



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 23, 2018 – 01:04 AM EST

PDB ID : 5MEI
Title : Crystal structure of Agelastatin A bound to the 80S ribosome
Authors : McClary, B.; Zinshteyn, B.; Meyer, M.; Jouanneau, M.; Pellegrino, S.;
Yusupova, G.; Schuller, A.; Reyes, J.C.P.; Lu, J.; Luo, C.; Dang, Y.; Romo,
D.; Yusupov, M.; Green, R.; Liu, J.O.
Deposited on : 2016-11-15
Resolution : 3.50 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

| | | |
|--------------------------------|---|--|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7.2 (RC1), CSD as538be (2017) |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | rb-20030736 |
| Percentile statistics | : | 20161228.v01 (using entries in the PDB archive December 28th 2016) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | rb-20030736 |

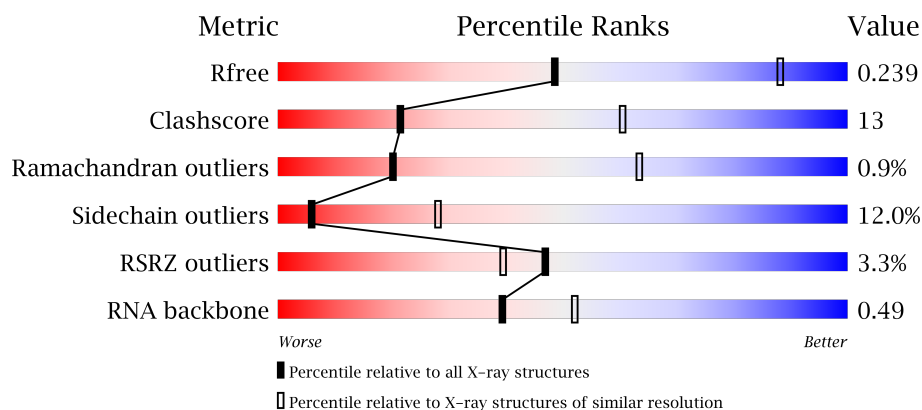
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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.











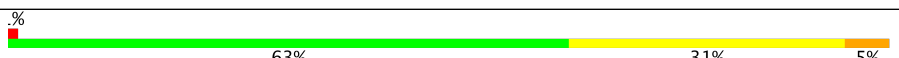
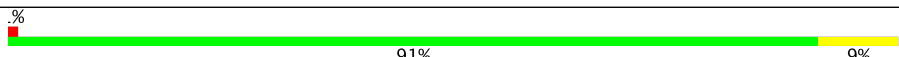
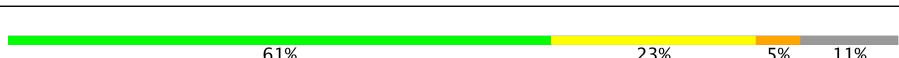
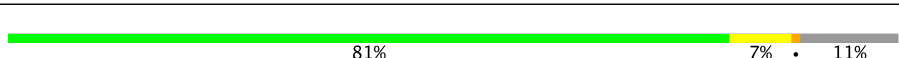
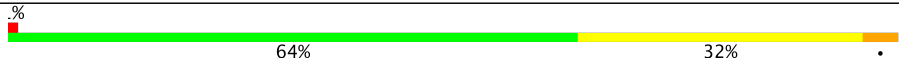
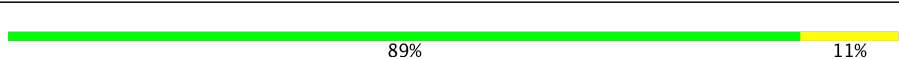

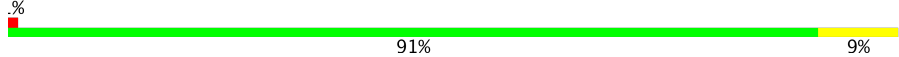





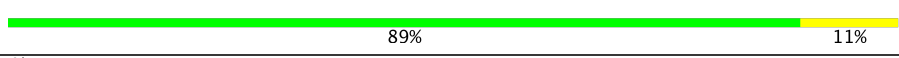

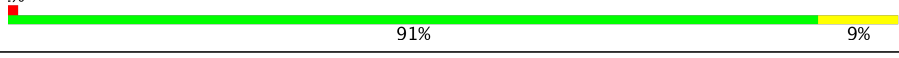
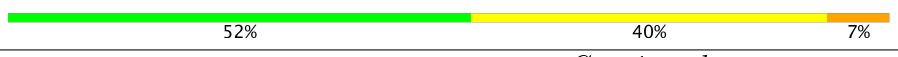
| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 100719 | 1195 (3.60-3.40) |
| Clashscore | 112137 | 1322 (3.60-3.40) |
| Ramachandran outliers | 110173 | 1283 (3.60-3.40) |
| Sidechain outliers | 110143 | 1284 (3.60-3.40) |
| RSRZ outliers | 101464 | 1226 (3.60-3.40) |
| RNA backbone | 2435 | 1024 (4.10-2.86) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | 1 | 3396 | <div> <div>2%</div> <div> <div></div> <div>45%</div> <div>37%</div> <div>10%</div> <div>7%</div> </div> </div> |
| 1 | AR | 3396 | <div> <div>2%</div> <div> <div></div> <div>42%</div> <div>39%</div> <div>11%</div> <div>7%</div> </div> </div> |
| 2 | 3 | 121 | <div> <div></div> <div> <div>59%</div> <div>36%</div> <div>6%</div> </div> </div> |
| 2 | AS | 121 | <div> <div>0%</div> <div> <div></div> <div>50%</div> <div>46%</div> <div>0%</div> </div> </div> |










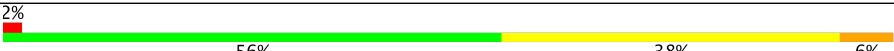
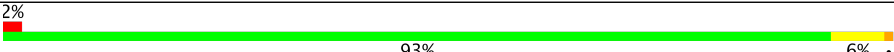








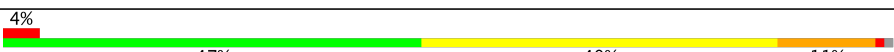
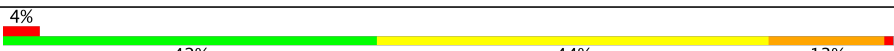

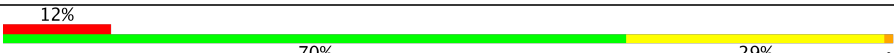
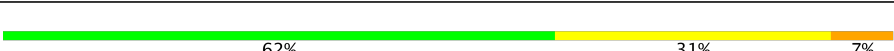

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 3 | 4 | 158 |  |
| 3 | AT | 158 |  |
| 4 | CD | 252 |  |
| 4 | j | 252 |  |
| 5 | CE | 386 |  |
| 5 | k | 386 |  |
| 6 | CF | 361 |  |
| 6 | l | 361 |  |
| 7 | CG | 296 |  |
| 7 | m | 296 |  |
| 8 | CH | 175 |  |
| 8 | n | 175 |  |
| 9 | CI | 222 |  |
| 9 | o | 222 |  |
| 10 | CJ | 233 |  |
| 10 | p | 233 |  |
| 11 | CK | 191 |  |
| 11 | q | 191 |  |
| 12 | CL | 220 |  |
| 12 | r | 220 |  |
| 13 | CM | 169 |  |
| 13 | s | 169 |  |
| 14 | CN | 193 |  |
| 14 | t | 193 |  |
| 15 | CO | 136 |  |

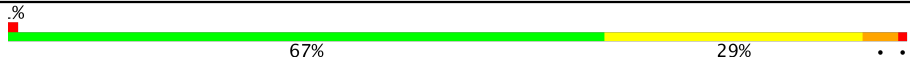

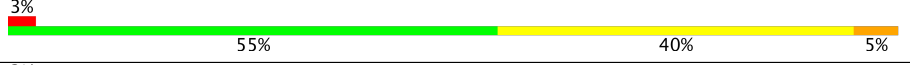

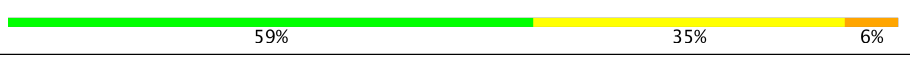
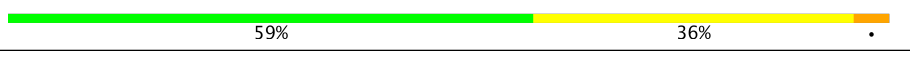
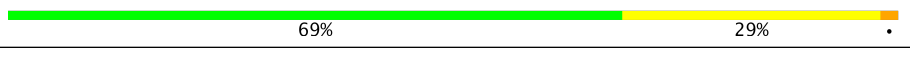

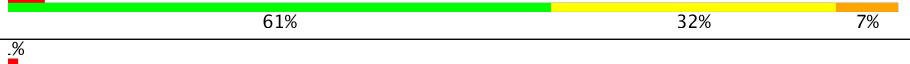


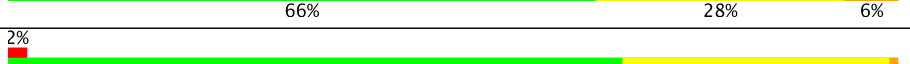
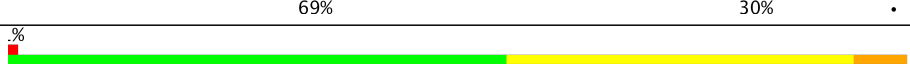
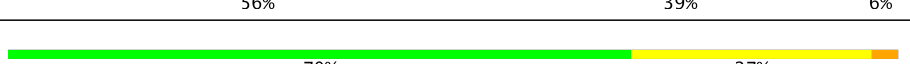

