 7/7 | 0.94 | 0.26 | 142,143,143,143 | 0 |
| 84 | OHX | AR | 3611 | 7/7 | 0.94 | 0.27 | 136,136,137,137 | 0 |
| 84 | OHX | AR | 3613 | 7/7 | 0.94 | 0.33 | 154,155,155,155 | 0 |
| 85 | MG | 1 | 4197 | 1/1 | 0.94 | 0.42 | 68,68,68,68 | 0 |
| 84 | OHX | A | 1980 | 7/7 | 0.94 | 0.22 | 166,166,167,167 | 0 |
| 85 | MG | d4 | 202 | 1/1 | 0.94 | 0.32 | 60,60,60,60 | 0 |
| 84 | OHX | 1 | 3511 | 7/7 | 0.94 | 0.21 | 118,118,119,119 | 0 |
| 85 | MG | AR | 4096 | 1/1 | 0.94 | 0.34 | 28,28,28,28 | 0 |
| 84 | OHX | AR | 3618 | 7/7 | 0.94 | 0.28 | 128,129,129,129 | 0 |
| 85 | MG | A | 2059 | 1/1 | 0.94 | 0.55 | 60,60,60,60 | 0 |
| 85 | MG | AR | 3879 | 1/1 | 0.94 | 0.39 | 30,30,30,30 | 0 |
| 87 | ZN | d7 | 101 | 1/1 | 0.94 | 0.45 | 180,180,180,180 | 0 |
| 84 | OHX | A | 1991 | 7/7 | 0.94 | 0.15 | 183,184,185,185 | 0 |
| 85 | MG | 1 | 4171 | 1/1 | 0.95 | 0.37 | 44,44,44,44 | 0 |
| 84 | OHX | AR | 3644 | 7/7 | 0.95 | 0.32 | 156,157,157,157 | 0 |
| 85 | MG | 1 | 3989 | 1/1 | 0.95 | 0.22 | 45,45,45,45 | 0 |
| 85 | MG | AR | 3849 | 1/1 | 0.95 | 0.40 | 40,40,40,40 | 0 |
| 85 | MG | A | 2055 | 1/1 | 0.95 | 0.40 | 61,61,61,61 | 0 |
| 84 | OHX | 1 | 3554 | 7/7 | 0.95 | 0.14 | 145,146,146,146 | 0 |
| 84 | OHX | 1 | 3599 | 7/7 | 0.95 | 0.35 | 146,146,146,147 | 0 |
| 84 | OHX | AR | 3738 | 7/7 | 0.95 | 0.26 | 129,130,130,130 | 0 |
| 84 | OHX | Q | 201 | 7/7 | 0.95 | 0.19 | 187,187,188,188 | 0 |
| 85 | MG | AR | 3855 | 1/1 | 0.95 | 0.35 | 56,56,56,56 | 0 |
| 85 | MG | 1 | 3996 | 1/1 | 0.95 | 0.30 | 46,46,46,46 | 0 |
| 85 | MG | AR | 4092 | 1/1 | 0.95 | 0.31 | 41,41,41,41 | 0 |
| 84 | OHX | 1 | 3661 | 7/7 | 0.95 | 0.21 | 145,145,146,146 | 0 |
| 85 | MG | 1 | 3998 | 1/1 | 0.95 | 0.18 | 54,54,54,54 | 0 |
| 84 | OHX | 1 | 3700 | 7/7 | 0.95 | 0.24 | 149,149,150,150 | 0 |
| 84 | OHX | AR | 3458 | 7/7 | 0.95 | 0.18 | 109,110,110,110 | 0 |
| 84 | OHX | AR | 3477 | 7/7 | 0.95 | 0.17 | 120,120,121,121 | 0 |
| 85 | MG | AR | 3871 | 1/1 | 0.95 | 0.78 | 44,44,44,44 | 0 |
| 85 | MG | AR | 3873 | 1/1 | 0.95 | 0.41 | 47,47,47,47 | 0 |
| 84 | OHX | sR | 1954 | 7/7 | 0.95 | 0.09 | 176,177,178,179 | 0 |
| 84 | OHX | 1 | 3701 | 7/7 | 0.95 | 0.33 | 147,148,148,148 | 0 |
| 84 | OHX | AR | 3656 | 7/7 | 0.95 | 0.37 | 152,152,153,153 | 0 |
| 84 | OHX | AR | 3503 | 7/7 | 0.95 | 0.14 | 118,119,119,120 | 0 |
| 85 | MG | 1 | 3793 | 1/1 | 0.95 | 0.47 | 25,25,25,25 | 0 |
| 84 | OHX | 1 | 3600 | 7/7 | 0.95 | 0.27 | 154,154,155,155 | 0 |
| 84 | OHX | AS | 207 | 7/7 | 0.95 | 0.10 | 152,153,154,154 | 0 |
| 84 | OHX | sR | 1973 | 7/7 | 0.95 | 0.17 | 145,145,146,147 | 0 |
| 85 | MG | AR | 3886 | 1/1 | 0.95 | 0.45 | 28,28,28,28 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | A | 2083 | 1/1 | 0.95 | 0.34 | 53,53,53,53 | 0 |
| 84 | OHX | 1 | 3482 | 7/7 | 0.95 | 0.17 | 99,99,100,100 | 0 |
| 84 | OHX | sR | 1977 | 7/7 | 0.95 | 0.12 | 159,160,161,161 | 0 |
| 85 | MG | AR | 4115 | 1/1 | 0.95 | 0.14 | 53,53,53,53 | 0 |
| 84 | OHX | AR | 3661 | 7/7 | 0.95 | 0.43 | 164,165,165,166 | 0 |
| 84 | OHX | AR | 3518 | 7/7 | 0.95 | 0.11 | 163,164,165,165 | 0 |
| 84 | OHX | AT | 206 | 7/7 | 0.95 | 0.15 | 128,128,128,128 | 0 |
| 84 | OHX | sR | 1982 | 7/7 | 0.95 | 0.31 | 140,140,140,140 | 0 |
| 85 | MG | A | 2093 | 1/1 | 0.95 | 0.33 | 54,54,54,54 | 0 |
| 84 | OHX | sR | 1985 | 7/7 | 0.95 | 0.17 | 137,137,138,138 | 0 |
| 85 | MG | AR | 4123 | 1/1 | 0.95 | 0.15 | 40,40,40,40 | 0 |
| 85 | MG | AR | 3896 | 1/1 | 0.95 | 0.71 | 46,46,46,46 | 0 |
| 85 | MG | AR | 4125 | 1/1 | 0.95 | 0.85 | 32,32,32,32 | 0 |
| 84 | OHX | sR | 1987 | 7/7 | 0.95 | 0.27 | 144,145,146,146 | 0 |
| 84 | OHX | sR | 1988 | 7/7 | 0.95 | 0.22 | 173,173,174,174 | 0 |
| 85 | MG | 1 | 4207 | 1/1 | 0.95 | 0.42 | 35,35,35,35 | 0 |
| 84 | OHX | AT | 211 | 7/7 | 0.95 | 0.15 | 163,163,164,164 | 0 |
| 85 | MG | 1 | 3812 | 1/1 | 0.95 | 0.50 | 60,60,60,60 | 0 |
| 85 | MG | 1 | 4211 | 1/1 | 0.95 | 0.29 | 22,22,22,22 | 0 |
| 85 | MG | AR | 4132 | 1/1 | 0.95 | 0.24 | 37,37,37,37 | 0 |
| 84 | OHX | sR | 1995 | 7/7 | 0.95 | 0.19 | 159,160,161,161 | 0 |
| 84 | OHX | AT | 212 | 7/7 | 0.95 | 0.26 | 152,152,152,152 | 0 |
| 85 | MG | 1 | 3815 | 1/1 | 0.95 | 0.49 | 47,47,47,47 | 0 |
| 84 | OHX | 1 | 3455 | 7/7 | 0.95 | 0.16 | 110,111,111,111 | 0 |
| 85 | MG | 1 | 4028 | 1/1 | 0.95 | 0.42 | 61,61,61,61 | 0 |
| 84 | OHX | sR | 1999 | 7/7 | 0.95 | 0.25 | 161,161,162,162 | 0 |
| 85 | MG | AR | 3918 | 1/1 | 0.95 | 0.42 | 24,24,24,24 | 0 |
| 85 | MG | A | 2116 | 1/1 | 0.95 | 0.45 | 76,76,76,76 | 0 |
| 85 | MG | AR | 4142 | 1/1 | 0.95 | 0.09 | 69,69,69,69 | 0 |
| 84 | OHX | 1 | 3515 | 7/7 | 0.95 | 0.18 | 124,124,124,125 | 0 |
| 84 | OHX | 1 | 3562 | 7/7 | 0.95 | 0.18 | 141,141,141,142 | 0 |
| 84 | OHX | 1 | 3633 | 7/7 | 0.95 | 0.23 | 178,179,179,180 | 0 |
| 85 | MG | 3 | 217 | 1/1 | 0.95 | 0.21 | 47,47,47,47 | 0 |
| 84 | OHX | AR | 3667 | 7/7 | 0.95 | 0.41 | 143,143,143,143 | 0 |
| 84 | OHX | AR | 3668 | 7/7 | 0.95 | 0.21 | 136,136,136,136 | 0 |
| 85 | MG | AR | 4153 | 1/1 | 0.95 | 0.34 | 36,36,36,36 | 0 |
| 84 | OHX | AR | 3536 | 7/7 | 0.95 | 0.13 | 139,139,139,139 | 0 |
| 84 | OHX | CF | 401 | 7/7 | 0.95 | 0.30 | 165,166,166,167 | 0 |
| 85 | MG | AR | 3938 | 1/1 | 0.95 | 0.54 | 52,52,52,52 | 0 |
| 84 | OHX | 1 | 3609 | 7/7 | 0.95 | 0.17 | 134,135,135,135 | 0 |
| 85 | MG | AR | 4158 | 1/1 | 0.95 | 0.23 | 52,52,52,52 | 0 |
| 85 | MG | 4 | 218 | 1/1 | 0.95 | 0.61 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 84 | OHX | AR | 3672 | 7/7 | 0.95 | 0.16 | 159,160,160,160 | 0 |
| 85 | MG | AR | 3942 | 1/1 | 0.95 | 0.66 | 34,34,34,34 | 0 |
| 84 | OHX | sR | 2011 | 7/7 | 0.95 | 0.26 | 172,172,173,173 | 0 |
| 84 | OHX | AR | 3542 | 7/7 | 0.95 | 0.14 | 145,146,147,147 | 0 |
| 85 | MG | A | 2136 | 1/1 | 0.95 | 0.12 | 96,96,96,96 | 0 |
| 85 | MG | AR | 4164 | 1/1 | 0.95 | 0.11 | 152,152,152,152 | 0 |
| 85 | MG | AR | 3945 | 1/1 | 0.95 | 0.40 | 43,43,43,43 | 0 |
| 85 | MG | 4 | 223 | 1/1 | 0.95 | 0.58 | 50,50,50,50 | 0 |
| 85 | MG | 1 | 3835 | 1/1 | 0.95 | 0.42 | 25,25,25,25 | 0 |
| 85 | MG | 1 | 3839 | 1/1 | 0.95 | 0.58 | 28,28,28,28 | 0 |
| 85 | MG | A | 2143 | 1/1 | 0.95 | 0.11 | 115,115,115,115 | 0 |
| 85 | MG | 1 | 3840 | 1/1 | 0.95 | 0.61 | 22,22,22,22 | 0 |
| 84 | OHX | sR | 2013 | 7/7 | 0.95 | 0.15 | 170,170,171,171 | 0 |
| 84 | OHX | CG | 303 | 7/7 | 0.95 | 0.35 | 158,159,159,160 | 0 |
| 84 | OHX | sR | 2015 | 7/7 | 0.95 | 0.31 | 158,159,159,160 | 0 |
| 85 | MG | 1 | 4052 | 1/1 | 0.95 | 0.17 | 51,51,51,51 | 0 |
| 84 | OHX | AR | 3543 | 7/7 | 0.95 | 0.16 | 137,138,138,139 | 0 |
| 85 | MG | A | 2151 | 1/1 | 0.95 | 0.14 | 67,67,67,67 | 0 |
| 84 | OHX | 1 | 3669 | 7/7 | 0.95 | 0.24 | 150,150,151,151 | 0 |
| 85 | MG | AR | 3961 | 1/1 | 0.95 | 0.27 | 28,28,28,28 | 0 |
| 84 | OHX | sR | 2018 | 7/7 | 0.95 | 0.27 | 157,158,158,159 | 0 |
| 84 | OHX | AR | 3549 | 7/7 | 0.95 | 0.16 | 137,138,138,138 | 0 |
| 85 | MG | 1 | 3857 | 1/1 | 0.95 | 0.48 | 33,33,33,33 | 0 |
| 85 | MG | AR | 4185 | 1/1 | 0.95 | 0.49 | 53,53,53,53 | 0 |
| 85 | MG | sR | 2053 | 1/1 | 0.95 | 0.65 | 49,49,49,49 | 0 |
| 84 | OHX | AR | 3553 | 7/7 | 0.95 | 0.15 | 136,136,137,137 | 0 |
| 85 | MG | 1 | 3861 | 1/1 | 0.95 | 0.30 | 44,44,44,44 | 0 |
| 84 | OHX | AR | 3558 | 7/7 | 0.95 | 0.25 | 121,121,121,122 | 0 |
| 85 | MG | AR | 4189 | 1/1 | 0.95 | 0.34 | 46,46,46,46 | 0 |
| 84 | OHX | CX | 202 | 7/7 | 0.95 | 0.20 | 131,132,132,132 | 0 |
| 85 | MG | l | 405 | 1/1 | 0.95 | 0.34 | 40,40,40,40 | 0 |
| 84 | OHX | AR | 3559 | 7/7 | 0.95 | 0.17 | 115,116,116,116 | 0 |
| 85 | MG | 1 | 3869 | 1/1 | 0.95 | 0.51 | 41,41,41,41 | 0 |
| 84 | OHX | 1 | 3711 | 7/7 | 0.95 | 0.42 | 157,157,158,158 | 0 |
| 85 | MG | AR | 4199 | 1/1 | 0.95 | 0.27 | 54,54,54,54 | 0 |
| 84 | OHX | AR | 3564 | 7/7 | 0.95 | 0.14 | 149,149,149,150 | 0 |
| 85 | MG | AR | 4201 | 1/1 | 0.95 | 0.66 | 40,40,40,40 | 0 |
| 84 | OHX | 1 | 3636 | 7/7 | 0.95 | 0.27 | 194,194,195,195 | 0 |
| 85 | MG | AR | 4205 | 1/1 | 0.95 | 0.14 | 36,36,36,36 | 0 |
| 84 | OHX | A | 1947 | 7/7 | 0.95 | 0.17 | 124,125,125,125 | 0 |
| 84 | OHX | 1 | 3637 | 7/7 | 0.95 | 0.26 | 143,144,144,144 | 0 |
| 84 | OHX | AR | 3686 | 7/7 | 0.95 | 0.32 | 173,174,175,175 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | sR | 2077 | 1/1 | 0.95 | 0.52 | 41,41,41,41 | 0 |
| 84 | OHX | AR | 3573 | 7/7 | 0.95 | 0.12 | 145,145,145,145 | 0 |
| 84 | OHX | A | 1963 | 7/7 | 0.95 | 0.22 | 165,166,167,167 | 0 |
| 84 | OHX | AR | 3577 | 7/7 | 0.95 | 0.16 | 156,156,157,157 | 0 |
| 85 | MG | 1 | 3882 | 1/1 | 0.95 | 0.42 | 22,22,22,22 | 0 |
| 84 | OHX | AR | 3689 | 7/7 | 0.95 | 0.34 | 152,153,153,153 | 0 |
| 85 | MG | 1 | 4078 | 1/1 | 0.95 | 0.26 | 38,38,38,38 | 0 |
| 85 | MG | AR | 3987 | 1/1 | 0.95 | 0.30 | 45,45,45,45 | 0 |
| 84 | OHX | A | 1968 | 7/7 | 0.95 | 0.28 | 146,147,147,148 | 0 |
| 85 | MG | 1 | 3886 | 1/1 | 0.95 | 0.63 | 31,31,31,31 | 0 |
| 85 | MG | 1 | 3887 | 1/1 | 0.95 | 0.45 | 31,31,31,31 | 0 |
| 85 | MG | sR | 2089 | 1/1 | 0.95 | 0.51 | 44,44,44,44 | 0 |
| 85 | MG | AR | 4220 | 1/1 | 0.95 | 0.35 | 47,47,47,47 | 0 |
| 84 | OHX | AR | 3580 | 7/7 | 0.95 | 0.19 | 132,132,133,133 | 0 |
| 84 | OHX | 1 | 3714 | 7/7 | 0.95 | 0.40 | 163,164,164,165 | 0 |
| 84 | OHX | 1 | 3519 | 7/7 | 0.95 | 0.17 | 110,110,111,111 | 0 |
| 85 | MG | sR | 2095 | 1/1 | 0.95 | 0.46 | 36,36,36,36 | 0 |
| 85 | MG | 1 | 4085 | 1/1 | 0.95 | 0.17 | 39,39,39,39 | 0 |
| 84 | OHX | A | 1978 | 7/7 | 0.95 | 0.17 | 167,168,169,169 | 0 |
| 85 | MG | sR | 2099 | 1/1 | 0.95 | 0.38 | 42,42,42,42 | 0 |
| 85 | MG | AR | 3999 | 1/1 | 0.95 | 0.23 | 42,42,42,42 | 0 |
| 85 | MG | AR | 4228 | 1/1 | 0.95 | 0.35 | 62,62,62,62 | 0 |
| 85 | MG | AR | 4229 | 1/1 | 0.95 | 0.64 | 92,92,92,92 | 0 |
| 84 | OHX | AR | 3597 | 7/7 | 0.95 | 0.34 | 126,127,127,127 | 0 |
| 84 | OHX | AR | 3694 | 7/7 | 0.95 | 0.38 | 147,148,148,149 | 0 |
| 85 | MG | AR | 3750 | 1/1 | 0.95 | 0.12 | 39,39,39,39 | 0 |
| 84 | OHX | AR | 3598 | 7/7 | 0.95 | 0.23 | 137,138,138,138 | 0 |
| 84 | OHX | AR | 3696 | 7/7 | 0.95 | 0.30 | 145,146,147,147 | 0 |
| 85 | MG | sR | 2112 | 1/1 | 0.95 | 0.23 | 62,62,62,62 | 0 |
| 85 | MG | sR | 2113 | 1/1 | 0.95 | 0.39 | 52,52,52,52 | 0 |
| 85 | MG | 1 | 4095 | 1/1 | 0.95 | 0.14 | 57,57,57,57 | 0 |
| 85 | MG | AR | 4007 | 1/1 | 0.95 | 0.45 | 52,52,52,52 | 0 |
| 84 | OHX | AR | 3600 | 7/7 | 0.95 | 0.25 | 157,158,158,159 | 0 |
| 84 | OHX | A | 1995 | 7/7 | 0.95 | 0.11 | 177,178,179,179 | 0 |
| 84 | OHX | 1 | 3640 | 7/7 | 0.95 | 0.25 | 145,145,146,146 | 0 |
| 85 | MG | 1 | 3919 | 1/1 | 0.95 | 0.66 | 23,23,23,23 | 0 |
| 84 | OHX | A | 1998 | 7/7 | 0.95 | 0.23 | 178,179,180,181 | 0 |
| 84 | OHX | A | 1999 | 7/7 | 0.95 | 0.21 | 169,170,170,171 | 0 |
| 84 | OHX | A | 2000 | 7/7 | 0.95 | 0.20 | 167,168,168,168 | 0 |
| 84 | OHX | 1 | 3643 | 7/7 | 0.95 | 0.25 | 157,158,158,158 | 0 |
| 85 | MG | AS | 214 | 1/1 | 0.95 | 0.35 | 57,57,57,57 | 0 |
| 85 | MG | AS | 216 | 1/1 | 0.95 | 0.55 | 26,26,26,26 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | sR | 2127 | 1/1 | 0.95 | 0.28 | 65,65,65,65 | 0 |
| 85 | MG | sR | 2128 | 1/1 | 0.95 | 0.31 | 38,38,38,38 | 0 |
| 85 | MG | 1 | 4106 | 1/1 | 0.95 | 0.15 | 37,37,37,37 | 0 |
| 84 | OHX | 1 | 3612 | 7/7 | 0.95 | 0.17 | 149,150,151,151 | 0 |
| 85 | MG | 1 | 3934 | 1/1 | 0.95 | 0.14 | 34,34,34,34 | 0 |
| 84 | OHX | A | 2003 | 7/7 | 0.95 | 0.26 | 153,154,155,155 | 0 |
| 84 | OHX | A | 2004 | 7/7 | 0.95 | 0.22 | 167,168,169,169 | 0 |
| 85 | MG | AS | 222 | 1/1 | 0.95 | 0.32 | 34,34,34,34 | 0 |
| 84 | OHX | 1 | 3613 | 7/7 | 0.95 | 0.35 | 140,141,141,141 | 0 |
| 85 | MG | AS | 224 | 1/1 | 0.95 | 0.15 | 88,88,88,88 | 0 |
| 84 | OHX | A | 2006 | 7/7 | 0.95 | 0.18 | 162,163,164,164 | 0 |
| 84 | OHX | AR | 3704 | 7/7 | 0.95 | 0.24 | 136,136,136,137 | 0 |
| 84 | OHX | 1 | 3677 | 7/7 | 0.95 | 0.16 | 196,197,197,198 | 0 |
| 84 | OHX | c5 | 201 | 7/7 | 0.95 | 0.26 | 179,180,181,181 | 0 |
| 85 | MG | 1 | 3945 | 1/1 | 0.95 | 0.36 | 34,34,34,34 | 0 |
| 84 | OHX | AR | 3706 | 7/7 | 0.95 | 0.29 | 146,146,146,147 | 0 |
| 84 | OHX | 1 | 3615 | 7/7 | 0.95 | 0.22 | 151,151,152,153 | 0 |
| 84 | OHX | 1 | 3537 | 7/7 | 0.95 | 0.23 | 127,128,128,128 | 0 |
| 84 | OHX | AR | 3610 | 7/7 | 0.95 | 0.13 | 155,155,156,156 | 0 |
| 85 | MG | 1 | 3736 | 1/1 | 0.95 | 0.34 | 53,53,53,53 | 0 |
| 84 | OHX | A | 2014 | 7/7 | 0.95 | 0.37 | 154,155,155,155 | 0 |
| 85 | MG | sR | 2149 | 1/1 | 0.95 | 0.51 | 59,59,59,59 | 0 |