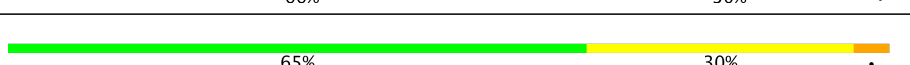
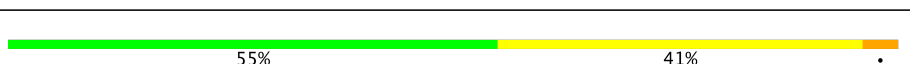
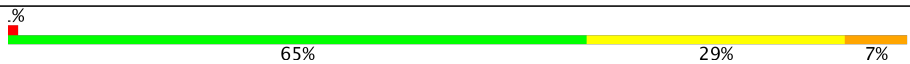
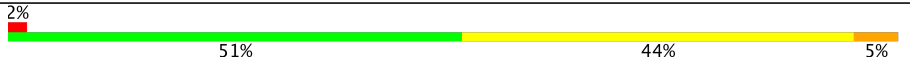


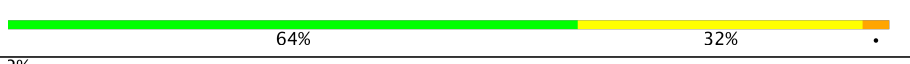
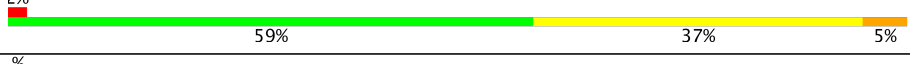


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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 15 | u | 136 |  |
| 16 | CP | 203 |  |
| 16 | v | 203 |  |
| 17 | CQ | 197 |  |
| 17 | w | 197 |  |
| 18 | CR | 183 |  |
| 18 | x | 183 |  |
| 19 | CS | 185 |  |
| 19 | y | 185 |  |
| 20 | CT | 188 |  |
| 20 | z | 188 |  |
| 21 | 0 | 172 |  |
| 21 | CU | 172 |  |
| 22 | 2 | 159 |  |
| 22 | CV | 159 |  |
| 23 | 5 | 100 |  |
| 23 | CW | 100 |  |
| 24 | CX | 136 |  |
| 24 | 12 | 136 |  |
| 25 | 6 | 1800 |  |
| 25 | A | 1800 |  |
| 26 | 7 | 98 |  |
| 26 | CY | 98 |  |
| 27 | 8 | 121 |  |
| 27 | CZ | 121 |  |



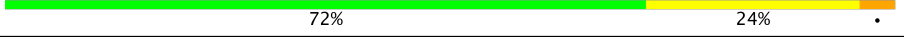

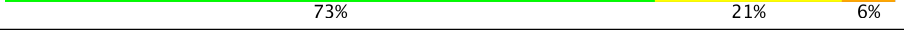
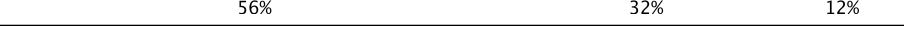
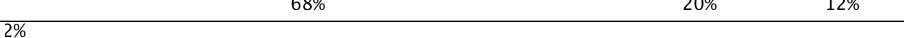
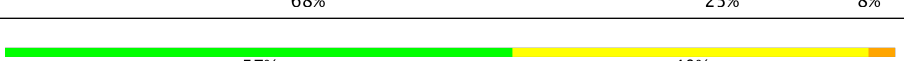



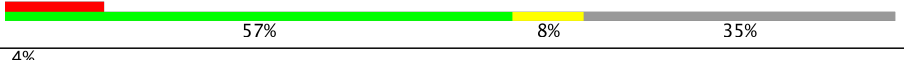
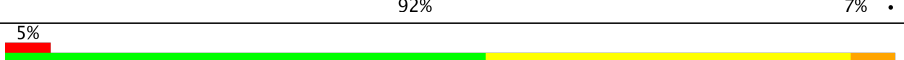



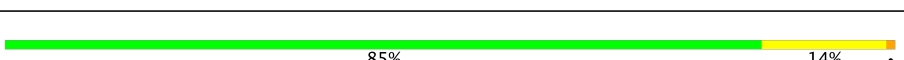
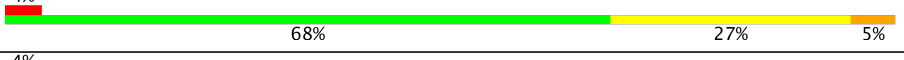
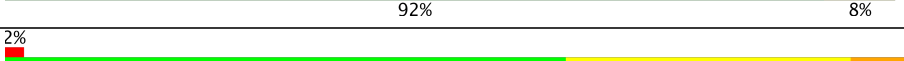

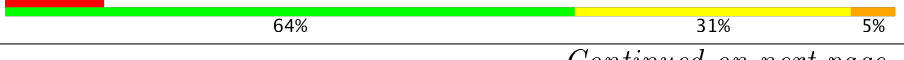


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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 28 | 9 | 126 |  |
| 28 | DA | 126 |  |
| 29 | AA | 135 |  |
| 29 | DB | 135 |  |
| 30 | AB | 148 |  |
| 30 | DC | 148 |  |
| 31 | AC | 58 |  |
| 31 | DD | 58 |  |
| 32 | AD | 97 |  |
| 32 | DE | 97 |  |
| 33 | AE | 109 |  |
| 33 | DF | 109 |  |
| 34 | AF | 127 |  |
| 34 | DG | 127 |  |
| 35 | AG | 106 |  |
| 35 | DH | 106 |  |
| 36 | AH | 112 |  |
| 36 | DI | 112 |  |
| 37 | AI | 119 |  |
| 37 | DJ | 119 |  |
| 38 | AJ | 99 |  |
| 38 | DK | 99 |  |
| 39 | AK | 87 |  |
| 39 | DL | 87 |  |
| 40 | AL | 77 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 40 | DM | 77 |  |
| 41 | AM | 50 |  |
| 41 | DN | 50 |  |
| 42 | AN | 52 |  |
| 42 | DO | 52 |  |
| 43 | AO | 25 |  |
| 43 | DP | 25 |  |
| 44 | AP | 105 |  |
| 44 | DQ | 105 |  |
| 45 | AQ | 91 |  |
| 45 | DR | 91 |  |
| 46 | i | 168 |  |
| 47 | p0 | 220 |  |
| 48 | sM | 104 |  |
| 49 | B | 206 |  |
| 49 | s0 | 206 |  |
| 50 | C | 216 |  |
| 50 | s1 | 216 |  |
| 51 | D | 217 |  |
| 51 | s2 | 217 |  |
| 52 | E | 223 |  |
| 52 | s3 | 223 |  |
| 53 | F | 260 |  |
| 53 | s4 | 260 | |
| 54 | G | 206 | |

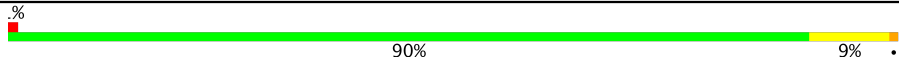
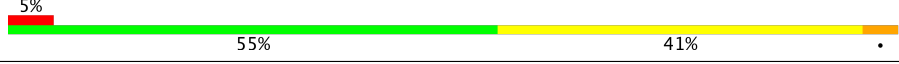
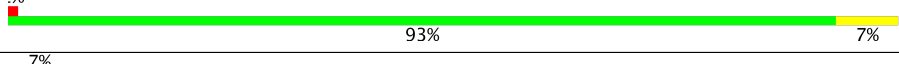


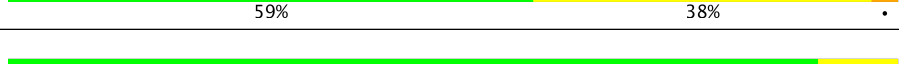
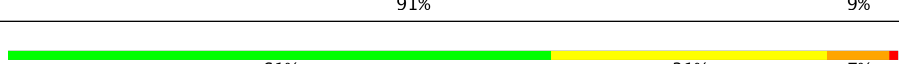
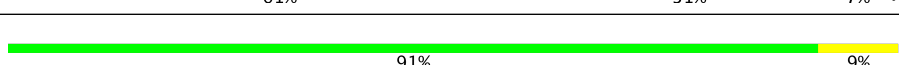

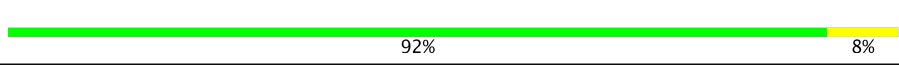

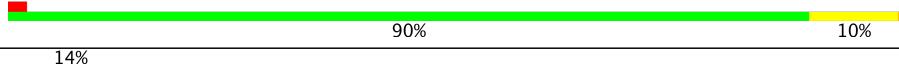
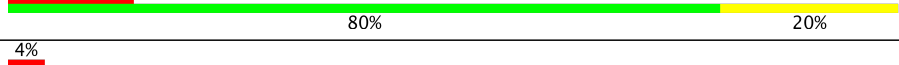
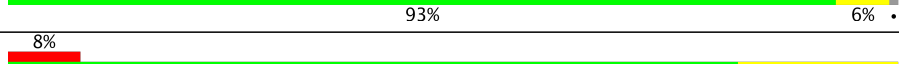
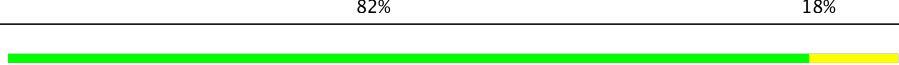
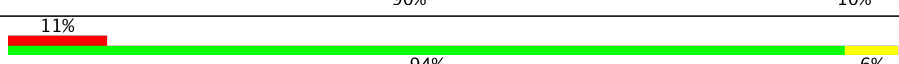
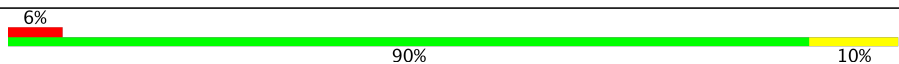
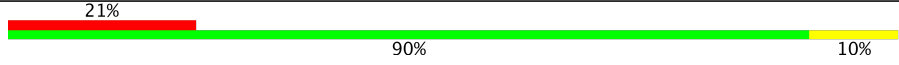
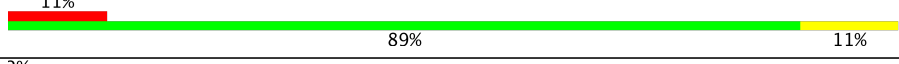

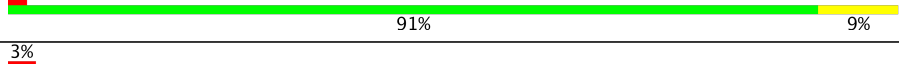




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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 54 | s5 | 206 | |
| 55 | H | 226 | |
| 55 | s6 | 226 | |
| 56 | I | 186 | |
| 56 | s7 | 186 | |
| 57 | J | 199 | |
| 57 | s8 | 199 | |
| 58 | K | 185 | |
| 58 | s9 | 185 | |
| 59 | L | 105 | |
| 59 | c0 | 105 | |
| 60 | M | 155 | |
| 60 | c1 | 155 | |
| 61 | N | 124 | |
| 61 | c2 | 124 | |
| 62 | O | 150 | |
| 62 | c3 | 150 | |
| 63 | P | 128 | |
| 63 | c4 | 128 | |
| 64 | Q | 141 | |
| 64 | c5 | 141 | |
| 65 | R | 142 | |
| 65 | c6 | 142 | |
| 66 | S | 125 | |
| 67 | T | 145 | |

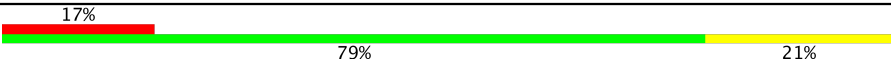
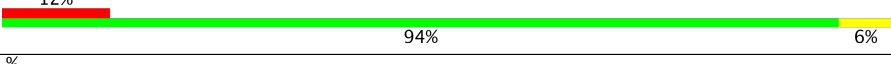
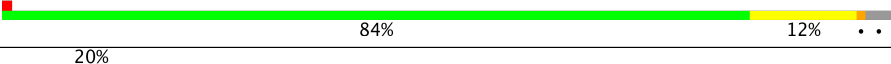
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 67 | c8 | 145 |  |
| 68 | U | 143 |  |
| 68 | c9 | 143 |  |
| 69 | V | 110 |  |
| 69 | d0 | 110 |  |
| 70 | W | 87 |  |
| 70 | d1 | 87 |  |
| 71 | X | 129 |  |
| 71 | d2 | 129 |  |
| 72 | Y | 144 |  |
| 72 | d3 | 144 |  |
| 73 | Z | 134 |  |
| 73 | d4 | 134 |  |
| 74 | a | 70 |  |
| 74 | d5 | 70 |  |
| 75 | b | 97 |  |
| 75 | d6 | 97 |  |
| 76 | c | 81 |  |
| 76 | d7 | 81 |  |
| 77 | d | 63 |  |
| 77 | d8 | 63 |  |
| 78 | d9 | 53 |  |
| 78 | e | 53 |  |
| 79 | e0 | 62 |  |
| 79 | f | 62 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 80 | g | 71 |  |
| 81 | h | 318 |  |
| 81 | sR | 318 |  |
| 82 | c7 | 121 |  |
| 83 | e1 | 51 |  |