| 84 | OHX | 1 | 3680 | 7/7 | 0.95 | 0.29 | 180,180,181,181 | 0 |
| 84 | OHX | AR | 3612 | 7/7 | 0.95 | 0.24 | 139,140,140,140 | 0 |
| 84 | OHX | 1 | 3582 | 7/7 | 0.95 | 0.29 | 125,125,126,126 | 0 |
| 85 | MG | 1 | 3743 | 1/1 | 0.95 | 0.59 | 42,42,42,42 | 0 |
| 84 | OHX | 1 | 3651 | 7/7 | 0.95 | 0.21 | 149,149,150,150 | 0 |
| 85 | MG | AR | 3799 | 1/1 | 0.95 | 0.36 | 46,46,46,46 | 0 |
| 85 | MG | AR | 3800 | 1/1 | 0.95 | 0.63 | 48,48,48,48 | 0 |
| 85 | MG | 1 | 4133 | 1/1 | 0.95 | 0.43 | 74,74,74,74 | 0 |
| 84 | OHX | AR | 3616 | 7/7 | 0.95 | 0.32 | 156,157,158,158 | 0 |
| 84 | OHX | 1 | 3685 | 7/7 | 0.95 | 0.26 | 172,172,173,173 | 0 |
| 84 | OHX | 1 | 3686 | 7/7 | 0.95 | 0.24 | 154,154,155,155 | 0 |
| 84 | OHX | 1 | 3689 | 7/7 | 0.95 | 0.31 | 131,132,132,132 | 0 |
| 85 | MG | 1 | 3961 | 1/1 | 0.95 | 0.37 | 67,67,67,67 | 0 |
| 85 | MG | CN | 201 | 1/1 | 0.95 | 0.17 | 72,72,72,72 | 0 |
| 84 | OHX | 1 | 3470 | 7/7 | 0.95 | 0.19 | 108,109,109,109 | 0 |
| 85 | MG | CP | 503 | 1/1 | 0.95 | 0.30 | 42,42,42,42 | 0 |
| 85 | MG | 1 | 4142 | 1/1 | 0.95 | 0.19 | 47,47,47,47 | 0 |
| 84 | OHX | AR | 3624 | 7/7 | 0.95 | 0.18 | 139,139,140,140 | 0 |
| 84 | OHX | AR | 3625 | 7/7 | 0.95 | 0.26 | 147,148,148,149 | 0 |
| 85 | MG | 1 | 3755 | 1/1 | 0.95 | 0.29 | 40,40,40,40 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | 1 | 4147 | 1/1 | 0.95 | 0.14 | 62,62,62,62 | 0 |
| 84 | OHX | A | 2027 | 7/7 | 0.95 | 0.20 | 197,198,199,199 | 0 |
| 84 | OHX | 1 | 3691 | 7/7 | 0.95 | 0.28 | 152,152,153,153 | 0 |
| 85 | MG | sR | 2181 | 1/1 | 0.95 | 0.13 | 108,108,108,108 | 0 |
| 84 | OHX | 3 | 203 | 7/7 | 0.95 | 0.16 | 113,114,114,114 | 0 |
| 85 | MG | 1 | 3759 | 1/1 | 0.95 | 0.33 | 55,55,55,55 | 0 |
| 84 | OHX | 1 | 3547 | 7/7 | 0.95 | 0.15 | 147,147,148,148 | 0 |
| 85 | MG | AR | 3823 | 1/1 | 0.95 | 0.12 | 80,80,80,80 | 0 |
| 84 | OHX | AR | 3629 | 7/7 | 0.95 | 0.24 | 157,157,158,158 | 0 |
| 84 | OHX | 3 | 207 | 7/7 | 0.95 | 0.16 | 158,158,159,159 | 0 |
| 85 | MG | sR | 2189 | 1/1 | 0.95 | 0.25 | 58,58,58,58 | 0 |
| 84 | OHX | AR | 3634 | 7/7 | 0.95 | 0.27 | 173,173,174,174 | 0 |
| 84 | OHX | AR | 3635 | 7/7 | 0.95 | 0.15 | 158,159,159,159 | 0 |
| 84 | OHX | 1 | 3620 | 7/7 | 0.95 | 0.17 | 148,148,149,149 | 0 |
| 85 | MG | AR | 3831 | 1/1 | 0.95 | 0.64 | 34,34,34,34 | 0 |
| 85 | MG | 1 | 3768 | 1/1 | 0.95 | 0.30 | 28,28,28,28 | 0 |
| 85 | MG | 1 | 3770 | 1/1 | 0.95 | 0.62 | 42,42,42,42 | 0 |
| 84 | OHX | 4 | 211 | 7/7 | 0.95 | 0.16 | 160,160,160,160 | 0 |
| 84 | OHX | 1 | 3621 | 7/7 | 0.95 | 0.11 | 200,201,201,201 | 0 |
| 84 | OHX | 1 | 3597 | 7/7 | 0.95 | 0.11 | 158,158,158,159 | 0 |
| 85 | MG | DH | 203 | 1/1 | 0.95 | 0.38 | 39,39,39,39 | 0 |
| 85 | MG | AR | 3837 | 1/1 | 0.95 | 0.64 | 25,25,25,25 | 0 |
| 85 | MG | AR | 3838 | 1/1 | 0.95 | 0.28 | 27,27,27,27 | 0 |
| 85 | MG | AR | 4078 | 1/1 | 0.95 | 0.54 | 34,34,34,34 | 0 |
| 85 | MG | A | 2043 | 1/1 | 0.95 | 0.37 | 55,55,55,55 | 0 |
| 85 | MG | A | 2045 | 1/1 | 0.95 | 0.56 | 45,45,45,45 | 0 |
| 84 | OHX | 1 | 3658 | 7/7 | 0.95 | 0.12 | 173,174,174,175 | 0 |
| 87 | ZN | g | 501 | 1/1 | 0.95 | 0.05 | 121,121,121,121 | 0 |
| 85 | MG | 1 | 3986 | 1/1 | 0.95 | 0.29 | 66,66,66,66 | 0 |
| 84 | OHX | l | 401 | 7/7 | 0.95 | 0.30 | 163,163,164,164 | 0 |
| 84 | OHX | 1 | 3528 | 7/7 | 0.96 | 0.15 | 138,139,139,139 | 0 |
| 84 | OHX | AR | 3576 | 7/7 | 0.96 | 0.21 | 138,139,139,140 | 0 |
| 84 | OHX | Rb | 401 | 7/7 | 0.96 | 0.16 | 195,195,197,197 | 0 |
| 84 | OHX | 1 | 3574 | 7/7 | 0.96 | 0.12 | 152,152,153,153 | 0 |
| 84 | OHX | 1 | 3576 | 7/7 | 0.96 | 0.24 | 130,130,130,131 | 0 |
| 85 | MG | AR | 4144 | 1/1 | 0.96 | 0.45 | 30,30,30,30 | 0 |
| 84 | OHX | AR | 3581 | 7/7 | 0.96 | 0.25 | 131,132,132,132 | 0 |
| 84 | OHX | AS | 208 | 7/7 | 0.96 | 0.24 | 135,135,136,136 | 0 |
| 84 | OHX | AR | 3582 | 7/7 | 0.96 | 0.33 | 145,145,146,146 | 0 |
| 84 | OHX | c8 | 201 | 7/7 | 0.96 | 0.14 | 166,166,167,167 | 0 |
| 85 | MG | AR | 4151 | 1/1 | 0.96 | 0.36 | 49,49,49,49 | 0 |
| 84 | OHX | d4 | 201 | 7/7 | 0.96 | 0.22 | 171,172,172,172 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | A | 2096 | 1/1 | 0.96 | 0.17 | 91,91,91,91 | 0 |
| 84 | OHX | AR | 3583 | 7/7 | 0.96 | 0.11 | 170,170,171,171 | 0 |
| 84 | OHX | AR | 3671 | 7/7 | 0.96 | 0.26 | 161,161,161,161 | 0 |
| 85 | MG | 1 | 3899 | 1/1 | 0.96 | 0.32 | 22,22,22,22 | 0 |
| 85 | MG | 1 | 3902 | 1/1 | 0.96 | 0.69 | 37,37,37,37 | 0 |
| 84 | OHX | AT | 205 | 7/7 | 0.96 | 0.12 | 136,137,137,137 | 0 |
| 85 | MG | 1 | 3905 | 1/1 | 0.96 | 0.41 | 36,36,36,36 | 0 |
| 84 | OHX | AR | 3585 | 7/7 | 0.96 | 0.24 | 156,156,156,156 | 0 |
| 85 | MG | AR | 3956 | 1/1 | 0.96 | 0.32 | 41,41,41,41 | 0 |
| 85 | MG | 1 | 3908 | 1/1 | 0.96 | 0.29 | 21,21,21,21 | 0 |
| 85 | MG | 1 | 3909 | 1/1 | 0.96 | 0.46 | 27,27,27,27 | 0 |
| 85 | MG | AR | 3959 | 1/1 | 0.96 | 0.36 | 30,30,30,30 | 0 |
| 85 | MG | 1 | 3735 | 1/1 | 0.96 | 0.47 | 50,50,50,50 | 0 |
| 84 | OHX | AT | 207 | 7/7 | 0.96 | 0.21 | 135,135,135,135 | 0 |
| 84 | OHX | AT | 209 | 7/7 | 0.96 | 0.20 | 133,133,134,134 | 0 |
| 85 | MG | 1 | 3915 | 1/1 | 0.96 | 0.31 | 39,39,39,39 | 0 |
| 85 | MG | AR | 3964 | 1/1 | 0.96 | 0.25 | 38,38,38,38 | 0 |
| 84 | OHX | AT | 210 | 7/7 | 0.96 | 0.19 | 136,136,137,137 | 0 |
| 85 | MG | AR | 4170 | 1/1 | 0.96 | 0.27 | 55,55,55,55 | 0 |
| 85 | MG | x | 207 | 1/1 | 0.96 | 0.33 | 42,42,42,42 | 0 |
| 84 | OHX | AR | 3673 | 7/7 | 0.96 | 0.25 | 179,180,181,181 | 0 |
| 84 | OHX | AR | 3587 | 7/7 | 0.96 | 0.20 | 120,121,121,121 | 0 |
| 84 | OHX | 1 | 3580 | 7/7 | 0.96 | 0.18 | 117,117,118,118 | 0 |
| 85 | MG | AB | 201 | 1/1 | 0.96 | 0.36 | 26,26,26,26 | 0 |
| 84 | OHX | AR | 3592 | 7/7 | 0.96 | 0.20 | 147,148,148,149 | 0 |
| 84 | OHX | AR | 3594 | 7/7 | 0.96 | 0.22 | 137,138,138,138 | 0 |
| 85 | MG | 1 | 3932 | 1/1 | 0.96 | 0.43 | 22,22,22,22 | 0 |
| 85 | MG | 1 | 3933 | 1/1 | 0.96 | 0.26 | 32,32,32,32 | 0 |
| 84 | OHX | AR | 3678 | 7/7 | 0.96 | 0.34 | 123,124,124,124 | 0 |
| 84 | OHX | e | 101 | 7/7 | 0.96 | 0.33 | 167,168,169,169 | 0 |
| 85 | MG | 1 | 3936 | 1/1 | 0.96 | 0.12 | 40,40,40,40 | 0 |
| 85 | MG | 1 | 3937 | 1/1 | 0.96 | 0.15 | 50,50,50,50 | 0 |
| 84 | OHX | h | 401 | 7/7 | 0.96 | 0.12 | 193,195,196,196 | 0 |
| 84 | OHX | 1 | 3481 | 7/7 | 0.96 | 0.13 | 120,120,121,121 | 0 |
| 85 | MG | AR | 4190 | 1/1 | 0.96 | 0.24 | 48,48,48,48 | 0 |
| 85 | MG | AR | 4191 | 1/1 | 0.96 | 0.19 | 26,26,26,26 | 0 |
| 85 | MG | AR | 4192 | 1/1 | 0.96 | 0.49 | 47,47,47,47 | 0 |
| 85 | MG | 1 | 3940 | 1/1 | 0.96 | 0.41 | 52,52,52,52 | 0 |
| 84 | OHX | sR | 1921 | 7/7 | 0.96 | 0.15 | 124,125,126,127 | 0 |
| 84 | OHX | sR | 1929 | 7/7 | 0.96 | 0.15 | 154,154,155,156 | 0 |
| 84 | OHX | 1 | 3583 | 7/7 | 0.96 | 0.19 | 139,140,140,140 | 0 |
| 84 | OHX | sR | 1933 | 7/7 | 0.96 | 0.17 | 106,106,107,107 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 84 | OHX | 1 | 3538 | 7/7 | 0.96 | 0.20 | 114,114,114,115 | 0 |
| 84 | OHX | sR | 1943 | 7/7 | 0.96 | 0.12 | 131,132,132,132 | 0 |
| 84 | OHX | 1 | 3591 | 7/7 | 0.96 | 0.15 | 169,170,171,171 | 0 |
| 85 | MG | AR | 3761 | 1/1 | 0.96 | 0.15 | 56,56,56,56 | 0 |
| 85 | MG | AR | 4203 | 1/1 | 0.96 | 0.22 | 40,40,40,40 | 0 |
| 84 | OHX | sR | 1952 | 7/7 | 0.96 | 0.10 | 159,159,160,160 | 0 |
| 85 | MG | AR | 3764 | 1/1 | 0.96 | 0.54 | 15,15,15,15 | 0 |
| 84 | OHX | 1 | 3592 | 7/7 | 0.96 | 0.21 | 118,119,119,119 | 0 |
| 84 | OHX | sR | 1955 | 7/7 | 0.96 | 0.11 | 168,169,170,171 | 0 |
| 85 | MG | AR | 3998 | 1/1 | 0.96 | 0.16 | 48,48,48,48 | 0 |
| 84 | OHX | sR | 1956 | 7/7 | 0.96 | 0.10 | 175,176,177,178 | 0 |
| 85 | MG | 1 | 4120 | 1/1 | 0.96 | 0.35 | 42,42,42,42 | 0 |
| 84 | OHX | 1 | 3539 | 7/7 | 0.96 | 0.13 | 130,131,131,132 | 0 |
| 84 | OHX | AR | 3603 | 7/7 | 0.96 | 0.16 | 142,143,143,143 | 0 |
| 84 | OHX | 1 | 3627 | 7/7 | 0.96 | 0.18 | 134,135,135,135 | 0 |
| 84 | OHX | sR | 1967 | 7/7 | 0.96 | 0.15 | 142,143,144,144 | 0 |
| 85 | MG | 1 | 3771 | 1/1 | 0.96 | 0.65 | 41,41,41,41 | 0 |
| 84 | OHX | 1 | 3595 | 7/7 | 0.96 | 0.14 | 183,183,184,185 | 0 |
| 85 | MG | sR | 2057 | 1/1 | 0.96 | 0.50 | 56,56,56,56 | 0 |
| 85 | MG | sR | 2058 | 1/1 | 0.96 | 0.36 | 51,51,51,51 | 0 |
| 84 | OHX | CL | 301 | 7/7 | 0.96 | 0.16 | 151,151,151,152 | 0 |
| 85 | MG | AR | 3779 | 1/1 | 0.96 | 0.27 | 49,49,49,49 | 0 |
| 84 | OHX | y | 201 | 7/7 | 0.96 | 0.18 | 151,152,153,154 | 0 |
| 84 | OHX | sR | 1975 | 7/7 | 0.96 | 0.39 | 135,135,136,136 | 0 |
| 85 | MG | AR | 3782 | 1/1 | 0.96 | 0.26 | 28,28,28,28 | 0 |
| 84 | OHX | 1 | 3705 | 7/7 | 0.96 | 0.25 | 123,124,124,125 | 0 |
| 85 | MG | 1 | 3962 | 1/1 | 0.96 | 0.22 | 93,93,93,93 | 0 |
| 84 | OHX | AR | 3608 | 7/7 | 0.96 | 0.17 | 128,128,128,128 | 0 |
| 85 | MG | AR | 3786 | 1/1 | 0.96 | 0.35 | 40,40,40,40 | 0 |
| 85 | MG | 1 | 3964 | 1/1 | 0.96 | 0.38 | 43,43,43,43 | 0 |
| 85 | MG | AR | 3790 | 1/1 | 0.96 | 0.41 | 40,40,40,40 | 0 |
| 84 | OHX | 1 | 3596 | 7/7 | 0.96 | 0.14 | 146,147,147,147 | 0 |
| 84 | OHX | AP | 502 | 7/7 | 0.96 | 0.20 | 102,102,103,104 | 0 |
| 85 | MG | 1 | 4139 | 1/1 | 0.96 | 0.48 | 35,35,35,35 | 0 |
| 84 | OHX | 1 | 3540 | 7/7 | 0.96 | 0.21 | 130,131,131,131 | 0 |
| 84 | OHX | AR | 3459 | 7/7 | 0.96 | 0.17 | 100,101,101,102 | 0 |
| 84 | OHX | sR | 1984 | 7/7 | 0.96 | 0.12 | 158,159,159,160 | 0 |
| 84 | OHX | AR | 3476 | 7/7 | 0.96 | 0.21 | 84,84,85,85 | 0 |
| 85 | MG | AR | 4239 | 1/1 | 0.96 | 0.29 | 38,38,38,38 | 0 |
| 84 | OHX | sR | 1986 | 7/7 | 0.96 | 0.16 | 172,173,174,174 | 0 |
| 85 | MG | AR | 4242 | 1/1 | 0.96 | 0.51 | 36,36,36,36 | 0 |
| 85 | MG | AR | 3801 | 1/1 | 0.96 | 0.68 | 41,41,41,41 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 84 | OHX | A | 1921 | 7/7 | 0.96 | 0.14 | 124,125,126,126 | 0 |
| 84 | OHX | A | 1932 | 7/7 | 0.96 | 0.14 | 143,144,144,145 | 0 |
| 84 | OHX | sR | 1989 | 7/7 | 0.96 | 0.15 | 151,151,152,152 | 0 |
| 84 | OHX | sR | 1990 | 7/7 | 0.96 | 0.11 | 159,159,160,161 | 0 |
| 84 | OHX | A | 1936 | 7/7 | 0.96 | 0.14 | 127,128,128,128 | 0 |
| 85 | MG | AR | 3810 | 1/1 | 0.96 | 0.54 | 25,25,25,25 | 0 |
| 85 | MG | 1 | 3791 | 1/1 | 0.96 | 0.55 | 37,37,37,37 | 0 |
| 85 | MG | sR | 2093 | 1/1 | 0.96 | 0.28 | 50,50,50,50 | 0 |
| 84 | OHX | sR | 1992 | 7/7 | 0.96 | 0.29 | 144,144,145,145 | 0 |
| 84 | OHX | sR | 1994 | 7/7 | 0.96 | 0.17 | 157,158,159,159 | 0 |
| 84 | OHX | 1 | 3541 | 7/7 | 0.96 | 0.15 | 141,141,142,142 | 0 |
| 84 | OHX | AR | 3478 | 7/7 | 0.96 | 0.19 | 99,99,100,100 | 0 |
| 85 | MG | 1 | 3797 | 1/1 | 0.96 | 0.59 | 54,54,54,54 | 0 |
| 84 | OHX | A | 1948 | 7/7 | 0.96 | 0.12 | 140,141,141,142 | 0 |
| 84 | OHX | AR | 3698 | 7/7 | 0.96 | 0.31 | 147,148,148,148 | 0 |
| 85 | MG | 1 | 3800 | 1/1 | 0.96 | 0.50 | 62,62,62,62 | 0 |
| 85 | MG | AR | 4047 | 1/1 | 0.96 | 0.23 | 45,45,45,45 | 0 |
| 84 | OHX | AR | 3617 | 7/7 | 0.96 | 0.15 | 146,146,147,147 | 0 |
| 84 | OHX | 1 | 3504 | 7/7 | 0.96 | 0.10 | 137,137,138,138 | 0 |
| 85 | MG | 1 | 3990 | 1/1 | 0.96 | 0.31 | 31,31,31,31 | 0 |
| 85 | MG | sR | 2108 | 1/1 | 0.96 | 0.34 | 55,55,55,55 | 0 |
| 84 | OHX | A | 1960 | 7/7 | 0.96 | 0.13 | 167,168,168,169 | 0 |
| 85 | MG | AT | 220 | 1/1 | 0.96 | 0.58 | 52,52,52,52 | 0 |
| 85 | MG | 1 | 3805 | 1/1 | 0.96 | 0.53 | 21,21,21,21 | 0 |
| 85 | MG | AR | 3825 | 1/1 | 0.96 | 0.39 | 27,27,27,27 | 0 |
| 84 | OHX | AR | 3619 | 7/7 | 0.96 | 0.24 | 138,139,139,139 | 0 |
| 85 | MG | 1 | 4170 | 1/1 | 0.96 | 0.13 | 50,50,50,50 | 0 |
| 85 | MG | 1 | 3807 | 1/1 | 0.96 | 0.25 | 33,33,33,33 | 0 |
| 85 | MG | AR | 3829 | 1/1 | 0.96 | 0.42 | 38,38,38,38 | 0 |
| 85 | MG | sR | 2119 | 1/1 | 0.96 | 0.46 | 67,67,67,67 | 0 |
| 84 | OHX | 1 | 3634 | 7/7 | 0.96 | 0.27 | 128,128,129,129 | 0 |
| 84 | OHX | A | 1965 | 7/7 | 0.96 | 0.12 | 148,149,150,150 | 0 |
| 85 | MG | 1 | 4174 | 1/1 | 0.96 | 0.27 | 60,60,60,60 | 0 |
| 85 | MG | 1 | 4175 | 1/1 | 0.96 | 0.38 | 54,54,54,54 | 0 |
| 84 | OHX | 1 | 3488 | 7/7 | 0.96 | 0.15 | 111,112,112,112 | 0 |
| 84 | OHX | AR | 3622 | 7/7 | 0.96 | 0.30 | 127,127,127,128 | 0 |
| 84 | OHX | 1 | 3602 | 7/7 | 0.96 | 0.10 | 168,168,169,169 | 0 |
| 84 | OHX | sR | 2010 | 7/7 | 0.96 | 0.17 | 138,139,140,140 | 0 |
| 84 | OHX | A | 1973 | 7/7 | 0.96 | 0.20 | 167,168,169,170 | 0 |
| 84 | OHX | 1 | 3603 | 7/7 | 0.96 | 0.25 | 136,136,137,137 | 0 |
| 85 | MG | AR | 3841 | 1/1 | 0.96 | 0.32 | 53,53,53,53 | 0 |
| 84 | OHX | A | 1975 | 7/7 | 0.96 | 0.10 | 169,171,172,172 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 84 | OHX | AR | 3519 | 7/7 | 0.96 | 0.17 | 108,108,109,109 | 0 |