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 | 3401 | - | - | - | X |
| 84 | OHX | 1 | 3402 | - | - | - | X |
| 84 | OHX | 1 | 3403 | - | - | - | X |
| 84 | OHX | 1 | 3405 | - | - | - | X |
| 84 | OHX | 1 | 3406 | - | - | X | X |
| 84 | OHX | 1 | 3407 | - | - | - | X |
| 84 | OHX | 1 | 3409 | - | - | - | X |
| 84 | OHX | 1 | 3411 | - | - | - | X |
| 84 | OHX | 1 | 3412 | - | - | - | X |
| 84 | OHX | 1 | 3417 | - | - | - | X |
| 84 | OHX | 1 | 3420 | - | - | - | X |
| 84 | OHX | 1 | 3441 | - | - | - | X |
| 84 | OHX | 1 | 3448 | - | - | - | X |
| 84 | OHX | 1 | 3471 | - | - | X | - |
| 84 | OHX | 1 | 3491 | - | - | - | X |
| 84 | OHX | 1 | 3496 | - | - | X | - |
| 84 | OHX | 1 | 3516 | - | - | - | X |
| 84 | OHX | 1 | 3529 | - | - | - | X |
| 84 | OHX | 1 | 3537 | - | - | - | X |
| 84 | OHX | 1 | 3542 | - | - | - | X |
| 84 | OHX | 1 | 3544 | - | - | - | X |
| 84 | OHX | 1 | 3546 | - | - | - | X |
| 84 | OHX | 1 | 3554 | - | - | - | X |
| 84 | OHX | 1 | 3566 | - | - | - | X |
| 84 | OHX | 1 | 3572 | - | - | - | X |
| 84 | OHX | 1 | 3575 | - | - | - | X |
| 84 | OHX | 1 | 3578 | - | - | - | X |
| 84 | OHX | 1 | 3581 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 84 | OHX | 1 | 3583 | - | - | - | X |
| 84 | OHX | 1 | 3584 | - | - | - | X |
| 84 | OHX | 1 | 3585 | - | - | - | X |
| 84 | OHX | 1 | 3587 | - | - | - | X |
| 84 | OHX | 1 | 3592 | - | - | - | X |
| 84 | OHX | 1 | 3594 | - | - | X | X |
| 84 | OHX | 1 | 3595 | - | - | - | X |
| 84 | OHX | 1 | 3596 | - | - | - | X |
| 84 | OHX | 1 | 3601 | - | - | - | X |
| 84 | OHX | 1 | 3602 | - | - | - | X |
| 84 | OHX | 1 | 3603 | - | - | - | X |
| 84 | OHX | 1 | 3605 | - | - | - | X |
| 84 | OHX | 1 | 3607 | - | - | - | X |
| 84 | OHX | 1 | 3608 | - | - | - | X |
| 84 | OHX | 1 | 3612 | - | - | - | X |
| 84 | OHX | 1 | 3613 | - | - | - | X |
| 84 | OHX | 1 | 3617 | - | - | - | X |
| 84 | OHX | 1 | 3620 | - | - | - | X |
| 84 | OHX | 1 | 3632 | - | - | - | X |
| 84 | OHX | 1 | 3635 | - | - | - | X |
| 84 | OHX | 1 | 3636 | - | - | - | X |
| 84 | OHX | 1 | 3644 | - | - | - | X |
| 84 | OHX | 1 | 3646 | - | - | - | X |
| 84 | OHX | 1 | 3647 | - | - | - | X |
| 84 | OHX | 1 | 3650 | - | - | - | X |
| 84 | OHX | 1 | 3651 | - | - | - | X |
| 84 | OHX | 1 | 3654 | - | - | - | X |
| 84 | OHX | 1 | 3657 | - | - | - | X |
| 84 | OHX | 1 | 3658 | - | - | - | X |
| 84 | OHX | 1 | 3660 | - | - | - | X |
| 84 | OHX | 1 | 3662 | - | - | - | X |
| 84 | OHX | 1 | 3664 | - | - | - | X |
| 84 | OHX | 1 | 3666 | - | - | - | X |
| 84 | OHX | 1 | 3667 | - | - | - | X |
| 84 | OHX | 1 | 3668 | - | - | - | X |
| 84 | OHX | 1 | 3672 | - | - | - | X |
| 84 | OHX | 1 | 3675 | - | - | - | X |
| 84 | OHX | 1 | 3679 | - | - | - | X |
| 84 | OHX | 1 | 3680 | - | - | - | X |
| 84 | OHX | 1 | 3681 | - | - | - | X |
| 84 | OHX | 1 | 3682 | - | - | - | X |
| 84 | OHX | 1 | 3684 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 84 | OHX | 1 | 3686 | - | - | - | X |
| 84 | OHX | 1 | 3687 | - | - | - | X |
| 84 | OHX | 1 | 3692 | - | - | - | X |
| 84 | OHX | 1 | 3693 | - | - | - | X |
| 84 | OHX | 1 | 3698 | - | - | - | X |
| 84 | OHX | 1 | 3700 | - | - | - | X |
| 84 | OHX | 1 | 3701 | - | - | - | X |
| 84 | OHX | 1 | 3702 | - | - | X | X |
| 84 | OHX | 1 | 3705 | - | - | - | X |
| 84 | OHX | 1 | 3708 | - | - | - | X |
| 84 | OHX | 1 | 3710 | - | - | - | X |
| 84 | OHX | 1 | 3712 | - | - | - | X |
| 84 | OHX | 1 | 3715 | - | - | - | X |
| 84 | OHX | 1 | 3717 | - | - | - | X |
| 84 | OHX | 1 | 3718 | - | - | - | X |
| 84 | OHX | 1 | 3721 | - | - | - | X |
| 84 | OHX | 1 | 3722 | - | - | - | X |
| 84 | OHX | 1 | 3727 | - | - | - | X |
| 84 | OHX | 1 | 3728 | - | - | - | X |
| 84 | OHX | 1 | 3729 | - | - | - | X |
| 84 | OHX | 1 | 3731 | - | - | - | X |
| 84 | OHX | 4 | 205 | - | - | - | X |
| 84 | OHX | 4 | 206 | - | - | - | X |
| 84 | OHX | 4 | 208 | - | - | - | X |
| 84 | OHX | 4 | 209 | - | - | - | X |
| 84 | OHX | 4 | 210 | - | - | - | X |
| 84 | OHX | 6 | 1901 | - | - | - | X |
| 84 | OHX | 6 | 1902 | - | - | - | X |
| 84 | OHX | 6 | 1903 | - | - | - | X |
| 84 | OHX | 6 | 1907 | - | - | - | X |
| 84 | OHX | 6 | 1958 | - | - | - | X |
| 84 | OHX | 6 | 1965 | - | - | - | X |
| 84 | OHX | 6 | 1971 | - | - | - | X |
| 84 | OHX | 6 | 1972 | - | - | - | X |
| 84 | OHX | 6 | 1979 | - | - | - | X |
| 84 | OHX | 6 | 1980 | - | - | - | X |
| 84 | OHX | 6 | 1981 | - | - | - | X |
| 84 | OHX | 6 | 1982 | - | - | - | X |
| 84 | OHX | 6 | 1983 | - | - | - | X |
| 84 | OHX | 6 | 1989 | - | - | - | X |
| 84 | OHX | 6 | 1991 | - | - | - | X |
| 84 | OHX | 6 | 1996 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 84 | OHX | 6 | 1997 | - | - | - | X |
| 84 | OHX | 6 | 1998 | - | - | - | X |
| 84 | OHX | 6 | 2005 | - | - | - | X |
| 84 | OHX | 6 | 2006 | - | - | - | X |
| 84 | OHX | 6 | 2015 | - | - | - | X |
| 84 | OHX | 6 | 2016 | - | - | - | X |
| 84 | OHX | 6 | 2019 | - | - | - | X |
| 84 | OHX | 6 | 2023 | - | - | - | X |
| 84 | OHX | 6 | 2027 | - | - | - | X |
| 84 | OHX | 6 | 2030 | - | - | - | X |
| 84 | OHX | 6 | 2032 | - | - | - | X |
| 84 | OHX | 6 | 2033 | - | - | - | X |
| 84 | OHX | 6 | 2035 | - | - | - | X |
| 84 | OHX | 6 | 2036 | - | - | - | X |
| 84 | OHX | 6 | 2037 | - | - | - | X |
| 84 | OHX | 6 | 2038 | - | - | - | X |
| 84 | OHX | 6 | 2040 | - | - | - | X |
| 84 | OHX | 6 | 2042 | - | - | - | X |
| 84 | OHX | 6 | 2045 | - | - | - | X |
| 84 | OHX | 6 | 2050 | - | - | - | X |
| 84 | OHX | A | 1903 | - | - | - | X |
| 84 | OHX | A | 1947 | - | - | - | X |
| 84 | OHX | A | 1954 | - | - | X | X |
| 84 | OHX | A | 1964 | - | - | - | X |
| 84 | OHX | A | 1970 | - | - | - | X |
| 84 | OHX | A | 1980 | - | - | - | X |
| 84 | OHX | A | 1982 | - | - | - | X |
| 84 | OHX | A | 1985 | - | - | - | X |
| 84 | OHX | A | 1986 | - | - | - | X |
| 84 | OHX | A | 1990 | - | - | - | X |
| 84 | OHX | A | 1993 | - | - | - | X |
| 84 | OHX | A | 1994 | - | - | - | X |
| 84 | OHX | A | 1996 | - | - | - | X |
| 84 | OHX | A | 1997 | - | - | - | X |
| 84 | OHX | A | 2003 | - | - | - | X |
| 84 | OHX | A | 2006 | - | - | - | X |
| 84 | OHX | A | 2009 | - | - | - | X |
| 84 | OHX | A | 2013 | - | - | - | X |
| 84 | OHX | A | 2014 | - | - | - | X |
| 84 | OHX | A | 2017 | - | - | - | X |
| 84 | OHX | A | 2021 | - | - | - | X |
| 84 | OHX | A | 2024 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 84 | OHX | A | 2026 | - | - | - | X |
| 84 | OHX | A | 2031 | - | - | - | X |
| 84 | OHX | A | 2035 | - | - | - | X |
| 84 | OHX | A | 2038 | - | - | - | X |
| 84 | OHX | AE | 201 | - | - | X | - |
| 84 | OHX | AR | 3402 | - | - | - | X |
| 84 | OHX | AR | 3403 | - | - | - | X |
| 84 | OHX | AR | 3406 | - | - | - | X |
| 84 | OHX | AR | 3407 | - | - | - | X |
| 84 | OHX | AR | 3409 | - | - | - | X |
| 84 | OHX | AR | 3415 | - | - | - | X |
| 84 | OHX | AR | 3443 | - | - | X | - |
| 84 | OHX | AR | 3485 | - | - | - | X |
| 84 | OHX | AR | 3494 | - | - | - | X |
| 84 | OHX | AR | 3497 | - | - | - | X |
| 84 | OHX | AR | 3524 | - | - | - | X |
| 84 | OHX | AR | 3526 | - | - | - | X |
| 84 | OHX | AR | 3545 | - | - | - | X |
| 84 | OHX | AR | 3554 | - | - | - | X |
| 84 | OHX | AR | 3572 | - | - | - | X |
| 84 | OHX | AR | 3575 | - | - | - | X |
| 84 | OHX | AR | 3577 | - | - | - | X |
| 84 | OHX | AR | 3578 | - | - | - | X |
| 84 | OHX | AR | 3581 | - | - | - | X |
| 84 | OHX | AR | 3584 | - | - | - | X |
| 84 | OHX | AR | 3587 | - | - | - | X |
| 84 | OHX | AR | 3589 | - | - | - | X |
| 84 | OHX | AR | 3591 | - | - | - | X |
| 84 | OHX | AR | 3594 | - | - | - | X |
| 84 | OHX | AR | 3597 | - | - | - | X |
| 84 | OHX | AR | 3601 | - | - | - | X |
| 84 | OHX | AR | 3602 | - | - | - | X |
| 84 | OHX | AR | 3604 | - | - | X | - |