| 84 | OHX | 1 | 3549 | 7/7 | 0.96 | 0.12 | 147,147,147,148 | 0 |
| 84 | OHX | 1 | 3605 | 7/7 | 0.96 | 0.13 | 141,142,142,142 | 0 |
| 84 | OHX | AR | 3531 | 7/7 | 0.96 | 0.14 | 121,121,122,122 | 0 |
| 84 | OHX | 1 | 3641 | 7/7 | 0.96 | 0.14 | 154,155,156,156 | 0 |
| 84 | OHX | AR | 3630 | 7/7 | 0.96 | 0.20 | 173,173,174,174 | 0 |
| 85 | MG | 1 | 4012 | 1/1 | 0.96 | 0.25 | 49,49,49,49 | 0 |
| 84 | OHX | AR | 3632 | 7/7 | 0.96 | 0.23 | 151,151,151,151 | 0 |
| 85 | MG | 1 | 3828 | 1/1 | 0.96 | 0.29 | 29,29,29,29 | 0 |
| 84 | OHX | 1 | 3552 | 7/7 | 0.96 | 0.21 | 130,131,132,132 | 0 |
| 84 | OHX | A | 1996 | 7/7 | 0.96 | 0.25 | 162,162,163,163 | 0 |
| 85 | MG | AR | 3858 | 1/1 | 0.96 | 0.49 | 29,29,29,29 | 0 |
| 84 | OHX | AR | 3535 | 7/7 | 0.96 | 0.20 | 107,107,108,108 | 0 |
| 84 | OHX | 1 | 3553 | 7/7 | 0.96 | 0.09 | 170,170,171,171 | 0 |
| 85 | MG | AR | 3863 | 1/1 | 0.96 | 0.23 | 49,49,49,49 | 0 |
| 85 | MG | sR | 2147 | 1/1 | 0.96 | 0.21 | 67,67,67,67 | 0 |
| 84 | OHX | AR | 3537 | 7/7 | 0.96 | 0.12 | 142,142,143,143 | 0 |
| 84 | OHX | AR | 3638 | 7/7 | 0.96 | 0.25 | 130,130,130,130 | 0 |
| 85 | MG | 1 | 3836 | 1/1 | 0.96 | 0.30 | 36,36,36,36 | 0 |
| 85 | MG | 1 | 3838 | 1/1 | 0.96 | 0.82 | 49,49,49,49 | 0 |
| 84 | OHX | AR | 3538 | 7/7 | 0.96 | 0.15 | 124,124,124,124 | 0 |
| 84 | OHX | AR | 3721 | 7/7 | 0.96 | 0.27 | 125,126,126,126 | 0 |
| 85 | MG | AR | 4093 | 1/1 | 0.96 | 0.30 | 33,33,33,33 | 0 |
| 85 | MG | 1 | 3841 | 1/1 | 0.96 | 0.33 | 40,40,40,40 | 0 |
| 85 | MG | 1 | 4205 | 1/1 | 0.96 | 0.42 | 58,58,58,58 | 0 |
| 85 | MG | 1 | 4026 | 1/1 | 0.96 | 0.67 | 47,47,47,47 | 0 |
| 84 | OHX | 1 | 3512 | 7/7 | 0.96 | 0.16 | 107,107,108,108 | 0 |
| 84 | OHX | 1 | 3432 | 7/7 | 0.96 | 0.23 | 84,85,85,85 | 0 |
| 85 | MG | sR | 2162 | 1/1 | 0.96 | 0.40 | 50,50,50,50 | 0 |
| 84 | OHX | 1 | 3499 | 7/7 | 0.96 | 0.15 | 106,107,107,107 | 0 |
| 85 | MG | DP | 101 | 1/1 | 0.96 | 0.34 | 52,52,52,52 | 0 |
| 84 | OHX | AR | 3547 | 7/7 | 0.96 | 0.11 | 157,157,158,158 | 0 |
| 85 | MG | 1 | 4214 | 1/1 | 0.96 | 0.42 | 36,36,36,36 | 0 |
| 85 | MG | sM | 201 | 1/1 | 0.96 | 0.25 | 44,44,44,44 | 0 |
| 85 | MG | 1 | 3850 | 1/1 | 0.96 | 0.62 | 40,40,40,40 | 0 |
| 85 | MG | A | 2044 | 1/1 | 0.96 | 0.64 | 40,40,40,40 | 0 |
| 85 | MG | AR | 4103 | 1/1 | 0.96 | 0.28 | 38,38,38,38 | 0 |
| 84 | OHX | 1 | 3683 | 7/7 | 0.96 | 0.27 | 135,136,136,137 | 0 |
| 85 | MG | 1 | 4217 | 1/1 | 0.96 | 0.14 | 36,36,36,36 | 0 |
| 84 | OHX | 1 | 3723 | 7/7 | 0.96 | 0.23 | 157,158,158,159 | 0 |
| 85 | MG | A | 2049 | 1/1 | 0.96 | 0.57 | 48,48,48,48 | 0 |
| 84 | OHX | AR | 3550 | 7/7 | 0.96 | 0.19 | 117,117,118,118 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | 3 | 211 | 1/1 | 0.96 | 0.48 | 33,33,33,33 | 0 |
| 84 | OHX | 1 | 3521 | 7/7 | 0.96 | 0.17 | 134,134,135,135 | 0 |
| 84 | OHX | AR | 3648 | 7/7 | 0.96 | 0.30 | 152,152,153,153 | 0 |
| 84 | OHX | AR | 3649 | 7/7 | 0.96 | 0.23 | 145,146,146,147 | 0 |
| 85 | MG | 1 | 3862 | 1/1 | 0.96 | 0.39 | 21,21,21,21 | 0 |
| 85 | MG | AR | 4114 | 1/1 | 0.96 | 0.51 | 37,37,37,37 | 0 |
| 85 | MG | 1 | 3863 | 1/1 | 0.96 | 0.49 | 42,42,42,42 | 0 |
| 84 | OHX | AR | 3554 | 7/7 | 0.96 | 0.16 | 125,125,125,126 | 0 |
| 85 | MG | 1 | 3865 | 1/1 | 0.96 | 0.67 | 29,29,29,29 | 0 |
| 84 | OHX | 1 | 3650 | 7/7 | 0.96 | 0.18 | 148,149,149,149 | 0 |
| 84 | OHX | A | 2016 | 7/7 | 0.96 | 0.18 | 161,162,162,163 | 0 |
| 85 | MG | AR | 3906 | 1/1 | 0.96 | 0.78 | 47,47,47,47 | 0 |
| 85 | MG | 1 | 3868 | 1/1 | 0.96 | 0.60 | 33,33,33,33 | 0 |
| 84 | OHX | 1 | 3687 | 7/7 | 0.96 | 0.32 | 149,150,150,150 | 0 |
| 84 | OHX | 1 | 3523 | 7/7 | 0.96 | 0.12 | 131,131,132,132 | 0 |
| 85 | MG | AR | 3910 | 1/1 | 0.96 | 0.49 | 38,38,38,38 | 0 |
| 85 | MG | 1 | 3872 | 1/1 | 0.96 | 0.34 | 31,31,31,31 | 0 |
| 85 | MG | AR | 3914 | 1/1 | 0.96 | 0.57 | 31,31,31,31 | 0 |
| 84 | OHX | AR | 3561 | 7/7 | 0.96 | 0.18 | 122,123,123,123 | 0 |
| 84 | OHX | AR | 3563 | 7/7 | 0.96 | 0.12 | 143,144,144,144 | 0 |
| 85 | MG | A | 2073 | 1/1 | 0.96 | 0.72 | 75,75,75,75 | 0 |
| 84 | OHX | 1 | 3614 | 7/7 | 0.96 | 0.19 | 133,133,134,134 | 0 |
| 85 | MG | 1 | 4056 | 1/1 | 0.96 | 0.42 | 50,50,50,50 | 0 |
| 86 | 7AL | 1 | 4210 | 26/26 | 0.96 | 0.23 | 31,31,32,32 | 0 |
| 86 | 7AL | AR | 4246 | 26/26 | 0.96 | 0.20 | 33,33,33,33 | 0 |
| 84 | OHX | AR | 3568 | 7/7 | 0.96 | 0.16 | 147,147,148,148 | 0 |
| 84 | OHX | 1 | 3653 | 7/7 | 0.96 | 0.28 | 133,133,133,134 | 0 |
| 84 | OHX | 1 | 3526 | 7/7 | 0.96 | 0.25 | 118,119,119,119 | 0 |
| 84 | OHX | AR | 3571 | 7/7 | 0.96 | 0.21 | 129,130,130,130 | 0 |
| 85 | MG | 1 | 3845 | 1/1 | 0.97 | 0.54 | 22,22,22,22 | 0 |
| 84 | OHX | AR | 3517 | 7/7 | 0.97 | 0.17 | 116,116,117,117 | 0 |
| 85 | MG | AR | 4039 | 1/1 | 0.97 | 0.34 | 47,47,47,47 | 0 |
| 84 | OHX | 1 | 3639 | 7/7 | 0.97 | 0.25 | 140,141,141,141 | 0 |
| 84 | OHX | 1 | 3584 | 7/7 | 0.97 | 0.18 | 149,149,150,150 | 0 |
| 84 | OHX | 1 | 3585 | 7/7 | 0.97 | 0.19 | 128,128,129,129 | 0 |
| 84 | OHX | AR | 3523 | 7/7 | 0.97 | 0.13 | 127,128,128,129 | 0 |
| 85 | MG | AR | 3775 | 1/1 | 0.97 | 0.19 | 38,38,38,38 | 0 |
| 84 | OHX | AR | 3651 | 7/7 | 0.97 | 0.36 | 150,151,151,151 | 0 |
| 85 | MG | 1 | 3856 | 1/1 | 0.97 | 0.40 | 23,23,23,23 | 0 |
| 84 | OHX | AR | 3524 | 7/7 | 0.97 | 0.18 | 117,117,117,117 | 0 |
| 85 | MG | 1 | 3858 | 1/1 | 0.97 | 0.65 | 37,37,37,37 | 0 |
| 84 | OHX | 1 | 3642 | 7/7 | 0.97 | 0.22 | 128,129,130,130 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | 1 | 3860 | 1/1 | 0.97 | 0.49 | 31,31,31,31 | 0 |
| 84 | OHX | sR | 1993 | 7/7 | 0.97 | 0.19 | 141,142,142,143 | 0 |
| 84 | OHX | AR | 3654 | 7/7 | 0.97 | 0.37 | 148,148,149,149 | 0 |
| 84 | OHX | AR | 3528 | 7/7 | 0.97 | 0.11 | 115,115,115,116 | 0 |
| 84 | OHX | AR | 3529 | 7/7 | 0.97 | 0.22 | 127,128,128,128 | 0 |
| 84 | OHX | 1 | 3586 | 7/7 | 0.97 | 0.16 | 132,132,132,132 | 0 |
| 85 | MG | AR | 3788 | 1/1 | 0.97 | 0.57 | 39,39,39,39 | 0 |
| 85 | MG | 1 | 4090 | 1/1 | 0.97 | 0.09 | 43,43,43,43 | 0 |
| 84 | OHX | 1 | 3587 | 7/7 | 0.97 | 0.13 | 142,142,143,143 | 0 |
| 85 | MG | 1 | 4092 | 1/1 | 0.97 | 0.40 | 46,46,46,46 | 0 |
| 84 | OHX | 1 | 3588 | 7/7 | 0.97 | 0.20 | 152,152,153,153 | 0 |
| 84 | OHX | AR | 3660 | 7/7 | 0.97 | 0.17 | 131,132,133,133 | 0 |
| 84 | OHX | 1 | 3485 | 7/7 | 0.97 | 0.11 | 121,121,122,122 | 0 |
| 85 | MG | A | 2058 | 1/1 | 0.97 | 0.54 | 49,49,49,49 | 0 |
| 85 | MG | 1 | 3870 | 1/1 | 0.97 | 0.56 | 27,27,27,27 | 0 |
| 84 | OHX | A | 1909 | 7/7 | 0.97 | 0.17 | 116,116,118,118 | 0 |
| 85 | MG | AR | 3798 | 1/1 | 0.97 | 0.32 | 30,30,30,30 | 0 |
| 84 | OHX | A | 1910 | 7/7 | 0.97 | 0.20 | 102,103,104,104 | 0 |
| 84 | OHX | A | 1911 | 7/7 | 0.97 | 0.18 | 110,111,112,112 | 0 |
| 84 | OHX | 1 | 3590 | 7/7 | 0.97 | 0.17 | 125,126,126,126 | 0 |
| 85 | MG | 1 | 4102 | 1/1 | 0.97 | 0.26 | 66,66,66,66 | 0 |
| 84 | OHX | 1 | 3449 | 7/7 | 0.97 | 0.19 | 91,91,92,92 | 0 |
| 84 | OHX | 1 | 3464 | 7/7 | 0.97 | 0.15 | 108,108,109,109 | 0 |
| 85 | MG | AR | 3805 | 1/1 | 0.97 | 0.60 | 38,38,38,38 | 0 |
| 85 | MG | AR | 3806 | 1/1 | 0.97 | 0.33 | 76,76,76,76 | 0 |
| 85 | MG | AR | 3807 | 1/1 | 0.97 | 0.50 | 32,32,32,32 | 0 |
| 84 | OHX | A | 1927 | 7/7 | 0.97 | 0.12 | 130,130,131,131 | 0 |
| 84 | OHX | A | 1928 | 7/7 | 0.97 | 0.12 | 128,129,130,130 | 0 |
| 84 | OHX | A | 1931 | 7/7 | 0.97 | 0.11 | 133,134,135,135 | 0 |
| 84 | OHX | AR | 3539 | 7/7 | 0.97 | 0.20 | 120,120,120,120 | 0 |
| 84 | OHX | A | 1933 | 7/7 | 0.97 | 0.16 | 119,120,120,120 | 0 |
| 85 | MG | 1 | 3883 | 1/1 | 0.97 | 0.59 | 30,30,30,30 | 0 |
| 84 | OHX | A | 1935 | 7/7 | 0.97 | 0.18 | 149,150,150,150 | 0 |
| 85 | MG | A | 2079 | 1/1 | 0.97 | 0.58 | 53,53,53,53 | 0 |
| 84 | OHX | AR | 3540 | 7/7 | 0.97 | 0.15 | 104,104,105,105 | 0 |
| 84 | OHX | A | 1937 | 7/7 | 0.97 | 0.13 | 134,135,136,136 | 0 |
| 84 | OHX | A | 1939 | 7/7 | 0.97 | 0.10 | 143,144,145,145 | 0 |
| 84 | OHX | A | 1940 | 7/7 | 0.97 | 0.19 | 126,127,127,128 | 0 |
| 84 | OHX | A | 1943 | 7/7 | 0.97 | 0.15 | 119,120,120,121 | 0 |
| 84 | OHX | A | 1944 | 7/7 | 0.97 | 0.13 | 135,136,136,137 | 0 |
| 84 | OHX | A | 1945 | 7/7 | 0.97 | 0.12 | 160,161,162,162 | 0 |
| 84 | OHX | 1 | 3532 | 7/7 | 0.97 | 0.19 | 113,114,114,114 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 84 | OHX | 1 | 3594 | 7/7 | 0.97 | 0.27 | 138,138,139,139 | 0 |
| 85 | MG | 1 | 3897 | 1/1 | 0.97 | 0.47 | 39,39,39,39 | 0 |
| 84 | OHX | 1 | 3533 | 7/7 | 0.97 | 0.11 | 160,161,162,162 | 0 |
| 85 | MG | A | 2092 | 1/1 | 0.97 | 0.19 | 80,80,80,80 | 0 |
| 85 | MG | 1 | 3901 | 1/1 | 0.97 | 0.46 | 18,18,18,18 | 0 |
| 84 | OHX | A | 1951 | 7/7 | 0.97 | 0.17 | 152,152,153,154 | 0 |
| 84 | OHX | A | 1952 | 7/7 | 0.97 | 0.21 | 139,140,140,141 | 0 |
| 85 | MG | 1 | 4129 | 1/1 | 0.97 | 0.46 | 26,26,26,26 | 0 |
| 84 | OHX | AR | 3544 | 7/7 | 0.97 | 0.12 | 140,140,141,142 | 0 |
| 84 | OHX | A | 1955 | 7/7 | 0.97 | 0.11 | 132,133,134,135 | 0 |
| 85 | MG | A | 2099 | 1/1 | 0.97 | 0.32 | 50,50,50,50 | 0 |
| 84 | OHX | A | 1956 | 7/7 | 0.97 | 0.12 | 145,146,147,147 | 0 |
| 84 | OHX | AR | 3546 | 7/7 | 0.97 | 0.15 | 138,139,139,139 | 0 |
| 84 | OHX | 1 | 3534 | 7/7 | 0.97 | 0.12 | 161,161,162,162 | 0 |
| 84 | OHX | 1 | 3535 | 7/7 | 0.97 | 0.21 | 126,126,126,126 | 0 |
| 85 | MG | AR | 4106 | 1/1 | 0.97 | 0.22 | 47,47,47,47 | 0 |
| 84 | OHX | 1 | 3468 | 7/7 | 0.97 | 0.16 | 109,110,110,111 | 0 |
| 84 | OHX | 1 | 3490 | 7/7 | 0.97 | 0.16 | 101,102,102,102 | 0 |
| 85 | MG | A | 2108 | 1/1 | 0.97 | 0.30 | 79,79,79,79 | 0 |
| 85 | MG | 1 | 3916 | 1/1 | 0.97 | 0.41 | 43,43,43,43 | 0 |
| 85 | MG | 1 | 3917 | 1/1 | 0.97 | 0.51 | 46,46,46,46 | 0 |
| 85 | MG | 1 | 3918 | 1/1 | 0.97 | 0.50 | 33,33,33,33 | 0 |
| 84 | OHX | AR | 3551 | 7/7 | 0.97 | 0.19 | 136,136,137,137 | 0 |
| 84 | OHX | AR | 3552 | 7/7 | 0.97 | 0.20 | 109,109,109,110 | 0 |
| 84 | OHX | A | 1967 | 7/7 | 0.97 | 0.13 | 136,137,137,138 | 0 |
| 85 | MG | 1 | 4145 | 1/1 | 0.97 | 0.08 | 44,44,44,44 | 0 |
| 85 | MG | AR | 3846 | 1/1 | 0.97 | 0.46 | 40,40,40,40 | 0 |
| 85 | MG | AR | 4117 | 1/1 | 0.97 | 0.07 | 41,41,41,41 | 0 |
| 84 | OHX | 1 | 3493 | 7/7 | 0.97 | 0.12 | 107,107,108,108 | 0 |
| 85 | MG | AR | 3848 | 1/1 | 0.97 | 0.29 | 29,29,29,29 | 0 |
| 85 | MG | 1 | 3925 | 1/1 | 0.97 | 0.54 | 27,27,27,27 | 0 |
| 85 | MG | AR | 4121 | 1/1 | 0.97 | 0.18 | 50,50,50,50 | 0 |
| 85 | MG | AR | 3850 | 1/1 | 0.97 | 0.36 | 21,21,21,21 | 0 |
| 85 | MG | 1 | 3927 | 1/1 | 0.97 | 0.61 | 20,20,20,20 | 0 |
| 84 | OHX | A | 1969 | 7/7 | 0.97 | 0.21 | 158,158,159,159 | 0 |
| 84 | OHX | A | 1970 | 7/7 | 0.97 | 0.19 | 136,136,137,137 | 0 |
| 84 | OHX | 1 | 3495 | 7/7 | 0.97 | 0.13 | 119,119,119,120 | 0 |
| 84 | OHX | AR | 3557 | 7/7 | 0.97 | 0.29 | 129,130,130,130 | 0 |
| 85 | MG | AR | 3856 | 1/1 | 0.97 | 0.47 | 34,34,34,34 | 0 |
| 84 | OHX | 1 | 3496 | 7/7 | 0.97 | 0.14 | 115,116,116,116 | 0 |
| 84 | OHX | 1 | 3542 | 7/7 | 0.97 | 0.18 | 123,124,125,125 | 0 |
| 84 | OHX | A | 1976 | 7/7 | 0.97 | 0.24 | 135,135,136,136 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | AR | 3860 | 1/1 | 0.97 | 0.43 | 26,26,26,26 | 0 |
| 84 | OHX | 1 | 3543 | 7/7 | 0.97 | 0.15 | 113,114,114,114 | 0 |
| 84 | OHX | 1 | 3544 | 7/7 | 0.97 | 0.23 | 120,121,121,121 | 0 |
| 85 | MG | AR | 4135 | 1/1 | 0.97 | 0.23 | 35,35,35,35 | 0 |
| 84 | OHX | A | 1979 | 7/7 | 0.97 | 0.17 | 154,155,156,157 | 0 |
| 85 | MG | AR | 3866 | 1/1 | 0.97 | 0.45 | 30,30,30,30 | 0 |
| 84 | OHX | AR | 3562 | 7/7 | 0.97 | 0.16 | 120,121,121,121 | 0 |
| 85 | MG | AR | 4139 | 1/1 | 0.97 | 0.13 | 51,51,51,51 | 0 |
| 84 | OHX | 1 | 3498 | 7/7 | 0.97 | 0.12 | 127,128,129,129 | 0 |
| 84 | OHX | A | 1982 | 7/7 | 0.97 | 0.28 | 135,136,136,137 | 0 |
| 85 | MG | AR | 3872 | 1/1 | 0.97 | 0.42 | 29,29,29,29 | 0 |
| 85 | MG | A | 2145 | 1/1 | 0.97 | 0.27 | 89,89,89,89 | 0 |
| 84 | OHX | A | 1983 | 7/7 | 0.97 | 0.17 | 161,162,163,163 | 0 |
| 85 | MG | AR | 3874 | 1/1 | 0.97 | 0.43 | 34,34,34,34 | 0 |
| 84 | OHX | 1 | 3546 | 7/7 | 0.97 | 0.13 | 145,145,146,146 | 0 |
| 84 | OHX | A | 1986 | 7/7 | 0.97 | 0.28 | 169,171,172,173 | 0 |
| 85 | MG | AR | 3877 | 1/1 | 0.97 | 0.75 | 36,36,36,36 | 0 |
| 84 | OHX | A | 1988 | 7/7 | 0.97 | 0.18 | 132,133,133,134 | 0 |
| 84 | OHX | 1 | 3451 | 7/7 | 0.97 | 0.17 | 101,101,102,102 | 0 |
| 85 | MG | AR | 3880 | 1/1 | 0.97 | 0.44 | 27,27,27,27 | 0 |
| 85 | MG | AR | 3881 | 1/1 | 0.97 | 0.67 | 28,28,28,28 | 0 |