| 84 | OHX | AR | 3606 | - | - | - | X |
| 84 | OHX | AR | 3608 | - | - | - | X |
| 84 | OHX | AR | 3609 | - | - | - | X |
| 84 | OHX | AR | 3611 | - | - | - | X |
| 84 | OHX | AR | 3613 | - | - | - | X |
| 84 | OHX | AR | 3617 | - | - | - | X |
| 84 | OHX | AR | 3620 | - | - | - | X |
| 84 | OHX | AR | 3626 | - | - | - | X |
| 84 | OHX | AR | 3633 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 84 | OHX | AR | 3635 | - | - | - | X |
| 84 | OHX | AR | 3638 | - | - | - | X |
| 84 | OHX | AR | 3640 | - | - | - | X |
| 84 | OHX | AR | 3641 | - | - | - | X |
| 84 | OHX | AR | 3643 | - | - | - | X |
| 84 | OHX | AR | 3644 | - | - | - | X |
| 84 | OHX | AR | 3645 | - | - | - | X |
| 84 | OHX | AR | 3646 | - | - | - | X |
| 84 | OHX | AR | 3648 | - | - | - | X |
| 84 | OHX | AR | 3650 | - | - | - | X |
| 84 | OHX | AR | 3652 | - | - | - | X |
| 84 | OHX | AR | 3653 | - | - | - | X |
| 84 | OHX | AR | 3655 | - | - | - | X |
| 84 | OHX | AR | 3659 | - | - | - | X |
| 84 | OHX | AR | 3660 | - | - | - | X |
| 84 | OHX | AR | 3661 | - | - | - | X |
| 84 | OHX | AR | 3663 | - | - | - | X |
| 84 | OHX | AR | 3668 | - | - | - | X |
| 84 | OHX | AR | 3671 | - | - | - | X |
| 84 | OHX | AR | 3672 | - | - | - | X |
| 84 | OHX | AR | 3674 | - | - | - | X |
| 84 | OHX | AR | 3677 | - | - | - | X |
| 84 | OHX | AR | 3683 | - | - | - | X |
| 84 | OHX | AR | 3684 | - | - | - | X |
| 84 | OHX | AR | 3685 | - | - | - | X |
| 84 | OHX | AR | 3686 | - | - | - | X |
| 84 | OHX | AR | 3689 | - | - | - | X |
| 84 | OHX | AR | 3690 | - | - | - | X |
| 84 | OHX | AR | 3691 | - | - | - | X |
| 84 | OHX | AR | 3692 | - | - | - | X |
| 84 | OHX | AR | 3694 | - | - | - | X |
| 84 | OHX | AR | 3695 | - | - | - | X |
| 84 | OHX | AR | 3696 | - | - | - | X |
| 84 | OHX | AR | 3699 | - | - | - | X |
| 84 | OHX | AR | 3700 | - | - | - | X |
| 84 | OHX | AR | 3701 | - | - | - | X |
| 84 | OHX | AR | 3703 | - | - | - | X |
| 84 | OHX | AR | 3705 | - | - | - | X |
| 84 | OHX | AR | 3712 | - | - | - | X |
| 84 | OHX | AR | 3714 | - | - | - | X |
| 84 | OHX | AR | 3715 | - | - | - | X |
| 84 | OHX | AR | 3717 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 84 | OHX | AR | 3721 | - | - | - | X |
| 84 | OHX | AR | 3728 | - | - | - | X |
| 84 | OHX | AR | 3729 | - | - | - | X |
| 84 | OHX | AR | 3730 | - | - | - | X |
| 84 | OHX | AR | 3731 | - | - | X | X |
| 84 | OHX | AR | 3734 | - | - | - | X |
| 84 | OHX | AR | 3739 | - | - | - | X |
| 84 | OHX | AS | 209 | - | - | - | X |
| 84 | OHX | AS | 210 | - | - | - | X |
| 84 | OHX | AT | 202 | - | - | - | X |
| 84 | OHX | AT | 203 | - | - | - | X |
| 84 | OHX | AT | 211 | - | - | - | X |
| 84 | OHX | AT | 215 | - | - | - | X |
| 84 | OHX | AT | 218 | - | - | - | X |
| 84 | OHX | AT | 219 | - | - | - | X |
| 84 | OHX | CE | 403 | - | - | - | X |
| 84 | OHX | CG | 302 | - | - | X | - |
| 84 | OHX | CG | 303 | - | - | - | X |
| 84 | OHX | DI | 201 | - | - | - | X |
| 84 | OHX | DL | 102 | - | - | - | X |
| 84 | OHX | x | 201 | - | - | - | X |
| 84 | OHX | y | 201 | - | - | - | X |
| 85 | MG | 1 | 3732 | - | - | - | X |
| 85 | MG | 1 | 3737 | - | - | - | X |
| 85 | MG | 1 | 3738 | - | - | - | X |
| 85 | MG | 1 | 3739 | - | - | - | X |
| 85 | MG | 1 | 3741 | - | - | - | X |
| 85 | MG | 1 | 3745 | - | - | - | X |
| 85 | MG | 1 | 3747 | - | - | - | X |
| 85 | MG | 1 | 3748 | - | - | - | X |
| 85 | MG | 1 | 3753 | - | - | - | X |
| 85 | MG | 1 | 3764 | - | - | - | X |
| 85 | MG | 1 | 3768 | - | - | - | X |
| 85 | MG | 1 | 3772 | - | - | - | X |
| 85 | MG | 1 | 3777 | - | - | - | X |
| 85 | MG | 1 | 3785 | - | - | - | X |
| 85 | MG | 1 | 3791 | - | - | - | X |
| 85 | MG | 1 | 3801 | - | - | - | X |
| 85 | MG | 1 | 3803 | - | - | - | X |
| 85 | MG | 1 | 3804 | - | - | - | X |
| 85 | MG | 1 | 3806 | - | - | - | X |
| 85 | MG | 1 | 3813 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 85 | MG | 1 | 3817 | - | - | - | X |
| 85 | MG | 1 | 3818 | - | - | - | X |
| 85 | MG | 1 | 3819 | - | - | - | X |
| 85 | MG | 1 | 3822 | - | - | - | X |
| 85 | MG | 1 | 3829 | - | - | - | X |
| 85 | MG | 1 | 3832 | - | - | - | X |
| 85 | MG | 1 | 3833 | - | - | - | X |
| 85 | MG | 1 | 3835 | - | - | - | X |
| 85 | MG | 1 | 3838 | - | - | - | X |
| 85 | MG | 1 | 3839 | - | - | - | X |
| 85 | MG | 1 | 3843 | - | - | - | X |
| 85 | MG | 1 | 3847 | - | - | - | X |
| 85 | MG | 1 | 3852 | - | - | - | X |
| 85 | MG | 1 | 3857 | - | - | - | X |
| 85 | MG | 1 | 3858 | - | - | - | X |
| 85 | MG | 1 | 3859 | - | - | - | X |
| 85 | MG | 1 | 3866 | - | - | - | X |
| 85 | MG | 1 | 3870 | - | - | - | X |
| 85 | MG | 1 | 3872 | - | - | - | X |
| 85 | MG | 1 | 3873 | - | - | - | X |
| 85 | MG | 1 | 3874 | - | - | - | X |
| 85 | MG | 1 | 3881 | - | - | - | X |
| 85 | MG | 1 | 3882 | - | - | - | X |
| 85 | MG | 1 | 3883 | - | - | - | X |
| 85 | MG | 1 | 3884 | - | - | - | X |
| 85 | MG | 1 | 3889 | - | - | - | X |
| 85 | MG | 1 | 3890 | - | - | - | X |
| 85 | MG | 1 | 3896 | - | - | - | X |
| 85 | MG | 1 | 3898 | - | - | - | X |
| 85 | MG | 1 | 3899 | - | - | - | X |
| 85 | MG | 1 | 3900 | - | - | - | X |
| 85 | MG | 1 | 3902 | - | - | - | X |
| 85 | MG | 1 | 3903 | - | - | - | X |
| 85 | MG | 1 | 3904 | - | - | - | X |
| 85 | MG | 1 | 3905 | - | - | - | X |
| 85 | MG | 1 | 3912 | - | - | - | X |
| 85 | MG | 1 | 3913 | - | - | - | X |
| 85 | MG | 1 | 3914 | - | - | - | X |
| 85 | MG | 1 | 3915 | - | - | - | X |
| 85 | MG | 1 | 3917 | - | - | - | X |
| 85 | MG | 1 | 3918 | - | - | - | X |
| 85 | MG | 1 | 3922 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 85 | MG | 1 | 3924 | - | - | - | X |
| 85 | MG | 1 | 3925 | - | - | - | X |
| 85 | MG | 1 | 3927 | - | - | - | X |
| 85 | MG | 1 | 3929 | - | - | - | X |
| 85 | MG | 1 | 3934 | - | - | - | X |
| 85 | MG | 1 | 3944 | - | - | - | X |
| 85 | MG | 1 | 3945 | - | - | - | X |
| 85 | MG | 1 | 3949 | - | - | - | X |
| 85 | MG | 1 | 3953 | - | - | - | X |
| 85 | MG | 1 | 3956 | - | - | - | X |
| 85 | MG | 1 | 3960 | - | - | - | X |
| 85 | MG | 1 | 3962 | - | - | - | X |
| 85 | MG | 1 | 3976 | - | - | - | X |
| 85 | MG | 1 | 3979 | - | - | - | X |
| 85 | MG | 1 | 3987 | - | - | - | X |
| 85 | MG | 1 | 3989 | - | - | - | X |
| 85 | MG | 1 | 3996 | - | - | - | X |
| 85 | MG | 1 | 4007 | - | - | - | X |
| 85 | MG | 1 | 4039 | - | - | - | X |
| 85 | MG | 1 | 4044 | - | - | - | X |
| 85 | MG | 1 | 4048 | - | - | - | X |
| 85 | MG | 1 | 4060 | - | - | - | X |
| 85 | MG | 1 | 4061 | - | - | - | X |
| 85 | MG | 1 | 4063 | - | - | - | X |
| 85 | MG | 1 | 4064 | - | - | - | X |
| 85 | MG | 1 | 4065 | - | - | - | X |
| 85 | MG | 1 | 4071 | - | - | - | X |
| 85 | MG | 1 | 4086 | - | - | - | X |
| 85 | MG | 1 | 4099 | - | - | - | X |
| 85 | MG | 1 | 4103 | - | - | - | X |
| 85 | MG | 1 | 4117 | - | - | - | X |
| 85 | MG | 1 | 4135 | - | - | - | X |
| 85 | MG | 1 | 4142 | - | - | - | X |
| 85 | MG | 1 | 4147 | - | - | - | X |
| 85 | MG | 1 | 4148 | - | - | - | X |
| 85 | MG | 1 | 4149 | - | - | - | X |
| 85 | MG | 1 | 4155 | - | - | - | X |
| 85 | MG | 1 | 4161 | - | - | - | X |
| 85 | MG | 1 | 4170 | - | - | - | X |
| 85 | MG | 1 | 4188 | - | - | - | X |
| 85 | MG | 1 | 4190 | - | - | - | X |
| 85 | MG | 1 | 4191 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 85 | MG | 1 | 4192 | - | - | - | X |
| 85 | MG | 1 | 4195 | - | - | - | X |
| 85 | MG | 1 | 4204 | - | - | - | X |
| 85 | MG | 1 | 4208 | - | - | - | X |
| 85 | MG | 1 | 4209 | - | - | - | X |
| 85 | MG | 1 | 4215 | - | - | - | X |
| 85 | MG | 1 | 4217 | - | - | - | X |
| 85 | MG | 1 | 4219 | - | - | - | X |
| 85 | MG | 1 | 4221 | - | - | - | X |
| 85 | MG | 4 | 217 | - | - | - | X |
| 85 | MG | 4 | 219 | - | - | - | X |
| 85 | MG | 6 | 2058 | - | - | - | X |
| 85 | MG | 6 | 2061 | - | - | - | X |
| 85 | MG | 6 | 2062 | - | - | - | X |
| 85 | MG | 6 | 2064 | - | - | - | X |
| 85 | MG | 6 | 2066 | - | - | - | X |
| 85 | MG | 6 | 2068 | - | - | - | X |
| 85 | MG | 6 | 2073 | - | - | - | X |
| 85 | MG | 6 | 2076 | - | - | - | X |
| 85 | MG | 6 | 2082 | - | - | - | X |
| 85 | MG | 6 | 2083 | - | - | - | X |
| 85 | MG | 6 | 2087 | - | - | - | X |
| 85 | MG | 6 | 2091 | - | - | - | X |
| 85 | MG | 6 | 2093 | - | - | - | X |
| 85 | MG | 6 | 2096 | - | - | - | X |
| 85 | MG | 6 | 2103 | - | - | - | X |
| 85 | MG | 6 | 2106 | - | - | - | X |
| 85 | MG | 6 | 2108 | - | - | - | X |
| 85 | MG | 6 | 2113 | - | - | - | X |
| 85 | MG | 6 | 2129 | - | - | - | X |
| 85 | MG | 6 | 2132 | - | - | - | X |
| 85 | MG | 6 | 2135 | - | - | - | X |
| 85 | MG | 6 | 2137 | - | - | - | X |
| 85 | MG | 6 | 2145 | - | - | - | X |
| 85 | MG | 6 | 2147 | - | - | - | X |
| 85 | MG | 6 | 2149 | - | - | - | X |
| 85 | MG | 6 | 2150 | - | - | - | X |
| 85 | MG | 6 | 2154 | - | - | - | X |
| 85 | MG | 6 | 2159 | - | - | - | X |
| 85 | MG | 6 | 2162 | - | - | - | X |
| 85 | MG | 6 | 2165 | - | - | - | X |
| 85 | MG | 6 | 2184 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 85 | MG | A | 2047 | - | - | - | X |
| 85 | MG | A | 2052 | - | - | - | X |
| 85 | MG | A | 2053 | - | - | - | X |
| 85 | MG | A | 2054 | - | - | - | X |
| 85 | MG | A | 2055 | - | - | - | X |
| 85 | MG | A | 2056 | - | - | - | X |
| 85 | MG | A | 2057 | - | - | - | X |
| 85 | MG | A | 2061 | - | - | - | X |
| 85 | MG | A | 2066 | - | - | - | X |
| 85 | MG | A | 2072 | - | - | - | X |
| 85 | MG | A | 2078 | - | - | - | X |
| 85 | MG | A | 2079 | - | - | - | X |
| 85 | MG | A | 2081 | - | - | - | X |
| 85 | MG | A | 2085 | - | - | - | X |
| 85 | MG | A | 2086 | - | - | - | X |
| 85 | MG | A | 2087 | - | - | - | X |
| 85 | MG | A | 2092 | - | - | - | X |
| 85 | MG | A | 2100 | - | - | - | X |
| 85 | MG | A | 2101 | - | - | - | X |
| 85 | MG | A | 2105 | - | - | - | X |
| 85 | MG | A | 2108 | - | - | - | X |
| 85 | MG | A | 2109 | - | - | - | X |
| 85 | MG | A | 2115 | - | - | - | X |
| 85 | MG | A | 2119 | - | - | - | X |
| 85 | MG | A | 2125 | - | - | - | X |
| 85 | MG | A | 2128 | - | - | - | X |
| 85 | MG | A | 2130 | - | - | - | X |
| 85 | MG | AB | 201 | - | - | - | X |
| 85 | MG | AB | 204 | - | - | - | X |
| 85 | MG | AF | 202 | - | - | - | X |
| 85 | MG | AK | 104 | - | - | - | X |
| 85 | MG | AR | 3741 | - | - | - | X |
| 85 | MG | AR | 3749 | - | - | - | X |
| 85 | MG | AR | 3756 | - | - | - | X |
| 85 | MG | AR | 3757 | - | - | - | X |
| 85 | MG | AR | 3763 | - | - | - | X |
| 85 | MG | AR | 3765 | - | - | - | X |
| 85 | MG | AR | 3768 | - | - | - | X |
| 85 | MG | AR | 3779 | - | - | - | X |
| 85 | MG | AR | 3783 | - | - | - | X |
| 85 | MG | AR | 3797 | - | - | - | X |
| 85 | MG | AR | 3801 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 85 | MG | AR | 3802 | - | - | - | X |
| 85 | MG | AR | 3810 | - | - | - | X |
| 85 | MG | AR | 3817 | - | - | - | X |
| 85 | MG | AR | 3836 | - | - | - | X |
| 85 | MG | AR | 3840 | - | - | - | X |
| 85 | MG | AR | 3842 | - | - | - | X |
| 85 | MG | AR | 3845 | - | - | - | X |
| 85 | MG | AR | 3846 | - | - | - | X |
| 85 | MG | AR | 3847 | - | - | - | X |
| 85 | MG | AR | 3850 | - | - | - | X |
| 85 | MG | AR | 3851 | - | - | - | X |
| 85 | MG | AR | 3852 | - | - | - | X |
| 85 | MG | AR | 3853 | - | - | - | X |
| 85 | MG | AR | 3856 | - | - | - | X |
| 85 | MG | AR | 3858 | - | - | - | X |
| 85 | MG | AR | 3862 | - | - | - | X |
| 85 | MG | AR | 3864 | - | - | - | X |
| 85 | MG | AR | 3866 | - | - | - | X |
| 85 | MG | AR | 3867 | - | - | - | X |
| 85 | MG | AR | 3872 | - | - | - | X |
| 85 | MG | AR | 3882 | - | - | - | X |
| 85 | MG | AR | 3885 | - | - | - | X |
| 85 | MG | AR | 3887 | - | - | - | X |
| 85 | MG | AR | 3889 | - | - | - | X |
| 85 | MG | AR | 3890 | - | - | - | X |
| 85 | MG | AR | 3891 | - | - | - | X |
| 85 | MG | AR | 3895 | - | - | - | X |
| 85 | MG | AR | 3896 | - | - | - | X |
| 85 | MG | AR | 3898 | - | - | - | X |
| 85 | MG | AR | 3900 | - | - | - | X |
| 85 | MG | AR | 3901 | - | - | - | X |
| 85 | MG | AR | 3905 | - | - | - | X |
| 85 | MG | AR | 3906 | - | - | - | X |
| 85 | MG | AR | 3909 | - | - | - | X |
| 85 | MG | AR | 3910 | - | - | - | X |
| 85 | MG | AR | 3911 | - | - | - | X |
| 85 | MG | AR | 3914 | - | - | - | X |
| 85 | MG | AR | 3915 | - | - | - | X |
| 85 | MG | AR | 3922 | - | - | - | X |
| 85 | MG | AR | 3925 | - | - | - | X |
| 85 | MG | AR | 3926 | - | - | - | X |
| 85 | MG | AR | 3927 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 85 | MG | AR | 3930 | - | - | - | X |
| 85 | MG | AR | 3933 | - | - | - | X |
| 85 | MG | AR | 3934 | - | - | - | X |
| 85 | MG | AR | 3935 | - | - | - | X |
| 85 | MG | AR | 3936 | - | - | - | X |
| 85 | MG | AR | 3937 | - | - | - | X |
| 85 | MG | AR | 3938 | - | - | - | X |
| 85 | MG | AR | 3939 | - | - | - | X |
| 85 | MG | AR | 3943 | - | - | - | X |
| 85 | MG | AR | 3946 | - | - | - | X |
| 85 | MG | AR | 3952 | - | - | - | X |
| 85 | MG | AR | 3957 | - | - | - | X |
| 85 | MG | AR | 3963 | - | - | - | X |
| 85 | MG | AR | 3964 | - | - | - | X |
| 85 | MG | AR | 3971 | - | - | - | X |
| 85 | MG | AR | 3973 | - | - | - | X |
| 85 | MG | AR | 3975 | - | - | - | X |
| 85 | MG | AR | 3983 | - | - | - | X |
| 85 | MG | AR | 3985 | - | - | - | X |
| 85 | MG | AR | 3991 | - | - | - | X |
| 85 | MG | AR | 3992 | - | - | - | X |
| 85 | MG | AR | 4000 | - | - | - | X |
| 85 | MG | AR | 4001 | - | - | - | X |
| 85 | MG | AR | 4011 | - | - | - | X |
| 85 | MG | AR | 4026 | - | - | - | X |
| 85 | MG | AR | 4030 | - | - | - | X |
| 85 | MG | AR | 4032 | - | - | - | X |
| 85 | MG | AR | 4033 | - | - | - | X |
| 85 | MG | AR | 4037 | - | - | - | X |
| 85 | MG | AR | 4040 | - | - | - | X |
| 85 | MG | AR | 4050 | - | - | - | X |
| 85 | MG | AR | 4081 | - | - | - | X |
| 85 | MG | AR | 4083 | - | - | - | X |
| 85 | MG | AR | 4084 | - | - | - | X |
| 85 | MG | AR | 4090 | - | - | - | X |
| 85 | MG | AR | 4092 | - | - | - | X |
| 85 | MG | AR | 4095 | - | - | - | X |
| 85 | MG | AR | 4102 | - | - | - | X |
| 85 | MG | AR | 4111 | - | - | - | X |
| 85 | MG | AR | 4135 | - | - | - | X |
| 85 | MG | AR | 4136 | - | - | - | X |
| 85 | MG | AR | 4138 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 85 | MG | AR | 4139 | - | - | - | X |
| 85 | MG | AR | 4173 | - | - | - | X |
| 85 | MG | AR | 4174 | - | - | - | X |
| 85 | MG | AR | 4177 | - | - | - | X |
| 85 | MG | AR | 4185 | - | - | - | X |
| 85 | MG | AR | 4187 | - | - | - | X |
| 85 | MG | AR | 4191 | - | - | - | X |
| 85 | MG | AR | 4200 | - | - | - | X |
| 85 | MG | AR | 4201 | - | - | - | X |
| 85 | MG | AR | 4205 | - | - | - | X |
| 85 | MG | AR | 4224 | - | - | - | X |
| 85 | MG | AR | 4225 | - | - | - | X |
| 85 | MG | AR | 4226 | - | - | - | X |
| 85 | MG | AR | 4228 | - | - | - | X |
| 85 | MG | AR | 4242 | - | - | - | X |
| 85 | MG | AT | 221 | - | - | - | X |
| 85 | MG | AT | 223 | - | - | - | X |
| 85 | MG | AT | 224 | - | - | - | X |
| 85 | MG | CE | 404 | - | - | - | X |
| 85 | MG | CE | 405 | - | - | - | X |
| 85 | MG | CE | 406 | - | - | - | X |
| 85 | MG | CI | 301 | - | - | - | X |
| 85 | MG | CP | 502 | - | - | - | X |
| 85 | MG | CQ | 201 | - | - | - | X |
| 85 | MG | CQ | 203 | - | - | - | X |
| 85 | MG | CR | 201 | - | - | - | X |
| 85 | MG | CR | 205 | - | - | - | X |
| 85 | MG | CU | 202 | - | - | - | X |
| 85 | MG | CX | 202 | - | - | - | X |
| 85 | MG | DG | 202 | - | - | - | X |
| 85 | MG | F | 301 | - | - | - | X |
| 85 | MG | d3 | 202 | - | - | - | X |
| 85 | MG | d9 | 102 | - | - | - | X |
| 85 | MG | l2 | 201 | - | - | - | X |
| 85 | MG | v | 302 | - | - | - | X |
| 85 | MG | x | 205 | - | - | - | X |