| 84 | OHX | 1 | 3610 | 7/7 | 0.97 | 0.20 | 136,137,137,137 | 0 |
| 84 | OHX | A | 1994 | 7/7 | 0.97 | 0.17 | 158,159,160,160 | 0 |
| 84 | OHX | 1 | 3472 | 7/7 | 0.97 | 0.18 | 97,98,98,98 | 0 |
| 84 | OHX | 1 | 3550 | 7/7 | 0.97 | 0.17 | 134,134,135,135 | 0 |
| 84 | OHX | AR | 3572 | 7/7 | 0.97 | 0.17 | 130,130,131,131 | 0 |
| 84 | OHX | 1 | 3503 | 7/7 | 0.97 | 0.17 | 109,110,110,110 | 0 |
| 84 | OHX | AR | 3574 | 7/7 | 0.97 | 0.20 | 114,115,115,116 | 0 |
| 84 | OHX | AR | 3575 | 7/7 | 0.97 | 0.17 | 161,161,161,161 | 0 |
| 84 | OHX | 1 | 3473 | 7/7 | 0.97 | 0.18 | 99,99,99,100 | 0 |
| 84 | OHX | 1 | 3507 | 7/7 | 0.97 | 0.26 | 118,118,118,119 | 0 |
| 85 | MG | AR | 3892 | 1/1 | 0.97 | 0.41 | 36,36,36,36 | 0 |
| 85 | MG | sR | 2061 | 1/1 | 0.97 | 0.32 | 84,84,84,84 | 0 |
| 84 | OHX | AR | 3578 | 7/7 | 0.97 | 0.20 | 132,133,133,134 | 0 |
| 85 | MG | 1 | 3739 | 1/1 | 0.97 | 0.45 | 31,31,31,31 | 0 |
| 85 | MG | 1 | 3740 | 1/1 | 0.97 | 0.49 | 27,27,27,27 | 0 |
| 85 | MG | sR | 2065 | 1/1 | 0.97 | 0.55 | 42,42,42,42 | 0 |
| 84 | OHX | AR | 3579 | 7/7 | 0.97 | 0.16 | 134,134,135,135 | 0 |
| 85 | MG | AR | 3898 | 1/1 | 0.97 | 0.29 | 45,45,45,45 | 0 |
| 84 | OHX | 1 | 3508 | 7/7 | 0.97 | 0.13 | 116,116,117,117 | 0 |
| 84 | OHX | 3 | 202 | 7/7 | 0.97 | 0.12 | 122,122,123,123 | 0 |
| 84 | OHX | 1 | 3509 | 7/7 | 0.97 | 0.12 | 124,124,125,125 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 84 | OHX | AR | 3703 | 7/7 | 0.97 | 0.22 | 106,106,107,107 | 0 |
| 84 | OHX | 1 | 3510 | 7/7 | 0.97 | 0.15 | 118,118,119,119 | 0 |
| 85 | MG | sR | 2073 | 1/1 | 0.97 | 0.61 | 58,58,58,58 | 0 |
| 85 | MG | AR | 4175 | 1/1 | 0.97 | 0.28 | 47,47,47,47 | 0 |
| 85 | MG | 1 | 3748 | 1/1 | 0.97 | 0.34 | 39,39,39,39 | 0 |
| 84 | OHX | 3 | 206 | 7/7 | 0.97 | 0.11 | 137,138,138,139 | 0 |
| 84 | OHX | AR | 3586 | 7/7 | 0.97 | 0.14 | 128,129,129,129 | 0 |
| 84 | OHX | 1 | 3474 | 7/7 | 0.97 | 0.17 | 118,119,119,119 | 0 |
| 84 | OHX | AR | 3588 | 7/7 | 0.97 | 0.28 | 124,124,125,125 | 0 |
| 84 | OHX | AR | 3589 | 7/7 | 0.97 | 0.15 | 121,122,122,122 | 0 |
| 84 | OHX | 1 | 3563 | 7/7 | 0.97 | 0.12 | 135,135,135,136 | 0 |
| 85 | MG | AR | 3913 | 1/1 | 0.97 | 0.71 | 36,36,36,36 | 0 |
| 85 | MG | 1 | 3974 | 1/1 | 0.97 | 0.09 | 59,59,59,59 | 0 |
| 85 | MG | AR | 3915 | 1/1 | 0.97 | 0.38 | 28,28,28,28 | 0 |
| 85 | MG | 1 | 3975 | 1/1 | 0.97 | 0.45 | 43,43,43,43 | 0 |
| 84 | OHX | AR | 3591 | 7/7 | 0.97 | 0.20 | 141,141,142,142 | 0 |
| 84 | OHX | 4 | 206 | 7/7 | 0.97 | 0.13 | 129,129,129,129 | 0 |
| 85 | MG | 1 | 4202 | 1/1 | 0.97 | 0.49 | 36,36,36,36 | 0 |
| 85 | MG | AR | 3922 | 1/1 | 0.97 | 0.59 | 41,41,41,41 | 0 |
| 85 | MG | AR | 3923 | 1/1 | 0.97 | 0.50 | 32,32,32,32 | 0 |
| 84 | OHX | AR | 3593 | 7/7 | 0.97 | 0.14 | 137,137,138,138 | 0 |
| 84 | OHX | 4 | 207 | 7/7 | 0.97 | 0.17 | 130,131,131,132 | 0 |
| 84 | OHX | 4 | 209 | 7/7 | 0.97 | 0.17 | 129,130,130,130 | 0 |
| 85 | MG | 1 | 4206 | 1/1 | 0.97 | 0.60 | 25,25,25,25 | 0 |
| 85 | MG | 1 | 3761 | 1/1 | 0.97 | 0.58 | 44,44,44,44 | 0 |
| 85 | MG | sR | 2098 | 1/1 | 0.97 | 0.49 | 62,62,62,62 | 0 |
| 84 | OHX | 4 | 210 | 7/7 | 0.97 | 0.20 | 123,123,123,123 | 0 |
| 84 | OHX | 1 | 3476 | 7/7 | 0.97 | 0.15 | 107,107,108,108 | 0 |
| 84 | OHX | 4 | 212 | 7/7 | 0.97 | 0.21 | 144,144,145,145 | 0 |
| 84 | OHX | 1 | 3565 | 7/7 | 0.97 | 0.24 | 155,155,155,156 | 0 |
| 85 | MG | 1 | 4213 | 1/1 | 0.97 | 0.08 | 72,72,72,72 | 0 |
| 84 | OHX | 1 | 3566 | 7/7 | 0.97 | 0.17 | 143,143,143,143 | 0 |
| 85 | MG | 1 | 3767 | 1/1 | 0.97 | 0.28 | 39,39,39,39 | 0 |
| 85 | MG | sR | 2106 | 1/1 | 0.97 | 0.29 | 41,41,41,41 | 0 |
| 84 | OHX | 1 | 3624 | 7/7 | 0.97 | 0.18 | 103,103,103,103 | 0 |
| 85 | MG | 1 | 3769 | 1/1 | 0.97 | 0.31 | 50,50,50,50 | 0 |
| 85 | MG | sR | 2109 | 1/1 | 0.97 | 0.53 | 48,48,48,48 | 0 |
| 84 | OHX | k | 401 | 7/7 | 0.97 | 0.18 | 123,123,124,124 | 0 |
| 85 | MG | sR | 2111 | 1/1 | 0.97 | 0.52 | 43,43,43,43 | 0 |
| 85 | MG | AR | 3948 | 1/1 | 0.97 | 0.50 | 37,37,37,37 | 0 |
| 84 | OHX | 1 | 3567 | 7/7 | 0.97 | 0.26 | 116,117,117,118 | 0 |
| 84 | OHX | r | 301 | 7/7 | 0.97 | 0.17 | 105,105,105,106 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 84 | OHX | v | 302 | 7/7 | 0.97 | 0.15 | 121,122,122,122 | 0 |
| 84 | OHX | 1 | 3441 | 7/7 | 0.97 | 0.17 | 88,88,89,89 | 0 |
| 84 | OHX | 1 | 3684 | 7/7 | 0.97 | 0.10 | 145,145,145,146 | 0 |
| 84 | OHX | 1 | 3570 | 7/7 | 0.97 | 0.21 | 125,126,126,126 | 0 |
| 84 | OHX | 1 | 3572 | 7/7 | 0.97 | 0.21 | 104,105,105,105 | 0 |
| 84 | OHX | AG | 201 | 7/7 | 0.97 | 0.21 | 127,127,128,128 | 0 |
| 84 | OHX | 1 | 3573 | 7/7 | 0.97 | 0.19 | 144,144,145,145 | 0 |
| 84 | OHX | 1 | 3688 | 7/7 | 0.97 | 0.23 | 122,122,123,123 | 0 |
| 84 | OHX | AR | 3429 | 7/7 | 0.97 | 0.21 | 81,81,81,81 | 0 |
| 84 | OHX | AR | 3443 | 7/7 | 0.97 | 0.14 | 105,105,106,106 | 0 |
| 84 | OHX | AR | 3444 | 7/7 | 0.97 | 0.16 | 91,91,92,92 | 0 |
| 85 | MG | 4 | 219 | 1/1 | 0.97 | 0.37 | 43,43,43,43 | 0 |
| 84 | OHX | AR | 3445 | 7/7 | 0.97 | 0.16 | 106,106,107,107 | 0 |
| 84 | OHX | AR | 3447 | 7/7 | 0.97 | 0.16 | 87,87,88,88 | 0 |
| 84 | OHX | J | 301 | 7/7 | 0.97 | 0.27 | 177,178,179,179 | 0 |
| 85 | MG | AR | 3967 | 1/1 | 0.97 | 0.34 | 38,38,38,38 | 0 |
| 84 | OHX | M | 201 | 7/7 | 0.97 | 0.30 | 145,146,147,147 | 0 |
| 85 | MG | 4 | 224 | 1/1 | 0.97 | 0.24 | 44,44,44,44 | 0 |
| 85 | MG | 1 | 4009 | 1/1 | 0.97 | 0.18 | 64,64,64,64 | 0 |
| 84 | OHX | AR | 3453 | 7/7 | 0.97 | 0.18 | 86,87,87,87 | 0 |
| 84 | OHX | 1 | 3518 | 7/7 | 0.97 | 0.16 | 109,110,110,111 | 0 |
| 84 | OHX | 1 | 3575 | 7/7 | 0.97 | 0.19 | 134,135,135,135 | 0 |
| 84 | OHX | AR | 3463 | 7/7 | 0.97 | 0.18 | 85,86,86,86 | 0 |
| 85 | MG | AR | 3975 | 1/1 | 0.97 | 0.33 | 31,31,31,31 | 0 |
| 84 | OHX | sR | 1905 | 7/7 | 0.97 | 0.25 | 96,97,97,97 | 0 |
| 84 | OHX | sR | 1911 | 7/7 | 0.97 | 0.21 | 98,98,98,99 | 0 |
| 84 | OHX | AR | 3466 | 7/7 | 0.97 | 0.16 | 97,98,98,98 | 0 |
| 84 | OHX | AR | 3469 | 7/7 | 0.97 | 0.14 | 101,102,102,103 | 0 |
| 85 | MG | AR | 4249 | 1/1 | 0.97 | 0.18 | 38,38,38,38 | 0 |
| 85 | MG | AR | 4250 | 1/1 | 0.97 | 0.43 | 28,28,28,28 | 0 |
| 84 | OHX | 1 | 3632 | 7/7 | 0.97 | 0.17 | 172,173,173,174 | 0 |
| 85 | MG | AS | 212 | 1/1 | 0.97 | 0.40 | 40,40,40,40 | 0 |
| 84 | OHX | 1 | 3458 | 7/7 | 0.97 | 0.19 | 83,83,83,83 | 0 |
| 84 | OHX | 1 | 3578 | 7/7 | 0.97 | 0.19 | 129,130,130,131 | 0 |
| 84 | OHX | sR | 1938 | 7/7 | 0.97 | 0.12 | 121,121,122,122 | 0 |
| 84 | OHX | sR | 1939 | 7/7 | 0.97 | 0.11 | 130,131,131,132 | 0 |
| 84 | OHX | AS | 203 | 7/7 | 0.97 | 0.18 | 114,115,115,115 | 0 |
| 85 | MG | 1 | 3804 | 1/1 | 0.97 | 0.26 | 21,21,21,21 | 0 |
| 84 | OHX | sR | 1941 | 7/7 | 0.97 | 0.17 | 110,111,111,112 | 0 |
| 84 | OHX | AS | 204 | 7/7 | 0.97 | 0.13 | 109,110,110,110 | 0 |
| 84 | OHX | sR | 1946 | 7/7 | 0.97 | 0.10 | 135,136,137,137 | 0 |
| 85 | MG | AR | 3990 | 1/1 | 0.97 | 0.73 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 84 | OHX | sR | 1947 | 7/7 | 0.97 | 0.12 | 124,124,125,125 | 0 |
| 85 | MG | r | 302 | 1/1 | 0.97 | 0.26 | 35,35,35,35 | 0 |
| 85 | MG | AS | 226 | 1/1 | 0.97 | 0.35 | 50,50,50,50 | 0 |
| 84 | OHX | AS | 206 | 7/7 | 0.97 | 0.12 | 114,114,115,115 | 0 |
| 85 | MG | t | 201 | 1/1 | 0.97 | 0.14 | 44,44,44,44 | 0 |
| 84 | OHX | AR | 3480 | 7/7 | 0.97 | 0.17 | 103,104,104,104 | 0 |
| 84 | OHX | AR | 3631 | 7/7 | 0.97 | 0.26 | 164,164,164,164 | 0 |
| 85 | MG | AR | 3997 | 1/1 | 0.97 | 0.34 | 37,37,37,37 | 0 |
| 84 | OHX | AR | 3482 | 7/7 | 0.97 | 0.18 | 102,102,102,102 | 0 |
| 84 | OHX | AR | 3484 | 7/7 | 0.97 | 0.16 | 105,105,106,106 | 0 |
| 85 | MG | 1 | 4035 | 1/1 | 0.97 | 0.08 | 91,91,91,91 | 0 |
| 84 | OHX | sR | 1957 | 7/7 | 0.97 | 0.13 | 125,126,126,127 | 0 |
| 85 | MG | AR | 4002 | 1/1 | 0.97 | 0.35 | 27,27,27,27 | 0 |
| 85 | MG | 1 | 4037 | 1/1 | 0.97 | 0.28 | 55,55,55,55 | 0 |
| 85 | MG | sR | 2175 | 1/1 | 0.97 | 0.25 | 36,36,36,36 | 0 |
| 84 | OHX | sR | 1959 | 7/7 | 0.97 | 0.14 | 141,142,143,143 | 0 |
| 85 | MG | sR | 2178 | 1/1 | 0.97 | 0.17 | 78,78,78,78 | 0 |
| 84 | OHX | AR | 3488 | 7/7 | 0.97 | 0.20 | 100,100,101,101 | 0 |
| 85 | MG | 1 | 3817 | 1/1 | 0.97 | 0.28 | 39,39,39,39 | 0 |
| 85 | MG | 1 | 3818 | 1/1 | 0.97 | 0.49 | 44,44,44,44 | 0 |
| 85 | MG | 1 | 3819 | 1/1 | 0.97 | 0.28 | 35,35,35,35 | 0 |
| 84 | OHX | AT | 202 | 7/7 | 0.97 | 0.14 | 134,134,134,134 | 0 |
| 84 | OHX | sR | 1963 | 7/7 | 0.97 | 0.12 | 126,126,127,127 | 0 |
| 84 | OHX | sR | 1964 | 7/7 | 0.97 | 0.12 | 137,137,138,138 | 0 |
| 84 | OHX | sR | 1965 | 7/7 | 0.97 | 0.21 | 124,125,125,125 | 0 |
| 85 | MG | 1 | 4048 | 1/1 | 0.97 | 0.58 | 37,37,37,37 | 0 |
| 84 | OHX | AT | 204 | 7/7 | 0.97 | 0.13 | 116,116,116,116 | 0 |
| 84 | OHX | AR | 3490 | 7/7 | 0.97 | 0.16 | 95,95,96,96 | 0 |
| 85 | MG | AR | 4016 | 1/1 | 0.97 | 0.29 | 28,28,28,28 | 0 |
| 85 | MG | 1 | 3826 | 1/1 | 0.97 | 0.22 | 38,38,38,38 | 0 |
| 84 | OHX | AR | 3636 | 7/7 | 0.97 | 0.14 | 127,127,128,128 | 0 |
| 84 | OHX | AR | 3492 | 7/7 | 0.97 | 0.12 | 127,128,128,129 | 0 |
| 84 | OHX | sR | 1972 | 7/7 | 0.97 | 0.33 | 168,169,170,170 | 0 |
| 84 | OHX | AT | 208 | 7/7 | 0.97 | 0.14 | 138,138,139,139 | 0 |
| 84 | OHX | sR | 1974 | 7/7 | 0.97 | 0.14 | 129,129,130,130 | 0 |
| 84 | OHX | AR | 3498 | 7/7 | 0.97 | 0.13 | 146,147,147,147 | 0 |
| 85 | MG | 1 | 3833 | 1/1 | 0.97 | 0.44 | 23,23,23,23 | 0 |
| 84 | OHX | 1 | 3579 | 7/7 | 0.97 | 0.19 | 115,115,116,116 | 0 |
| 84 | OHX | AR | 3500 | 7/7 | 0.97 | 0.24 | 108,109,109,109 | 0 |
| 84 | OHX | 1 | 3520 | 7/7 | 0.97 | 0.18 | 113,113,114,114 | 0 |
| 85 | MG | 1 | 3837 | 1/1 | 0.97 | 0.33 | 33,33,33,33 | 0 |
| 84 | OHX | 1 | 3484 | 7/7 | 0.97 | 0.12 | 113,113,114,114 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 84 | OHX | sR | 1980 | 7/7 | 0.97 | 0.31 | 161,162,163,163 | 0 |
| 84 | OHX | 1 | 3522 | 7/7 | 0.97 | 0.13 | 128,129,130,130 | 0 |
| 85 | MG | AR | 3763 | 1/1 | 0.97 | 0.17 | 25,25,25,25 | 0 |
| 84 | OHX | AR | 3512 | 7/7 | 0.97 | 0.11 | 133,134,134,134 | 0 |
| 84 | OHX | sR | 1983 | 7/7 | 0.97 | 0.20 | 155,155,156,156 | 0 |
| 84 | OHX | AR | 3516 | 7/7 | 0.97 | 0.28 | 114,115,115,115 | 0 |
| 85 | MG | 1 | 3881 | 1/1 | 0.98 | 0.31 | 29,29,29,29 | 0 |
| 84 | OHX | AR | 3449 | 7/7 | 0.98 | 0.17 | 82,82,82,82 | 0 |
| 85 | MG | r | 303 | 1/1 | 0.98 | 0.12 | 43,43,43,43 | 0 |
| 84 | OHX | AR | 3450 | 7/7 | 0.98 | 0.17 | 92,93,93,93 | 0 |
| 84 | OHX | AR | 3451 | 7/7 | 0.98 | 0.13 | 103,103,104,104 | 0 |
| 85 | MG | A | 2091 | 1/1 | 0.98 | 0.69 | 56,56,56,56 | 0 |
| 85 | MG | AR | 3933 | 1/1 | 0.98 | 0.57 | 42,42,42,42 | 0 |
| 85 | MG | AR | 3934 | 1/1 | 0.98 | 0.49 | 38,38,38,38 | 0 |
| 85 | MG | AR | 4147 | 1/1 | 0.98 | 0.08 | 55,55,55,55 | 0 |
| 85 | MG | AR | 3935 | 1/1 | 0.98 | 0.60 | 35,35,35,35 | 0 |
| 85 | MG | AR | 3936 | 1/1 | 0.98 | 0.71 | 22,22,22,22 | 0 |
| 85 | MG | AR | 3937 | 1/1 | 0.98 | 0.38 | 25,25,25,25 | 0 |
| 85 | MG | 1 | 4068 | 1/1 | 0.98 | 0.62 | 33,33,33,33 | 0 |
| 84 | OHX | AR | 3452 | 7/7 | 0.98 | 0.13 | 107,107,108,108 | 0 |
| 84 | OHX | 1 | 3556 | 7/7 | 0.98 | 0.17 | 127,127,127,128 | 0 |
| 84 | OHX | AR | 3454 | 7/7 | 0.98 | 0.15 | 109,110,110,110 | 0 |
| 84 | OHX | AR | 3455 | 7/7 | 0.98 | 0.13 | 110,111,111,111 | 0 |
| 84 | OHX | AR | 3565 | 7/7 | 0.98 | 0.19 | 128,128,128,128 | 0 |
| 85 | MG | 1 | 3890 | 1/1 | 0.98 | 0.43 | 27,27,27,27 | 0 |
| 84 | OHX | AR | 3566 | 7/7 | 0.98 | 0.09 | 156,156,157,157 | 0 |
| 85 | MG | AR | 3946 | 1/1 | 0.98 | 0.48 | 21,21,21,21 | 0 |
| 85 | MG | A | 2107 | 1/1 | 0.98 | 0.10 | 147,147,147,147 | 0 |
| 85 | MG | 1 | 3892 | 1/1 | 0.98 | 0.68 | 34,34,34,34 | 0 |
| 85 | MG | 1 | 3893 | 1/1 | 0.98 | 0.55 | 28,28,28,28 | 0 |
| 84 | OHX | AR | 3567 | 7/7 | 0.98 | 0.20 | 111,112,112,112 | 0 |
| 84 | OHX | CE | 401 | 7/7 | 0.98 | 0.12 | 110,110,111,111 | 0 |
| 84 | OHX | AR | 3457 | 7/7 | 0.98 | 0.16 | 100,101,101,101 | 0 |
| 85 | MG | AR | 3952 | 1/1 | 0.98 | 0.13 | 59,59,59,59 | 0 |
| 84 | OHX | 1 | 3497 | 7/7 | 0.98 | 0.14 | 104,105,105,105 | 0 |
| 85 | MG | 1 | 3898 | 1/1 | 0.98 | 0.39 | 29,29,29,29 | 0 |
| 84 | OHX | 1 | 3558 | 7/7 | 0.98 | 0.19 | 127,127,128,128 | 0 |
| 85 | MG | 1 | 3900 | 1/1 | 0.98 | 0.50 | 25,25,25,25 | 0 |
| 84 | OHX | AR | 3461 | 7/7 | 0.98 | 0.15 | 95,95,95,96 | 0 |
| 85 | MG | 1 | 4086 | 1/1 | 0.98 | 0.08 | 40,40,40,40 | 0 |
| 84 | OHX | AR | 3462 | 7/7 | 0.98 | 0.21 | 83,83,83,84 | 0 |