2 Entry composition [i](#)

There are 87 unique types of molecules in this entry. The entry contains 409590 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 |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 1 | 1 | 3149 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 67355 | 30086 | 12142 | 21978 | 3149 | | | |
| 1 | AR | 3149 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 67355 | 30086 | 12142 | 21978 | 3149 | | | |

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24 | 12 | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1003 | 628 | 189 | 179 | 7 | | | |
| 24 | CX | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1003 | 628 | 189 | 179 | 7 | | | |

- Molecule 25 is a RNA chain called 18S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 25 | 6 | 1783 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 37990 | 16984 | 6723 | 12500 | 1783 | | | |
| 25 | A | 1781 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 37948 | 16965 | 6715 | 12487 | 1781 | | | |

- Molecule 26 is a protein called 60S ribosomal protein L24-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26 | 7 | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 699 | 443 | 137 | 118 | 1 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26 | CY | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 699 | 443 | 137 | 118 | 1 | | | |

- Molecule 27 is a protein called 60S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 27 | 8 | 121 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 964 | 620 | 169 | 173 | 2 | | | |
| 27 | CZ | 121 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 964 | 620 | 169 | 173 | 2 | | | |

- Molecule 28 is a protein called 60S ribosomal protein L26-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 28 | 9 | 126 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 993 | 625 | 192 | 176 | | | | |
| 28 | DA | 126 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 993 | 625 | 192 | 176 | | | | |

- Molecule 29 is a protein called 60S ribosomal protein L27-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 29 | AA | 135 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 1092 | 710 | 202 | 180 | | | | |
| 29 | DB | 135 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 1092 | 710 | 202 | 180 | | | | |

- Molecule 30 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30 | AB | 148 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1173 | 749 | 231 | 190 | 3 | | | |
| 30 | DC | 148 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1173 | 749 | 231 | 190 | 3 | | | |

- Molecule 31 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|--|---------|---------|-------|
| 31 | AC | 58 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 462 | 289 | 100 | 73 | | | | |
| 31 | DD | 58 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 462 | 289 | 100 | 73 | | | | |

- Molecule 32 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32 | AD | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 743 | 479 | 124 | 139 | 1 | | | |
| 32 | DE | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 743 | 479 | 124 | 139 | 1 | | | |

- Molecule 33 is a protein called 60S ribosomal protein L31-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33 | AE | 109 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 876 | 556 | 167 | 152 | 1 | | | |
| 33 | DF | 109 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 876 | 556 | 167 | 152 | 1 | | | |

- Molecule 34 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34 | AF | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1020 | 647 | 205 | 167 | 1 | | | |
| 34 | DG | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1020 | 647 | 205 | 167 | 1 | | | |

- Molecule 35 is a protein called 60S ribosomal protein L33-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35 | AG | 106 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 850 | 540 | 165 | 144 | 1 | | | |
| 35 | DH | 106 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 850 | 540 | 165 | 144 | 1 | | | |

- Molecule 36 is a protein called 60S ribosomal protein L34-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36 | AH | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 880 | 545 | 179 | 152 | 4 | | | |
| 36 | DI | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 880 | 545 | 179 | 152 | 4 | | | |

- Molecule 37 is a protein called 60S ribosomal protein L35-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37 | AI | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 969 | 615 | 186 | 167 | 1 | | | |
| 37 | DJ | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 969 | 615 | 186 | 167 | 1 | | | |

- Molecule 38 is a protein called 60S ribosomal protein L36-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38 | AJ | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 771 | 481 | 156 | 132 | 2 | | | |
| 38 | DK | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 771 | 481 | 156 | 132 | 2 | | | |

- Molecule 39 is a protein called 60S ribosomal protein L37-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39 | AK | 87 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 681 | 414 | 148 | 114 | 5 | | | |
| 39 | DL | 87 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 681 | 414 | 148 | 114 | 5 | | | |

- Molecule 40 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 40 | AL | 77 | Total | C | N | O | 0 | 0 | 0 |
| | | | 612 | 391 | 115 | 106 | | | |
| 40 | DM | 77 | Total | C | N | O | 0 | 0 | 0 |
| | | | 612 | 391 | 115 | 106 | | | |

- Molecule 41 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 41 | AM | 50 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 436 | 272 | 97 | 65 | 2 | | | |
| 41 | DN | 50 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 436 | 272 | 97 | 65 | 2 | | | |

- Molecule 42 is a protein called Ubiquitin-60S ribosomal protein L40.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 42 | AN | 52 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 417 | 259 | 86 | 67 | 5 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 42 | DO | 52 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 417 | 259 | 86 | 67 | 5 | | | |

- Molecule 43 is a protein called 60S ribosomal protein L41-B.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 43 | AO | 25 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 233 | 142 | 63 | 27 | 1 | | | |
| 43 | DP | 25 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 233 | 142 | 63 | 27 | 1 | | | |

- Molecule 44 is a protein called 60S ribosomal protein L42-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44 | AP | 105 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 847 | 534 | 170 | 138 | 5 | | | |
| 44 | DQ | 105 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 847 | 534 | 170 | 138 | 5 | | | |

- Molecule 45 is a protein called 60S ribosomal protein L43-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45 | AQ | 91 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 694 | 429 | 138 | 121 | 6 | | | |
| 45 | DR | 91 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 694 | 429 | 138 | 121 | 6 | | | |

- Molecule 46 is a protein called Suppressor protein STM1.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 46 | i | 159 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1104 | 652 | 221 | 231 | | | |

- Molecule 47 is a protein called 60S acidic ribosomal protein P0.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47 | p0 | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1077 | 687 | 192 | 195 | 3 | | | |