| 85 | MG | AR | 3747 | 1/1 | 0.98 | 0.19 | 46,46,46,46 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | 1 | 3903 | 1/1 | 0.98 | 0.38 | 29,29,29,29 | 0 |
| 85 | MG | A | 2123 | 1/1 | 0.98 | 0.46 | 50,50,50,50 | 0 |
| 85 | MG | 1 | 4089 | 1/1 | 0.98 | 0.45 | 23,23,23,23 | 0 |
| 84 | OHX | 1 | 3559 | 7/7 | 0.98 | 0.13 | 156,156,157,157 | 0 |
| 84 | OHX | 1 | 3525 | 7/7 | 0.98 | 0.16 | 112,112,113,113 | 0 |
| 85 | MG | 1 | 3906 | 1/1 | 0.98 | 0.65 | 23,23,23,23 | 0 |
| 84 | OHX | AR | 3467 | 7/7 | 0.98 | 0.15 | 84,84,84,84 | 0 |
| 84 | OHX | 1 | 3601 | 7/7 | 0.98 | 0.28 | 118,118,119,119 | 0 |
| 84 | OHX | AR | 3470 | 7/7 | 0.98 | 0.15 | 95,96,96,96 | 0 |
| 84 | OHX | AR | 3472 | 7/7 | 0.98 | 0.13 | 102,103,103,103 | 0 |
| 84 | OHX | CP | 501 | 7/7 | 0.98 | 0.18 | 137,137,138,138 | 0 |
| 84 | OHX | AR | 3474 | 7/7 | 0.98 | 0.14 | 97,97,97,97 | 0 |
| 85 | MG | 1 | 3914 | 1/1 | 0.98 | 0.56 | 31,31,31,31 | 0 |
| 85 | MG | AR | 3760 | 1/1 | 0.98 | 0.57 | 33,33,33,33 | 0 |
| 84 | OHX | AR | 3475 | 7/7 | 0.98 | 0.15 | 90,91,91,91 | 0 |
| 84 | OHX | DH | 201 | 7/7 | 0.98 | 0.15 | 119,119,120,120 | 0 |
| 84 | OHX | 1 | 3561 | 7/7 | 0.98 | 0.15 | 116,116,116,116 | 0 |
| 84 | OHX | DQ | 201 | 7/7 | 0.98 | 0.14 | 107,107,107,108 | 0 |
| 84 | OHX | A | 1903 | 7/7 | 0.98 | 0.26 | 107,108,108,108 | 0 |
| 85 | MG | AR | 4195 | 1/1 | 0.98 | 0.12 | 81,81,81,81 | 0 |
| 85 | MG | 1 | 3920 | 1/1 | 0.98 | 0.38 | 25,25,25,25 | 0 |
| 84 | OHX | T | 201 | 7/7 | 0.98 | 0.15 | 115,116,117,117 | 0 |
| 85 | MG | 1 | 3922 | 1/1 | 0.98 | 0.46 | 34,34,34,34 | 0 |
| 84 | OHX | A | 1906 | 7/7 | 0.98 | 0.17 | 102,103,104,104 | 0 |
| 84 | OHX | 1 | 3644 | 7/7 | 0.98 | 0.22 | 144,145,145,145 | 0 |
| 84 | OHX | 1 | 3475 | 7/7 | 0.98 | 0.14 | 105,105,106,106 | 0 |
| 84 | OHX | sR | 1907 | 7/7 | 0.98 | 0.24 | 98,99,99,100 | 0 |
| 84 | OHX | sR | 1909 | 7/7 | 0.98 | 0.18 | 102,103,103,104 | 0 |
| 84 | OHX | AR | 3584 | 7/7 | 0.98 | 0.14 | 109,109,110,110 | 0 |
| 85 | MG | 1 | 3931 | 1/1 | 0.98 | 0.14 | 29,29,29,29 | 0 |
| 84 | OHX | sR | 1913 | 7/7 | 0.98 | 0.17 | 97,98,98,98 | 0 |
| 85 | MG | 1 | 3752 | 1/1 | 0.98 | 0.50 | 36,36,36,36 | 0 |
| 85 | MG | 1 | 4119 | 1/1 | 0.98 | 0.10 | 69,69,69,69 | 0 |
| 84 | OHX | sR | 1916 | 7/7 | 0.98 | 0.15 | 93,93,94,94 | 0 |
| 84 | OHX | sR | 1918 | 7/7 | 0.98 | 0.14 | 93,94,94,94 | 0 |
| 84 | OHX | A | 1912 | 7/7 | 0.98 | 0.13 | 105,105,106,106 | 0 |
| 84 | OHX | sR | 1920 | 7/7 | 0.98 | 0.14 | 114,115,116,116 | 0 |
| 84 | OHX | A | 1913 | 7/7 | 0.98 | 0.15 | 114,114,115,115 | 0 |
| 84 | OHX | sR | 1924 | 7/7 | 0.98 | 0.12 | 111,111,112,112 | 0 |
| 85 | MG | AR | 3787 | 1/1 | 0.98 | 0.55 | 31,31,31,31 | 0 |
| 84 | OHX | sR | 1926 | 7/7 | 0.98 | 0.12 | 114,115,115,116 | 0 |
| 84 | OHX | sR | 1928 | 7/7 | 0.98 | 0.12 | 126,127,127,127 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 84 | OHX | AR | 3479 | 7/7 | 0.98 | 0.13 | 110,111,111,112 | 0 |
| 84 | OHX | sR | 1930 | 7/7 | 0.98 | 0.16 | 98,99,99,100 | 0 |
| 84 | OHX | sR | 1931 | 7/7 | 0.98 | 0.12 | 115,115,116,116 | 0 |
| 85 | MG | AR | 3793 | 1/1 | 0.98 | 0.48 | 53,53,53,53 | 0 |
| 84 | OHX | 1 | 3527 | 7/7 | 0.98 | 0.21 | 124,124,124,124 | 0 |
| 84 | OHX | AR | 3481 | 7/7 | 0.98 | 0.21 | 96,97,97,97 | 0 |
| 84 | OHX | sR | 1934 | 7/7 | 0.98 | 0.12 | 123,123,124,124 | 0 |
| 84 | OHX | sR | 1936 | 7/7 | 0.98 | 0.16 | 101,101,101,102 | 0 |
| 84 | OHX | sR | 1937 | 7/7 | 0.98 | 0.13 | 110,110,111,111 | 0 |
| 85 | MG | 1 | 4137 | 1/1 | 0.98 | 0.13 | 62,62,62,62 | 0 |
| 84 | OHX | A | 1922 | 7/7 | 0.98 | 0.13 | 110,111,111,111 | 0 |
| 84 | OHX | A | 1923 | 7/7 | 0.98 | 0.14 | 115,116,116,116 | 0 |
| 84 | OHX | A | 1926 | 7/7 | 0.98 | 0.12 | 122,123,123,123 | 0 |
| 84 | OHX | 1 | 3447 | 7/7 | 0.98 | 0.12 | 93,93,93,94 | 0 |
| 84 | OHX | sR | 1942 | 7/7 | 0.98 | 0.13 | 130,131,131,132 | 0 |
| 85 | MG | sR | 2075 | 1/1 | 0.98 | 0.16 | 63,63,63,63 | 0 |
| 84 | OHX | AR | 3483 | 7/7 | 0.98 | 0.14 | 102,102,102,102 | 0 |
| 84 | OHX | sR | 1944 | 7/7 | 0.98 | 0.09 | 145,146,147,147 | 0 |
| 84 | OHX | A | 1929 | 7/7 | 0.98 | 0.16 | 113,113,114,114 | 0 |
| 84 | OHX | A | 1930 | 7/7 | 0.98 | 0.14 | 120,121,121,121 | 0 |
| 84 | OHX | sR | 1948 | 7/7 | 0.98 | 0.13 | 118,119,119,120 | 0 |
| 85 | MG | AR | 4243 | 1/1 | 0.98 | 0.26 | 27,27,27,27 | 0 |
| 84 | OHX | sR | 1949 | 7/7 | 0.98 | 0.12 | 144,145,146,146 | 0 |
| 84 | OHX | 3 | 201 | 7/7 | 0.98 | 0.15 | 95,95,96,96 | 0 |
| 85 | MG | sR | 2084 | 1/1 | 0.98 | 0.31 | 52,52,52,52 | 0 |
| 84 | OHX | sR | 1951 | 7/7 | 0.98 | 0.13 | 137,138,139,139 | 0 |
| 85 | MG | 1 | 3782 | 1/1 | 0.98 | 0.47 | 35,35,35,35 | 0 |
| 85 | MG | AR | 4025 | 1/1 | 0.98 | 0.19 | 36,36,36,36 | 0 |
| 84 | OHX | AR | 3485 | 7/7 | 0.98 | 0.14 | 98,98,98,98 | 0 |
| 84 | OHX | sR | 1953 | 7/7 | 0.98 | 0.12 | 132,133,134,134 | 0 |
| 84 | OHX | AR | 3487 | 7/7 | 0.98 | 0.25 | 110,110,110,110 | 0 |
| 84 | OHX | A | 1934 | 7/7 | 0.98 | 0.13 | 138,139,140,140 | 0 |
| 85 | MG | 1 | 4157 | 1/1 | 0.98 | 0.10 | 57,57,57,57 | 0 |
| 85 | MG | AS | 215 | 1/1 | 0.98 | 0.57 | 77,77,77,77 | 0 |
| 84 | OHX | 1 | 3529 | 7/7 | 0.98 | 0.12 | 131,132,132,132 | 0 |
| 84 | OHX | 1 | 3530 | 7/7 | 0.98 | 0.19 | 114,115,115,115 | 0 |
| 84 | OHX | sR | 1958 | 7/7 | 0.98 | 0.14 | 119,119,120,120 | 0 |
| 84 | OHX | AR | 3491 | 7/7 | 0.98 | 0.16 | 103,103,104,104 | 0 |
| 84 | OHX | A | 1938 | 7/7 | 0.98 | 0.15 | 121,122,122,123 | 0 |
| 85 | MG | 1 | 3792 | 1/1 | 0.98 | 0.50 | 20,20,20,20 | 0 |
| 84 | OHX | AR | 3596 | 7/7 | 0.98 | 0.14 | 109,110,110,110 | 0 |
| 84 | OHX | sR | 1962 | 7/7 | 0.98 | 0.20 | 148,148,149,149 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 84 | OHX | 3 | 204 | 7/7 | 0.98 | 0.13 | 119,119,120,120 | 0 |
| 84 | OHX | A | 1941 | 7/7 | 0.98 | 0.15 | 146,146,147,147 | 0 |
| 84 | OHX | A | 1942 | 7/7 | 0.98 | 0.17 | 127,128,128,129 | 0 |
| 84 | OHX | AR | 3495 | 7/7 | 0.98 | 0.13 | 99,100,100,100 | 0 |
| 84 | OHX | AR | 3599 | 7/7 | 0.98 | 0.19 | 130,130,131,131 | 0 |
| 84 | OHX | sR | 1968 | 7/7 | 0.98 | 0.22 | 132,133,134,134 | 0 |
| 85 | MG | AR | 4045 | 1/1 | 0.98 | 0.23 | 74,74,74,74 | 0 |
| 84 | OHX | AR | 3496 | 7/7 | 0.98 | 0.14 | 106,107,107,107 | 0 |
| 84 | OHX | sR | 1970 | 7/7 | 0.98 | 0.15 | 135,135,136,136 | 0 |
| 84 | OHX | AR | 3497 | 7/7 | 0.98 | 0.20 | 104,104,105,105 | 0 |
| 84 | OHX | 1 | 3531 | 7/7 | 0.98 | 0.11 | 124,125,126,126 | 0 |
| 84 | OHX | 1 | 3501 | 7/7 | 0.98 | 0.14 | 106,107,107,108 | 0 |
| 84 | OHX | A | 1949 | 7/7 | 0.98 | 0.09 | 144,146,146,146 | 0 |
| 85 | MG | AR | 3839 | 1/1 | 0.98 | 0.54 | 45,45,45,45 | 0 |
| 84 | OHX | 1 | 3569 | 7/7 | 0.98 | 0.28 | 122,122,123,123 | 0 |
| 84 | OHX | AR | 3501 | 7/7 | 0.98 | 0.09 | 133,134,134,135 | 0 |
| 84 | OHX | 1 | 3477 | 7/7 | 0.98 | 0.14 | 103,103,104,104 | 0 |
| 84 | OHX | AR | 3504 | 7/7 | 0.98 | 0.19 | 106,106,106,107 | 0 |
| 84 | OHX | AR | 3505 | 7/7 | 0.98 | 0.14 | 121,121,121,122 | 0 |
| 84 | OHX | A | 1957 | 7/7 | 0.98 | 0.21 | 139,140,140,141 | 0 |
| 84 | OHX | AR | 3506 | 7/7 | 0.98 | 0.26 | 117,118,118,118 | 0 |
| 85 | MG | 1 | 3995 | 1/1 | 0.98 | 0.12 | 29,29,29,29 | 0 |
| 84 | OHX | AR | 3507 | 7/7 | 0.98 | 0.18 | 90,90,91,91 | 0 |
| 84 | OHX | 4 | 201 | 7/7 | 0.98 | 0.28 | 79,80,80,80 | 0 |
| 84 | OHX | A | 1961 | 7/7 | 0.98 | 0.11 | 154,155,156,157 | 0 |
| 84 | OHX | A | 1962 | 7/7 | 0.98 | 0.15 | 133,134,135,135 | 0 |
| 85 | MG | AR | 4066 | 1/1 | 0.98 | 0.20 | 71,71,71,71 | 0 |
| 84 | OHX | AR | 3509 | 7/7 | 0.98 | 0.16 | 97,97,97,97 | 0 |
| 84 | OHX | AR | 3510 | 7/7 | 0.98 | 0.14 | 117,118,118,118 | 0 |
| 84 | OHX | 4 | 204 | 7/7 | 0.98 | 0.14 | 103,103,103,104 | 0 |
| 84 | OHX | 4 | 205 | 7/7 | 0.98 | 0.13 | 111,111,111,111 | 0 |
| 84 | OHX | AR | 3514 | 7/7 | 0.98 | 0.11 | 110,110,110,111 | 0 |
| 84 | OHX | AR | 3515 | 7/7 | 0.98 | 0.12 | 116,116,116,117 | 0 |
| 84 | OHX | 1 | 3571 | 7/7 | 0.98 | 0.09 | 155,155,155,155 | 0 |
| 84 | OHX | 1 | 3480 | 7/7 | 0.98 | 0.15 | 95,96,96,96 | 0 |
| 85 | MG | CR | 201 | 1/1 | 0.98 | 0.60 | 35,35,35,35 | 0 |
| 84 | OHX | 4 | 208 | 7/7 | 0.98 | 0.23 | 126,126,126,126 | 0 |
| 85 | MG | AR | 3861 | 1/1 | 0.98 | 0.53 | 30,30,30,30 | 0 |
| 84 | OHX | A | 1972 | 7/7 | 0.98 | 0.12 | 163,164,165,165 | 0 |
| 84 | OHX | 1 | 3459 | 7/7 | 0.98 | 0.16 | 93,94,94,94 | 0 |
| 85 | MG | AR | 3864 | 1/1 | 0.98 | 0.61 | 27,27,27,27 | 0 |
| 84 | OHX | sR | 1997 | 7/7 | 0.98 | 0.19 | 151,152,153,153 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 84 | OHX | AR | 3520 | 7/7 | 0.98 | 0.15 | 112,112,113,113 | 0 |
| 84 | OHX | AR | 3521 | 7/7 | 0.98 | 0.14 | 112,112,113,113 | 0 |
| 84 | OHX | 1 | 3536 | 7/7 | 0.98 | 0.16 | 100,100,101,101 | 0 |
| 85 | MG | AR | 3870 | 1/1 | 0.98 | 0.35 | 35,35,35,35 | 0 |
| 84 | OHX | 1 | 3505 | 7/7 | 0.98 | 0.14 | 108,108,109,109 | 0 |
| 84 | OHX | 1 | 3506 | 7/7 | 0.98 | 0.14 | 120,120,121,121 | 0 |
| 84 | OHX | AR | 3525 | 7/7 | 0.98 | 0.20 | 119,120,120,120 | 0 |
| 84 | OHX | sR | 2004 | 7/7 | 0.98 | 0.14 | 124,125,126,126 | 0 |
| 84 | OHX | 1 | 3577 | 7/7 | 0.98 | 0.14 | 146,147,147,148 | 0 |
| 85 | MG | DC | 206 | 1/1 | 0.98 | 0.15 | 38,38,38,38 | 0 |
| 84 | OHX | AR | 3527 | 7/7 | 0.98 | 0.11 | 120,121,121,122 | 0 |
| 84 | OHX | 1 | 3461 | 7/7 | 0.98 | 0.16 | 103,103,104,104 | 0 |
| 84 | OHX | 1 | 3483 | 7/7 | 0.98 | 0.20 | 117,118,118,119 | 0 |
| 84 | OHX | A | 1984 | 7/7 | 0.98 | 0.13 | 130,131,131,132 | 0 |
| 84 | OHX | 1 | 3462 | 7/7 | 0.98 | 0.13 | 92,92,93,93 | 0 |
| 84 | OHX | 1 | 3581 | 7/7 | 0.98 | 0.30 | 120,120,121,121 | 0 |
| 84 | OHX | A | 1987 | 7/7 | 0.98 | 0.16 | 146,146,147,147 | 0 |
| 85 | MG | 3 | 212 | 1/1 | 0.98 | 0.42 | 47,47,47,47 | 0 |
| 84 | OHX | 1 | 3448 | 7/7 | 0.98 | 0.14 | 89,89,90,90 | 0 |
| 85 | MG | 1 | 3847 | 1/1 | 0.98 | 0.55 | 38,38,38,38 | 0 |
| 85 | MG | sR | 2166 | 1/1 | 0.98 | 0.09 | 59,59,59,59 | 0 |
| 84 | OHX | A | 1989 | 7/7 | 0.98 | 0.27 | 183,183,184,184 | 0 |
| 85 | MG | 1 | 3849 | 1/1 | 0.98 | 0.40 | 27,27,27,27 | 0 |
| 85 | MG | 1 | 4031 | 1/1 | 0.98 | 0.19 | 33,33,33,33 | 0 |
| 84 | OHX | A | 1990 | 7/7 | 0.98 | 0.21 | 150,151,152,152 | 0 |
| 85 | MG | sR | 2171 | 1/1 | 0.98 | 0.15 | 101,101,101,101 | 0 |
| 84 | OHX | AR | 3534 | 7/7 | 0.98 | 0.13 | 104,104,105,105 | 0 |
| 85 | MG | A | 2050 | 1/1 | 0.98 | 0.45 | 66,66,66,66 | 0 |
| 84 | OHX | A | 1992 | 7/7 | 0.98 | 0.19 | 142,143,143,144 | 0 |
| 85 | MG | 1 | 3854 | 1/1 | 0.98 | 0.60 | 29,29,29,29 | 0 |
| 84 | OHX | 1 | 3436 | 7/7 | 0.98 | 0.18 | 87,88,88,88 | 0 |
| 84 | OHX | 1 | 3487 | 7/7 | 0.98 | 0.14 | 90,91,91,92 | 0 |
| 85 | MG | AR | 3895 | 1/1 | 0.98 | 0.31 | 25,25,25,25 | 0 |
| 84 | OHX | 1 | 3513 | 7/7 | 0.98 | 0.19 | 104,105,105,105 | 0 |
| 84 | OHX | 1 | 3514 | 7/7 | 0.98 | 0.12 | 116,117,117,117 | 0 |
| 85 | MG | sR | 2182 | 1/1 | 0.98 | 0.20 | 60,60,60,60 | 0 |
| 84 | OHX | 1 | 3467 | 7/7 | 0.98 | 0.15 | 102,102,103,103 | 0 |
| 84 | OHX | 1 | 3548 | 7/7 | 0.98 | 0.09 | 124,125,126,126 | 0 |
| 85 | MG | AR | 3900 | 1/1 | 0.98 | 0.42 | 35,35,35,35 | 0 |
| 85 | MG | 1 | 4042 | 1/1 | 0.98 | 0.08 | 57,57,57,57 | 0 |
| 84 | OHX | 1 | 3516 | 7/7 | 0.98 | 0.12 | 102,102,102,102 | 0 |
| 84 | OHX | AK | 103 | 7/7 | 0.98 | 0.14 | 100,100,101,101 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 84 | OHX | 1 | 3426 | 7/7 | 0.98 | 0.19 | 79,79,80,80 | 0 |
| 84 | OHX | AS | 202 | 7/7 | 0.98 | 0.17 | 91,92,93,93 | 0 |
| 84 | OHX | AR | 3413 | 7/7 | 0.98 | 0.25 | 77,78,78,78 | 0 |
| 84 | OHX | AR | 3545 | 7/7 | 0.98 | 0.21 | 104,105,105,105 | 0 |
| 84 | OHX | AS | 205 | 7/7 | 0.98 | 0.11 | 112,113,113,113 | 0 |
| 84 | OHX | 1 | 3551 | 7/7 | 0.98 | 0.15 | 122,123,123,123 | 0 |
| 84 | OHX | AR | 3432 | 7/7 | 0.98 | 0.17 | 79,80,80,80 | 0 |
| 84 | OHX | A | 2008 | 7/7 | 0.98 | 0.16 | 132,133,133,133 | 0 |
| 84 | OHX | AR | 3434 | 7/7 | 0.98 | 0.20 | 85,85,85,85 | 0 |
| 84 | OHX | AR | 3435 | 7/7 | 0.98 | 0.17 | 90,90,91,91 | 0 |
| 84 | OHX | AR | 3440 | 7/7 | 0.98 | 0.17 | 79,79,79,79 | 0 |
| 84 | OHX | 1 | 3452 | 7/7 | 0.98 | 0.16 | 99,99,99,100 | 0 |
| 85 | MG | AR | 3917 | 1/1 | 0.98 | 0.62 | 34,34,34,34 | 0 |
| 84 | OHX | 1 | 3453 | 7/7 | 0.98 | 0.13 | 101,102,102,102 | 0 |
| 85 | MG | A | 2078 | 1/1 | 0.98 | 0.53 | 43,43,43,43 | 0 |
| 85 | MG | AR | 3919 | 1/1 | 0.98 | 0.47 | 34,34,34,34 | 0 |
| 84 | OHX | 1 | 3417 | 7/7 | 0.98 | 0.23 | 85,85,86,86 | 0 |
| 84 | OHX | AR | 3446 | 7/7 | 0.98 | 0.16 | 88,88,88,88 | 0 |
| 87 | ZN | AQ | 501 | 1/1 | 0.98 | 0.11 | 60,60,60,60 | 0 |
| 87 | ZN | DQ | 202 | 1/1 | 0.98 | 0.04 | 82,82,82,82 | 0 |
| 84 | OHX | AR | 3555 | 7/7 | 0.98 | 0.14 | 116,116,117,117 | 0 |
| 84 | OHX | AR | 3556 | 7/7 | 0.98 | 0.11 | 142,142,143,143 | 0 |
| 84 | OHX | 1 | 3456 | 7/7 | 0.98 | 0.14 | 96,97,97,97 | 0 |
| 85 | MG | AR | 3925 | 1/1 | 0.98 | 0.53 | 32,32,32,32 | 0 |
| 85 | MG | A | 2141 | 1/1 | 0.99 | 0.28 | 78,78,78,78 | 0 |
| 85 | MG | 1 | 4118 | 1/1 | 0.99 | 0.16 | 100,100,100,100 | 0 |
| 84 | OHX | 1 | 3445 | 7/7 | 0.99 | 0.17 | 85,85,85,85 | 0 |
| 84 | OHX | AR | 3430 | 7/7 | 0.99 | 0.15 | 84,84,85,85 | 0 |
| 85 | MG | 1 | 4121 | 1/1 | 0.99 | 0.18 | 66,66,66,66 | 0 |
| 84 | OHX | AR | 3431 | 7/7 | 0.99 | 0.17 | 81,81,82,82 | 0 |
| 84 | OHX | 1 | 3406 | 7/7 | 0.99 | 0.26 | 79,79,79,79 | 0 |
| 84 | OHX | AR | 3433 | 7/7 | 0.99 | 0.19 | 80,80,80,80 | 0 |
| 84 | OHX | 1 | 3407 | 7/7 | 0.99 | 0.23 | 78,78,78,78 | 0 |
| 84 | OHX | 1 | 3408 | 7/7 | 0.99 | 0.27 | 83,83,83,83 | 0 |
| 84 | OHX | AR | 3436 | 7/7 | 0.99 | 0.15 | 80,81,81,81 | 0 |
| 84 | OHX | AR | 3437 | 7/7 | 0.99 | 0.14 | 83,83,83,84 | 0 |
| 84 | OHX | AR | 3438 | 7/7 | 0.99 | 0.14 | 84,84,85,85 | 0 |
| 84 | OHX | AR | 3439 | 7/7 | 0.99 | 0.17 | 79,79,79,79 | 0 |
| 84 | OHX | 1 | 3500 | 7/7 | 0.99 | 0.13 | 81,82,82,82 | 0 |
| 84 | OHX | AR | 3441 | 7/7 | 0.99 | 0.16 | 87,87,87,88 | 0 |
| 84 | OHX | AR | 3442 | 7/7 | 0.99 | 0.12 | 95,96,96,97 | 0 |
| 84 | OHX | 1 | 3409 | 7/7 | 0.99 | 0.25 | 85,86,86,86 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 84 | OHX | 1 | 3450 | 7/7 | 0.99 | 0.14 | 97,98,99,99 | 0 |
| 84 | OHX | 1 | 3410 | 7/7 | 0.99 | 0.24 | 82,83,83,83 | 0 |
| 84 | OHX | 1 | 3412 | 7/7 | 0.99 | 0.24 | 83,83,84,84 | 0 |
| 84 | OHX | 1 | 3413 | 7/7 | 0.99 | 0.24 | 82,83,83,83 | 0 |
| 85 | MG | AR | 3928 | 1/1 | 0.99 | 0.67 | 42,42,42,42 | 0 |
| 85 | MG | AR | 3929 | 1/1 | 0.99 | 0.49 | 31,31,31,31 | 0 |
| 84 | OHX | AR | 3448 | 7/7 | 0.99 | 0.16 | 86,86,86,87 | 0 |
| 84 | OHX | 1 | 3454 | 7/7 | 0.99 | 0.13 | 90,91,91,91 | 0 |
| 84 | OHX | 1 | 3414 | 7/7 | 0.99 | 0.20 | 80,81,81,81 | 0 |
| 84 | OHX | 1 | 3415 | 7/7 | 0.99 | 0.24 | 90,90,91,91 | 0 |
| 84 | OHX | 1 | 3457 | 7/7 | 0.99 | 0.14 | 94,95,95,95 | 0 |
| 84 | OHX | 1 | 3416 | 7/7 | 0.99 | 0.18 | 80,80,80,80 | 0 |
| 85 | MG | AR | 3770 | 1/1 | 0.99 | 0.29 | 55,55,55,55 | 0 |
| 84 | OHX | 1 | 3401 | 7/7 | 0.99 | 0.30 | 84,84,84,85 | 0 |
| 84 | OHX | 1 | 3460 | 7/7 | 0.99 | 0.13 | 82,82,83,83 | 0 |
| 85 | MG | AR | 3773 | 1/1 | 0.99 | 0.59 | 43,43,43,43 | 0 |
| 84 | OHX | AR | 3456 | 7/7 | 0.99 | 0.15 | 83,83,83,83 | 0 |
| 84 | OHX | 1 | 3418 | 7/7 | 0.99 | 0.21 | 84,84,84,84 | 0 |
| 84 | OHX | CV | 201 | 7/7 | 0.99 | 0.26 | 85,85,85,85 | 0 |
| 84 | OHX | CX | 201 | 7/7 | 0.99 | 0.15 | 93,94,94,94 | 0 |
| 84 | OHX | 1 | 3419 | 7/7 | 0.99 | 0.20 | 79,79,79,79 | 0 |
| 85 | MG | 1 | 3842 | 1/1 | 0.99 | 0.44 | 27,27,27,27 | 0 |
| 84 | OHX | DD | 102 | 7/7 | 0.99 | 0.23 | 82,82,83,83 | 0 |
| 84 | OHX | 1 | 3420 | 7/7 | 0.99 | 0.21 | 86,86,86,87 | 0 |
| 84 | OHX | AR | 3460 | 7/7 | 0.99 | 0.12 | 90,91,91,91 | 0 |
| 85 | MG | 1 | 4156 | 1/1 | 0.99 | 0.12 | 83,83,83,83 | 0 |
| 84 | OHX | 1 | 3422 | 7/7 | 0.99 | 0.20 | 85,86,86,86 | 0 |
| 84 | OHX | A | 1901 | 7/7 | 0.99 | 0.21 | 92,93,93,93 | 0 |
| 84 | OHX | A | 1902 | 7/7 | 0.99 | 0.18 | 88,89,89,89 | 0 |
| 84 | OHX | 1 | 3517 | 7/7 | 0.99 | 0.11 | 117,117,118,118 | 0 |
| 84 | OHX | A | 1904 | 7/7 | 0.99 | 0.17 | 97,97,97,97 | 0 |
| 85 | MG | 1 | 3851 | 1/1 | 0.99 | 0.17 | 38,38,38,38 | 0 |
| 84 | OHX | A | 1905 | 7/7 | 0.99 | 0.18 | 93,94,94,94 | 0 |
| 84 | OHX | 1 | 3465 | 7/7 | 0.99 | 0.14 | 93,93,94,94 | 0 |
| 84 | OHX | A | 1907 | 7/7 | 0.99 | 0.15 | 99,100,100,101 | 0 |
| 84 | OHX | A | 1908 | 7/7 | 0.99 | 0.17 | 103,104,105,105 | 0 |
| 84 | OHX | AR | 3464 | 7/7 | 0.99 | 0.11 | 98,98,98,99 | 0 |
| 85 | MG | 1 | 4169 | 1/1 | 0.99 | 0.16 | 39,39,39,39 | 0 |
| 84 | OHX | AR | 3465 | 7/7 | 0.99 | 0.11 | 102,103,103,103 | 0 |
| 84 | OHX | 1 | 3466 | 7/7 | 0.99 | 0.13 | 94,95,95,95 | 0 |
| 84 | OHX | 1 | 3423 | 7/7 | 0.99 | 0.18 | 88,88,88,88 | 0 |
| 84 | OHX | AR | 3468 | 7/7 | 0.99 | 0.11 | 101,101,102,102 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 84 | OHX | A | 1914 | 7/7 | 0.99 | 0.15 | 101,102,103,103 | 0 |
| 84 | OHX | 1 | 3424 | 7/7 | 0.99 | 0.16 | 84,84,84,84 | 0 |
| 84 | OHX | A | 1916 | 7/7 | 0.99 | 0.13 | 106,107,108,108 | 0 |
| 84 | OHX | A | 1917 | 7/7 | 0.99 | 0.12 | 105,106,106,107 | 0 |
| 84 | OHX | 1 | 3469 | 7/7 | 0.99 | 0.23 | 85,85,85,86 | 0 |
| 84 | OHX | A | 1919 | 7/7 | 0.99 | 0.13 | 100,100,101,101 | 0 |
| 84 | OHX | A | 1920 | 7/7 | 0.99 | 0.12 | 102,102,103,103 | 0 |
| 84 | OHX | sR | 1901 | 7/7 | 0.99 | 0.27 | 87,87,87,87 | 0 |
| 84 | OHX | sR | 1902 | 7/7 | 0.99 | 0.24 | 98,99,99,99 | 0 |
| 84 | OHX | sR | 1903 | 7/7 | 0.99 | 0.21 | 86,86,86,87 | 0 |
| 84 | OHX | sR | 1904 | 7/7 | 0.99 | 0.19 | 90,90,90,91 | 0 |
| 84 | OHX | AR | 3471 | 7/7 | 0.99 | 0.14 | 90,91,91,92 | 0 |
| 84 | OHX | sR | 1906 | 7/7 | 0.99 | 0.20 | 90,90,90,90 | 0 |
| 84 | OHX | 1 | 3425 | 7/7 | 0.99 | 0.21 | 87,88,88,88 | 0 |
| 85 | MG | AR | 4146 | 1/1 | 0.99 | 0.07 | 42,42,42,42 | 0 |
| 84 | OHX | sR | 1908 | 7/7 | 0.99 | 0.18 | 87,88,88,88 | 0 |
| 85 | MG | 1 | 4189 | 1/1 | 0.99 | 0.14 | 46,46,46,46 | 0 |
| 84 | OHX | AR | 3473 | 7/7 | 0.99 | 0.13 | 103,103,104,104 | 0 |
| 84 | OHX | sR | 1910 | 7/7 | 0.99 | 0.20 | 87,88,88,88 | 0 |
| 84 | OHX | A | 1924 | 7/7 | 0.99 | 0.08 | 121,121,122,123 | 0 |
| 84 | OHX | sR | 1912 | 7/7 | 0.99 | 0.16 | 89,89,90,90 | 0 |
| 84 | OHX | A | 1925 | 7/7 | 0.99 | 0.11 | 135,135,136,136 | 0 |
| 84 | OHX | sR | 1914 | 7/7 | 0.99 | 0.15 | 104,104,105,106 | 0 |
| 84 | OHX | sR | 1915 | 7/7 | 0.99 | 0.16 | 92,93,93,94 | 0 |
| 84 | OHX | 1 | 3524 | 7/7 | 0.99 | 0.14 | 107,107,108,108 | 0 |
| 84 | OHX | sR | 1917 | 7/7 | 0.99 | 0.13 | 98,99,100,100 | 0 |
| 84 | OHX | 4 | 202 | 7/7 | 0.99 | 0.24 | 83,83,83,83 | 0 |
| 84 | OHX | 4 | 203 | 7/7 | 0.99 | 0.14 | 83,83,84,84 | 0 |
| 84 | OHX | 1 | 3471 | 7/7 | 0.99 | 0.12 | 98,99,99,99 | 0 |
| 84 | OHX | 1 | 3402 | 7/7 | 0.99 | 0.30 | 84,84,84,84 | 0 |
| 84 | OHX | sR | 1922 | 7/7 | 0.99 | 0.16 | 103,103,104,104 | 0 |
| 84 | OHX | sR | 1923 | 7/7 | 0.99 | 0.14 | 92,93,93,94 | 0 |
| 84 | OHX | 1 | 3427 | 7/7 | 0.99 | 0.20 | 88,88,89,89 | 0 |
| 84 | OHX | sR | 1925 | 7/7 | 0.99 | 0.16 | 101,101,102,102 | 0 |
| 84 | OHX | 1 | 3428 | 7/7 | 0.99 | 0.18 | 83,83,83,83 | 0 |
| 85 | MG | 1 | 3744 | 1/1 | 0.99 | 0.76 | 52,52,52,52 | 0 |
| 84 | OHX | sR | 1927 | 7/7 | 0.99 | 0.15 | 100,100,101,101 | 0 |
| 84 | OHX | 1 | 3429 | 7/7 | 0.99 | 0.20 | 93,93,94,94 | 0 |
| 84 | OHX | 1 | 3430 | 7/7 | 0.99 | 0.13 | 86,86,86,86 | 0 |
| 84 | OHX | 1 | 3431 | 7/7 | 0.99 | 0.15 | 81,81,82,82 | 0 |
| 84 | OHX | 1 | 3478 | 7/7 | 0.99 | 0.15 | 93,93,93,94 | 0 |
| 84 | OHX | 1 | 3479 | 7/7 | 0.99 | 0.11 | 108,108,109,109 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 84 | OHX | AR | 3486 | 7/7 | 0.99 | 0.16 | 87,87,88,88 | 0 |
| 84 | OHX | 1 | 3403 | 7/7 | 0.99 | 0.30 | 83,83,83,83 | 0 |
| 84 | OHX | sR | 1935 | 7/7 | 0.99 | 0.13 | 109,109,110,110 | 0 |
| 84 | OHX | 1 | 3433 | 7/7 | 0.99 | 0.18 | 86,86,87,87 | 0 |
| 84 | OHX | AR | 3489 | 7/7 | 0.99 | 0.15 | 95,95,95,96 | 0 |
| 85 | MG | AR | 4179 | 1/1 | 0.99 | 0.14 | 70,70,70,70 | 0 |
| 85 | MG | AR | 4180 | 1/1 | 0.99 | 0.15 | 66,66,66,66 | 0 |
| 84 | OHX | 1 | 3434 | 7/7 | 0.99 | 0.18 | 86,87,87,87 | 0 |
| 84 | OHX | 1 | 3435 | 7/7 | 0.99 | 0.20 | 92,92,93,93 | 0 |
| 84 | OHX | 1 | 3404 | 7/7 | 0.99 | 0.29 | 89,89,89,89 | 0 |
| 85 | MG | AR | 4184 | 1/1 | 0.99 | 0.14 | 43,43,43,43 | 0 |
| 84 | OHX | AR | 3493 | 7/7 | 0.99 | 0.19 | 83,83,83,83 | 0 |
| 85 | MG | sR | 2150 | 1/1 | 0.99 | 0.09 | 76,76,76,76 | 0 |
| 85 | MG | 1 | 4063 | 1/1 | 0.99 | 0.52 | 35,35,35,35 | 0 |
| 85 | MG | sR | 2152 | 1/1 | 0.99 | 0.08 | 110,110,110,110 | 0 |
| 85 | MG | 1 | 3910 | 1/1 | 0.99 | 0.44 | 31,31,31,31 | 0 |
| 84 | OHX | AR | 3494 | 7/7 | 0.99 | 0.10 | 106,107,107,107 | 0 |
| 84 | OHX | 1 | 3437 | 7/7 | 0.99 | 0.20 | 85,85,85,85 | 0 |
| 84 | OHX | v | 301 | 7/7 | 0.99 | 0.15 | 92,92,92,93 | 0 |
| 84 | OHX | sR | 1945 | 7/7 | 0.99 | 0.12 | 118,119,119,120 | 0 |
| 84 | OHX | 1 | 3438 | 7/7 | 0.99 | 0.18 | 85,86,86,86 | 0 |
| 84 | OHX | A | 1950 | 7/7 | 0.99 | 0.14 | 116,117,117,118 | 0 |
| 84 | OHX | 1 | 3439 | 7/7 | 0.99 | 0.18 | 86,86,86,86 | 0 |
| 84 | OHX | 1 | 3440 | 7/7 | 0.99 | 0.17 | 82,83,83,83 | 0 |
| 84 | OHX | 1 | 3405 | 7/7 | 0.99 | 0.28 | 91,91,91,91 | 0 |
| 84 | OHX | A | 1954 | 7/7 | 0.99 | 0.15 | 129,130,130,130 | 0 |
| 84 | OHX | 1 | 3442 | 7/7 | 0.99 | 0.15 | 88,89,89,89 | 0 |
| 84 | OHX | AR | 3502 | 7/7 | 0.99 | 0.12 | 112,112,113,113 | 0 |
| 84 | OHX | AC | 101 | 7/7 | 0.99 | 0.24 | 84,84,84,85 | 0 |
| 84 | OHX | 1 | 3491 | 7/7 | 0.99 | 0.14 | 97,97,98,98 | 0 |
| 84 | OHX | 1 | 3492 | 7/7 | 0.99 | 0.11 | 106,106,107,107 | 0 |
| 85 | MG | AR | 3867 | 1/1 | 0.99 | 0.34 | 37,37,37,37 | 0 |
| 85 | MG | 1 | 3926 | 1/1 | 0.99 | 0.63 | 23,23,23,23 | 0 |
| 84 | OHX | AR | 3615 | 7/7 | 0.99 | 0.18 | 107,107,107,107 | 0 |
| 84 | OHX | 1 | 3443 | 7/7 | 0.99 | 0.15 | 89,90,90,91 | 0 |
| 84 | OHX | 1 | 3494 | 7/7 | 0.99 | 0.14 | 89,90,90,90 | 0 |
| 85 | MG | 1 | 3930 | 1/1 | 0.99 | 0.52 | 26,26,26,26 | 0 |
| 84 | OHX | AR | 3401 | 7/7 | 0.99 | 0.34 | 88,88,88,88 | 0 |
| 84 | OHX | AR | 3402 | 7/7 | 0.99 | 0.31 | 82,82,82,82 | 0 |
| 85 | MG | sR | 2177 | 1/1 | 0.99 | 0.15 | 84,84,84,84 | 0 |
| 84 | OHX | AR | 3403 | 7/7 | 0.99 | 0.29 | 80,80,80,80 | 0 |
| 84 | OHX | AR | 3404 | 7/7 | 0.99 | 0.29 | 81,81,82,82 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 84 | OHX | AR | 3405 | 7/7 | 0.99 | 0.27 | 86,86,87,87 | 0 |
| 84 | OHX | AR | 3513 | 7/7 | 0.99 | 0.15 | 81,81,81,82 | 0 |
| 84 | OHX | AR | 3406 | 7/7 | 0.99 | 0.26 | 82,82,82,82 | 0 |
| 84 | OHX | AR | 3407 | 7/7 | 0.99 | 0.25 | 80,80,80,80 | 0 |
| 84 | OHX | AR | 3408 | 7/7 | 0.99 | 0.24 | 77,77,77,77 | 0 |
| 84 | OHX | AR | 3409 | 7/7 | 0.99 | 0.24 | 82,82,83,83 | 0 |
| 85 | MG | AR | 4221 | 1/1 | 0.99 | 0.15 | 40,40,40,40 | 0 |
| 84 | OHX | AR | 3410 | 7/7 | 0.99 | 0.24 | 78,79,79,79 | 0 |
| 84 | OHX | AR | 3411 | 7/7 | 0.99 | 0.26 | 87,87,88,88 | 0 |
| 84 | OHX | AR | 3412 | 7/7 | 0.99 | 0.26 | 80,80,80,80 | 0 |
| 84 | OHX | 1 | 3444 | 7/7 | 0.99 | 0.18 | 90,90,91,91 | 0 |
| 84 | OHX | AR | 3414 | 7/7 | 0.99 | 0.24 | 80,80,80,80 | 0 |
| 84 | OHX | AR | 3415 | 7/7 | 0.99 | 0.21 | 78,78,79,79 | 0 |
| 84 | OHX | AR | 3416 | 7/7 | 0.99 | 0.21 | 82,82,82,82 | 0 |
| 84 | OHX | AR | 3417 | 7/7 | 0.99 | 0.22 | 79,80,80,80 | 0 |
| 84 | OHX | AR | 3418 | 7/7 | 0.99 | 0.17 | 84,84,84,84 | 0 |
| 85 | MG | AR | 4231 | 1/1 | 0.99 | 0.14 | 80,80,80,80 | 0 |
| 84 | OHX | AS | 201 | 7/7 | 0.99 | 0.17 | 88,88,88,89 | 0 |
| 84 | OHX | AR | 3419 | 7/7 | 0.99 | 0.20 | 81,82,82,82 | 0 |
| 84 | OHX | AR | 3420 | 7/7 | 0.99 | 0.23 | 84,84,84,84 | 0 |
| 84 | OHX | AR | 3421 | 7/7 | 0.99 | 0.20 | 89,89,89,89 | 0 |
| 84 | OHX | AR | 3530 | 7/7 | 0.99 | 0.07 | 128,129,129,130 | 0 |
| 85 | MG | x | 205 | 1/1 | 0.99 | 0.63 | 31,31,31,31 | 0 |
| 85 | MG | AR | 4064 | 1/1 | 0.99 | 0.12 | 84,84,84,84 | 0 |
| 84 | OHX | AR | 3422 | 7/7 | 0.99 | 0.22 | 83,84,84,84 | 0 |
| 84 | OHX | AR | 3423 | 7/7 | 0.99 | 0.20 | 82,82,82,82 | 0 |
| 85 | MG | AR | 4241 | 1/1 | 0.99 | 0.67 | 41,41,41,41 | 0 |
| 87 | ZN | AK | 101 | 1/1 | 0.99 | 0.16 | 39,39,39,39 | 0 |
| 87 | ZN | AP | 501 | 1/1 | 0.99 | 0.03 | 75,75,75,75 | 0 |
| 84 | OHX | AR | 3424 | 7/7 | 0.99 | 0.23 | 82,82,82,82 | 0 |
| 87 | ZN | DL | 102 | 1/1 | 0.99 | 0.18 | 44,44,44,44 | 0 |
| 84 | OHX | AR | 3425 | 7/7 | 0.99 | 0.21 | 81,81,81,82 | 0 |
| 87 | ZN | DR | 501 | 1/1 | 0.99 | 0.11 | 62,62,62,62 | 0 |
| 87 | ZN | b | 102 | 1/1 | 0.99 | 0.10 | 84,84,84,84 | 0 |
| 84 | OHX | AR | 3426 | 7/7 | 0.99 | 0.20 | 82,82,83,83 | 0 |
| 87 | ZN | e | 103 | 1/1 | 0.99 | 0.09 | 82,82,82,82 | 0 |
| 84 | OHX | AR | 3427 | 7/7 | 0.99 | 0.17 | 77,77,77,77 | 0 |
| 84 | OHX | AR | 3428 | 7/7 | 0.99 | 0.20 | 81,81,81,81 | 0 |
| 84 | OHX | AT | 203 | 7/7 | 0.99 | 0.13 | 104,104,104,104 | 0 |
| 87 | ZN | DO | 201 | 1/1 | 1.00 | 0.16 | 29,29,29,29 | 0 |
| 85 | MG | AR | 4204 | 1/1 | 1.00 | 0.17 | 63,63,63,63 | 0 |
| 84 | OHX | 1 | 3411 | 7/7 | 1.00 | 0.22 | 81,82,82,82 | 0 |

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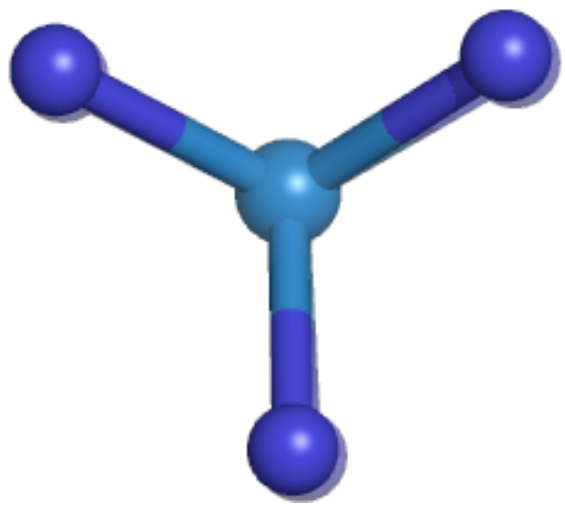
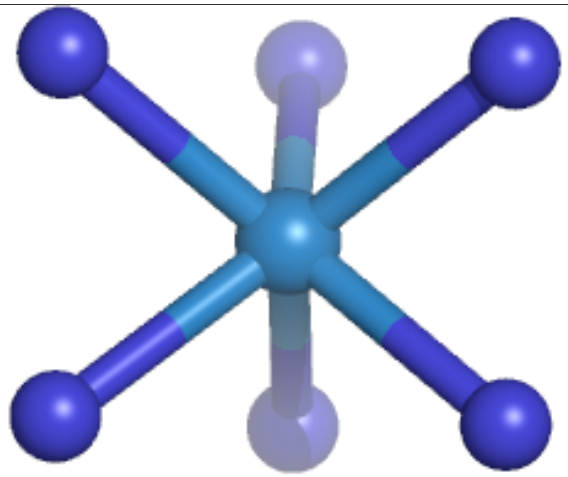
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 85 | MG | 1 | 4158 | 1/1 | 1.00 | 0.15 | 57,57,57,57 | 0 |
| 84 | OHX | 1 | 3421 | 7/7 | 1.00 | 0.21 | 84,84,85,85 | 0 |
| 87 | ZN | AN | 500 | 1/1 | 1.00 | 0.15 | 43,43,43,43 | 0 |
| 85 | MG | AR | 4208 | 1/1 | 1.00 | 0.17 | 73,73,73,73 | 0 |
| 87 | ZN | d6 | 103 | 1/1 | 1.00 | 0.12 | 68,68,68,68 | 0 |
| 85 | MG | AR | 3912 | 1/1 | 1.00 | 0.58 | 29,29,29,29 | 0 |
| 87 | ZN | d9 | 103 | 1/1 | 1.00 | 0.12 | 81,81,81,81 | 0 |
| 85 | MG | 1 | 4099 | 1/1 | 1.00 | 0.17 | 68,68,68,68 | 0 |

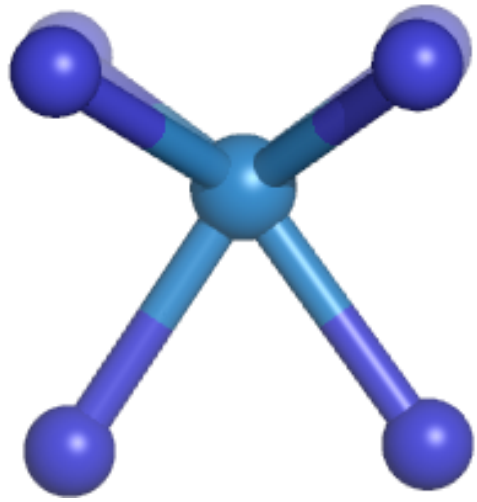
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around OHX AR 3740:**

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

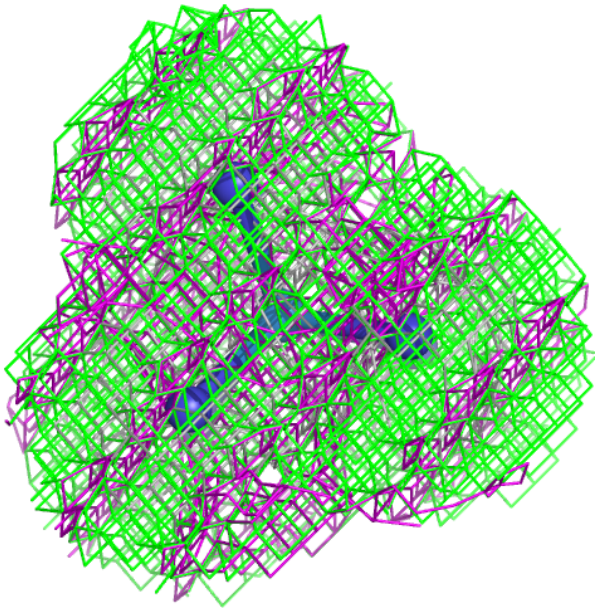


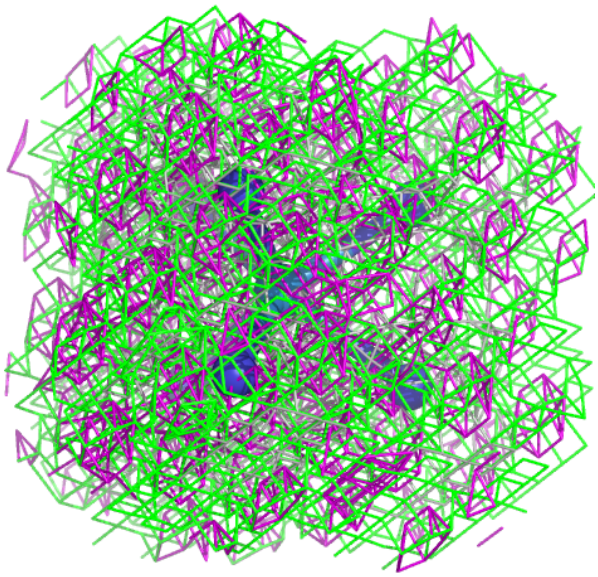


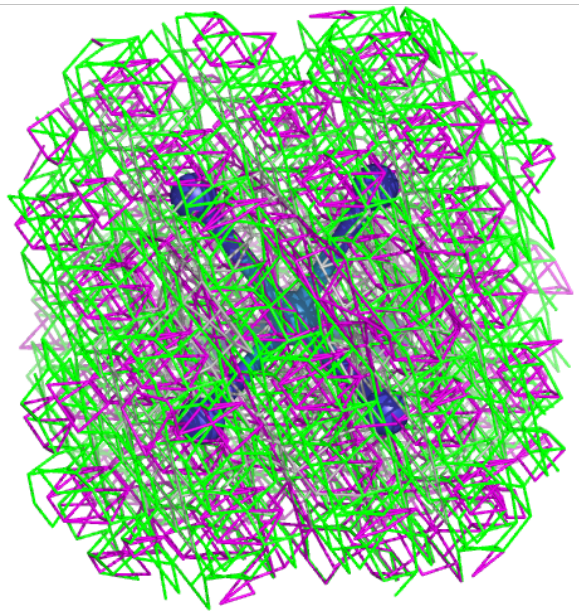


**Electron density around OHX 1 3673:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

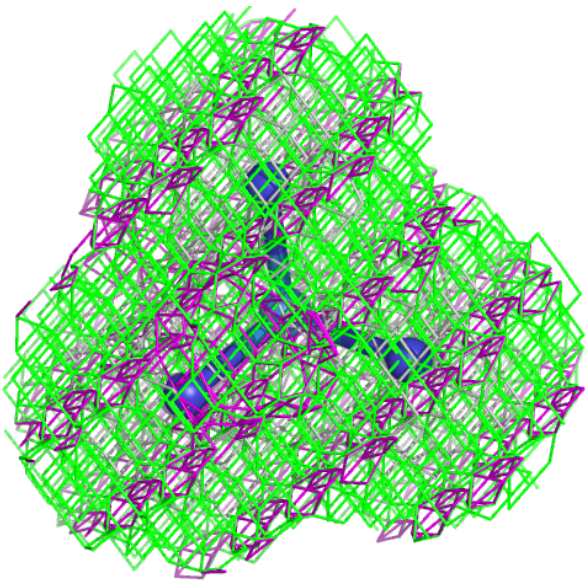


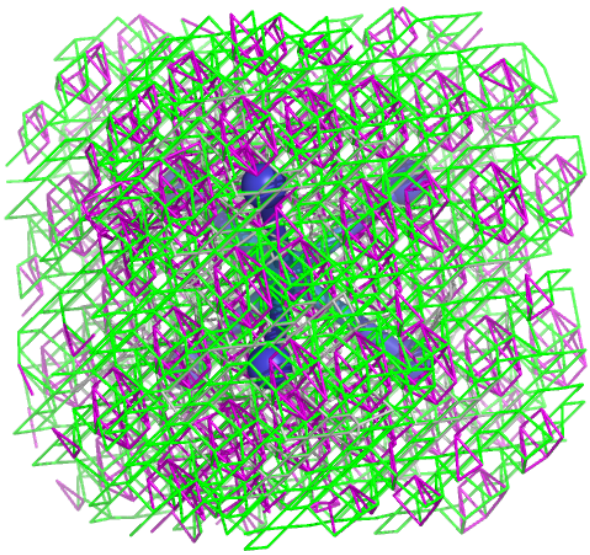


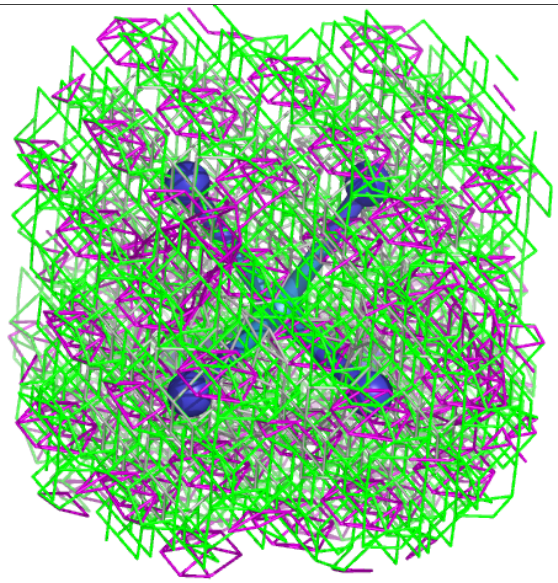


**Electron density around OHX 1 3718:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

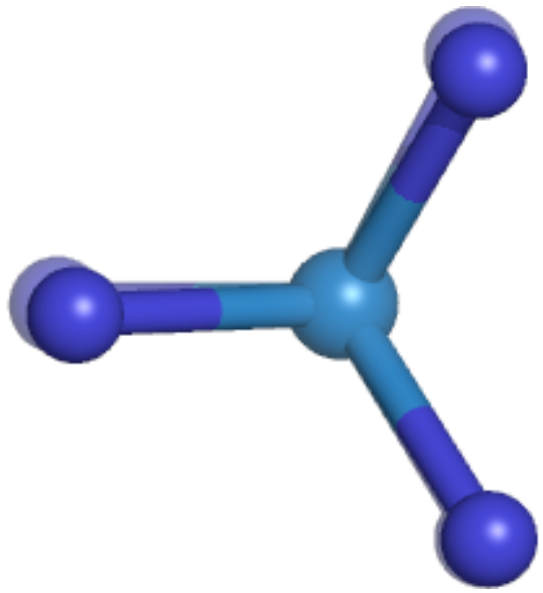


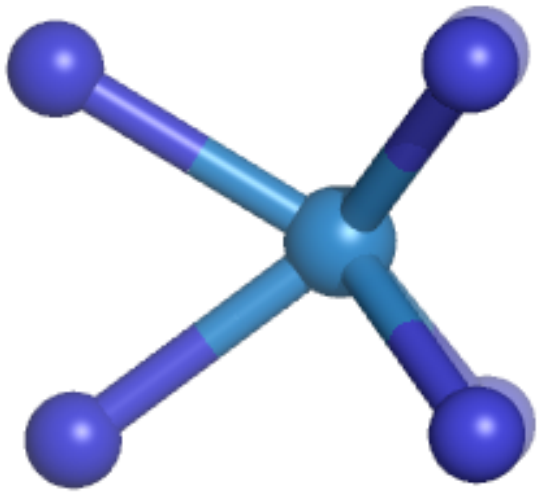


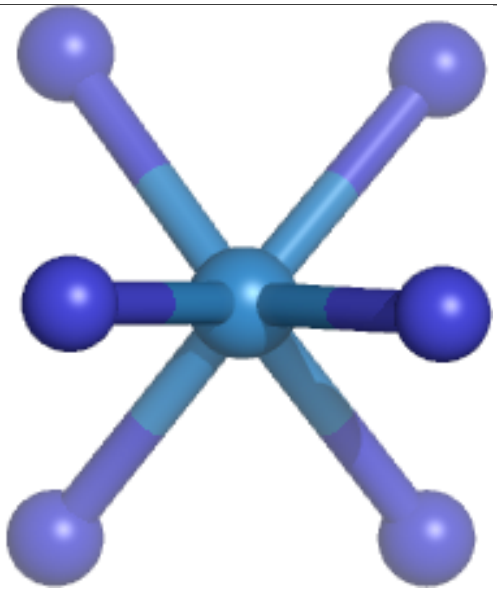


**Electron density around OHX A 2039:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

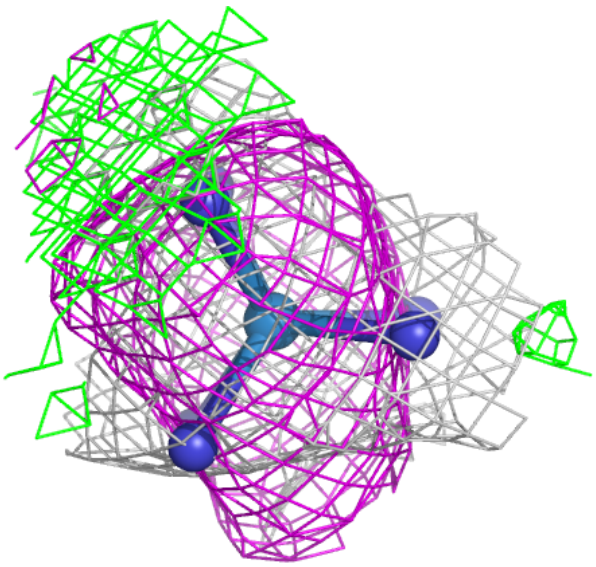


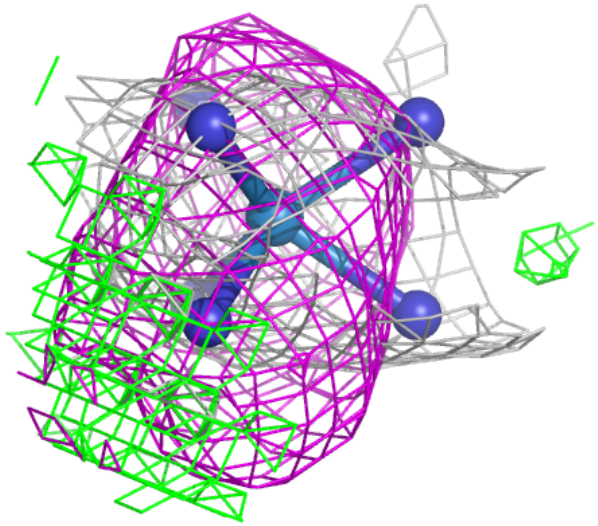


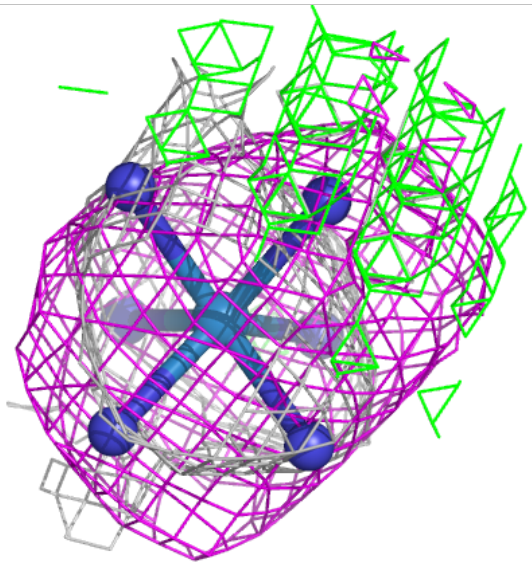


**Electron density around OHX sR 2040:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

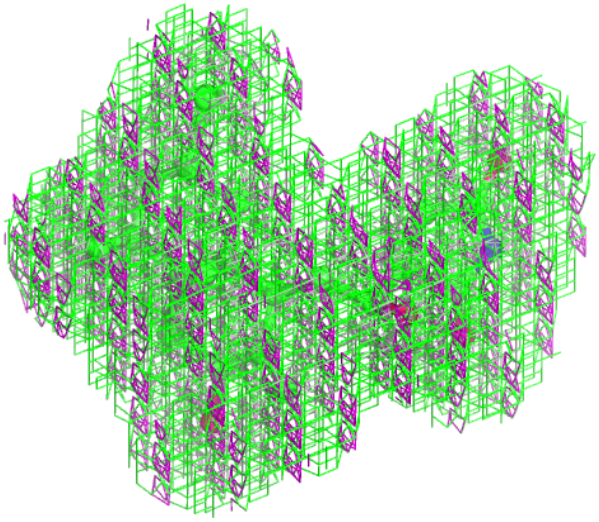


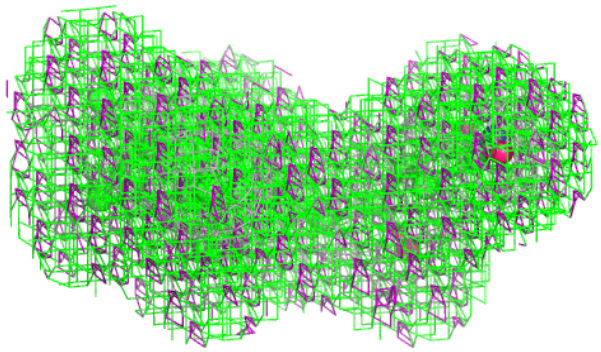


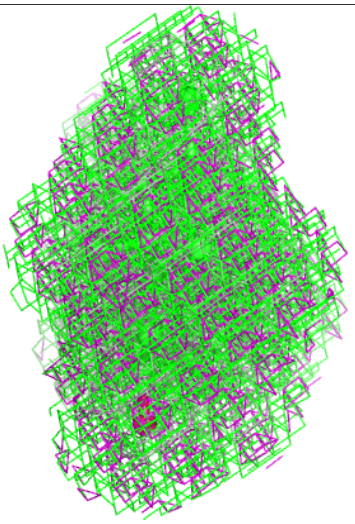


**Electron density around 7AL 1 4210:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

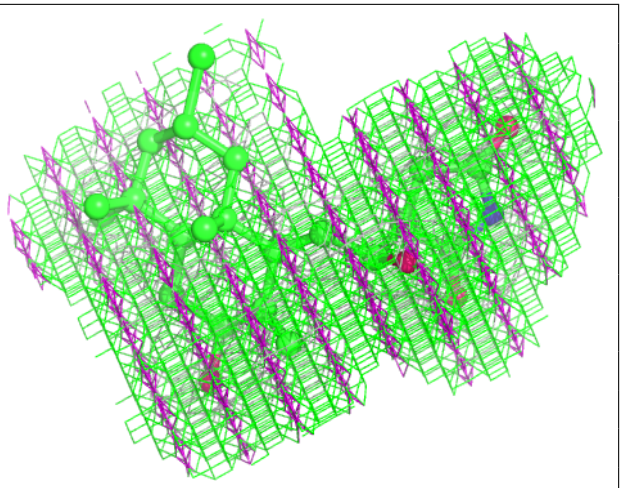


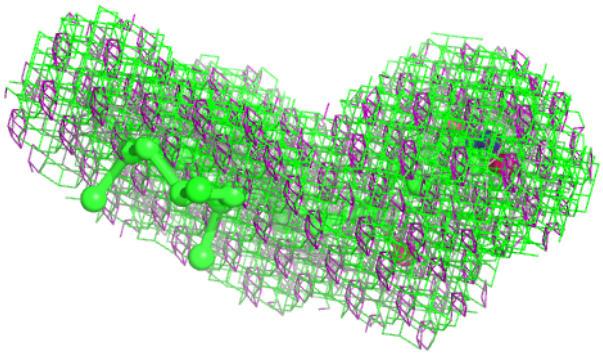


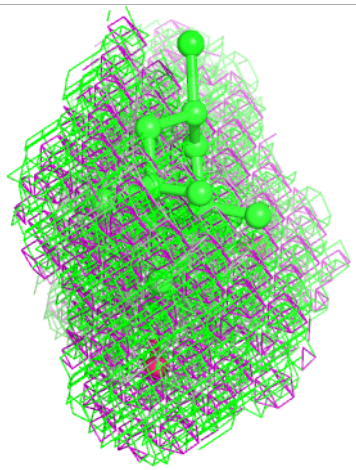


**Electron density around 7AL AR 4246:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)







## 6.5 Other polymers (i)

There are no such residues in this entry.