- Molecule 48 is a protein called Suppressor protein STM1,Suppressor protein STM1,Suppressor protein Stm1 - Mol B.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 48 | sM | 104 | Total | C | N | O | | | |
| | | | 680 | 403 | 140 | 137 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 49 | B | 206 | Total | C | N | O | S | | | |
| | | | 1577 | 1014 | 278 | 283 | 2 | 0 | 0 | 0 |
| 49 | s0 | 206 | Total | C | N | O | S | | | |
| | | | 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 |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 50 | C | 214 | Total | C | N | O | S | | | |
| | | | 1709 | 1084 | 310 | 311 | 4 | 0 | 0 | 0 |
| 50 | s1 | 216 | Total | C | N | O | S | | | |
| | | | 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 |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 51 | D | 217 | Total | C | N | O | S | | | |
| | | | 1635 | 1047 | 289 | 297 | 2 | 0 | 0 | 0 |
| 51 | s2 | 217 | Total | C | N | O | S | | | |
| | | | 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 |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 52 | E | 223 | Total | C | N | O | S | | | |
| | | | 1734 | 1101 | 313 | 314 | 6 | 0 | 0 | 0 |
| 52 | s3 | 223 | Total | C | N | O | S | | | |
| | | | 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 |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 53 | F | 260 | Total | C | N | O | S | | | |
| | | | 2068 | 1316 | 389 | 360 | 3 | 0 | 0 | 0 |
| 53 | s4 | 260 | Total | C | N | O | S | | | |
| | | | 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 |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 54 | G | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1609 | 1007 | 300 | 299 | 3 | | | |
| 54 | s5 | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1609 | 1007 | 300 | 299 | 3 | | | |

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 59 | L | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 772 | 499 | 126 | 145 | 2 | | | |
| 59 | c0 | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 761 | 490 | 125 | 144 | 2 | | | |

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 63 | P | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 891 | 545 | 182 | 163 | 1 | | | |
| 63 | c4 | 128 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 949 | 582 | 188 | 176 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 64 | Q | 124 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 977 | 622 | 182 | 166 | 7 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 64 | c5 | 135 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1039 | 658 | 196 | 178 | 7 | | | |

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 74 | a | 70 | Total | C | N | O | 0 | 0 | 0 |
| | | | 563 | 360 | 104 | 99 | | | |
| 74 | d5 | 69 | Total | C | N | O | 0 | 0 | 0 |
| | | | 558 | 357 | 103 | 98 | | | |

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

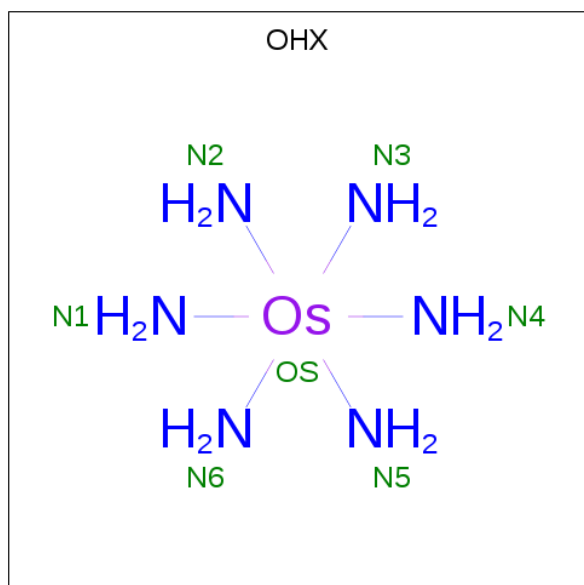
- Molecule 82 is a protein called 40S ribosomal protein S17-A.

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

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

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

- Molecule 84 is osmium (III) hexammine (three-letter code: OHX) (formula: $\text{H}_{12}\text{N}_6\text{Os}$).



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

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

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

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

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

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 84 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 1 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 3 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 3 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 3 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 3 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 3 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 3 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 3 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 84 | 4 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 4 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 4 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 4 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 4 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 4 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 4 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 4 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 4 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 4 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | k | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | k | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | l | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | r | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | v | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | x | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | x | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | y | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | z | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 84 | 2 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |

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

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

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
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| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
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| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
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| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
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| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
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| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
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| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
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| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
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| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
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| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
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| 84 | 6 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | AC | 1 | Total | N | Os | 0 | 0 |
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| 84 | AE | 1 | Total | N | Os | 0 | 0 |
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| 84 | AR | 1 | Total | N | Os | 0 | 0 |
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| 84 | AR | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | AR | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | AR | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | AR | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | AR | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | AR | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | AR | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | AR | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |

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

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

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

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

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

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

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 84 | AT | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | AT | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | AT | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | AT | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | AT | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | AT | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | AT | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | CE | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | CE | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | CF | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | CF | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | CG | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | CG | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | CG | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | CK | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | CL | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | CL | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | CM | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | CO | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | CP | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | CV | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 84 | CX | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | CZ | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | DD | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | DG | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | DH | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | DI | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | DL | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | DL | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | A | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | A | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | A | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | A | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | A | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | A | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | A | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | A | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | A | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | A | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | A | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |

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

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

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

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

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

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

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 84 | A | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | A | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | A | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | H | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | J | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | M | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | O | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | Q | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | T | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | e | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | h | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | s8 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | c3 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | c5 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | c8 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | d9 | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |
| 84 | sR | 1 | Total | N | Os | 0 | 0 |
| | | | 7 | 6 | 1 | | |

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

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 85 | AP | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 85 | AK | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 85 | AB | 4 | Total 4 | Mg 4 | 0 | 0 |
| 85 | DF | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | c6 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | 6 | 141 | Total 141 | Mg 141 | 0 | 0 |
| 85 | DO | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | sM | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | d5 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | t | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | CD | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | CR | 6 | Total 6 | Mg 6 | 0 | 0 |
| 85 | o | 3 | Total 3 | Mg 3 | 0 | 0 |
| 85 | DC | 4 | Total 4 | Mg 4 | 0 | 0 |
| 85 | AS | 20 | Total 20 | Mg 20 | 0 | 0 |
| 85 | DH | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | c9 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | k | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | CO | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | DG | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | CU | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | b | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | DR | 2 | Total 2 | Mg 2 | 0 | 0 |

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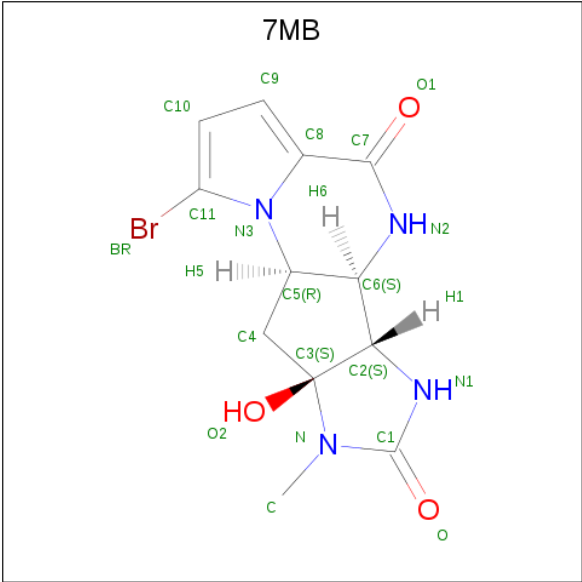
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 85 | w | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | CK | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | CQ | 4 | Total 4 | Mg 4 | 0 | 0 |
| 85 | x | 5 | Total 5 | Mg 5 | 0 | 0 |
| 85 | AR | 504 | Total 504 | Mg 504 | 0 | 0 |
| 85 | d6 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | s6 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | s | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | DI | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | j | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | 1 | 490 | Total 490 | Mg 490 | 0 | 0 |
| 85 | D | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | DD | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | s2 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | d3 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 85 | v | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | A | 111 | Total 111 | Mg 111 | 0 | 0 |
| 85 | CP | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | 4 | 21 | Total 21 | Mg 21 | 0 | 0 |
| 85 | DA | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | r | 1 | Total 1 | Mg 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|----------|---------|---------|
| 85 | 9 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | CF | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | CX | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | DE | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | s1 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | AH | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | DP | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | s8 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | i | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | CI | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | d9 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | z | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | AT | 12 | Total 12 | Mg 12 | 0 | 0 |
| 85 | F | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | l2 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | CE | 4 | Total 4 | Mg 4 | 0 | 0 |
| 85 | Y | 1 | Total 1 | Mg 1 | 0 | 0 |
| 85 | l | 2 | Total 2 | Mg 2 | 0 | 0 |
| 85 | 3 | 12 | Total 12 | Mg 12 | 0 | 0 |
| 85 | AF | 2 | Total 2 | Mg 2 | 0 | 0 |

- Molecule 86 is Agelastatin A (three-letter code: 7MB) (formula: $C_{12}H_{13}BrN_4O_3$).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 86 | 1 | 1 | Total | Br | C | N | O | 0 | 0 |
| | | | 20 | 1 | 12 | 4 | 3 | | |
| 86 | AR | 1 | Total | Br | C | N | O | 0 | 0 |
| | | | 20 | 1 | 12 | 4 | 3 | | |

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

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 87 | AP | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 87 | g | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 87 | AQ | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 87 | AK | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 87 | DQ | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 87 | e | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 87 | b | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 87 | e1 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 87 | c | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 87 | DL | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

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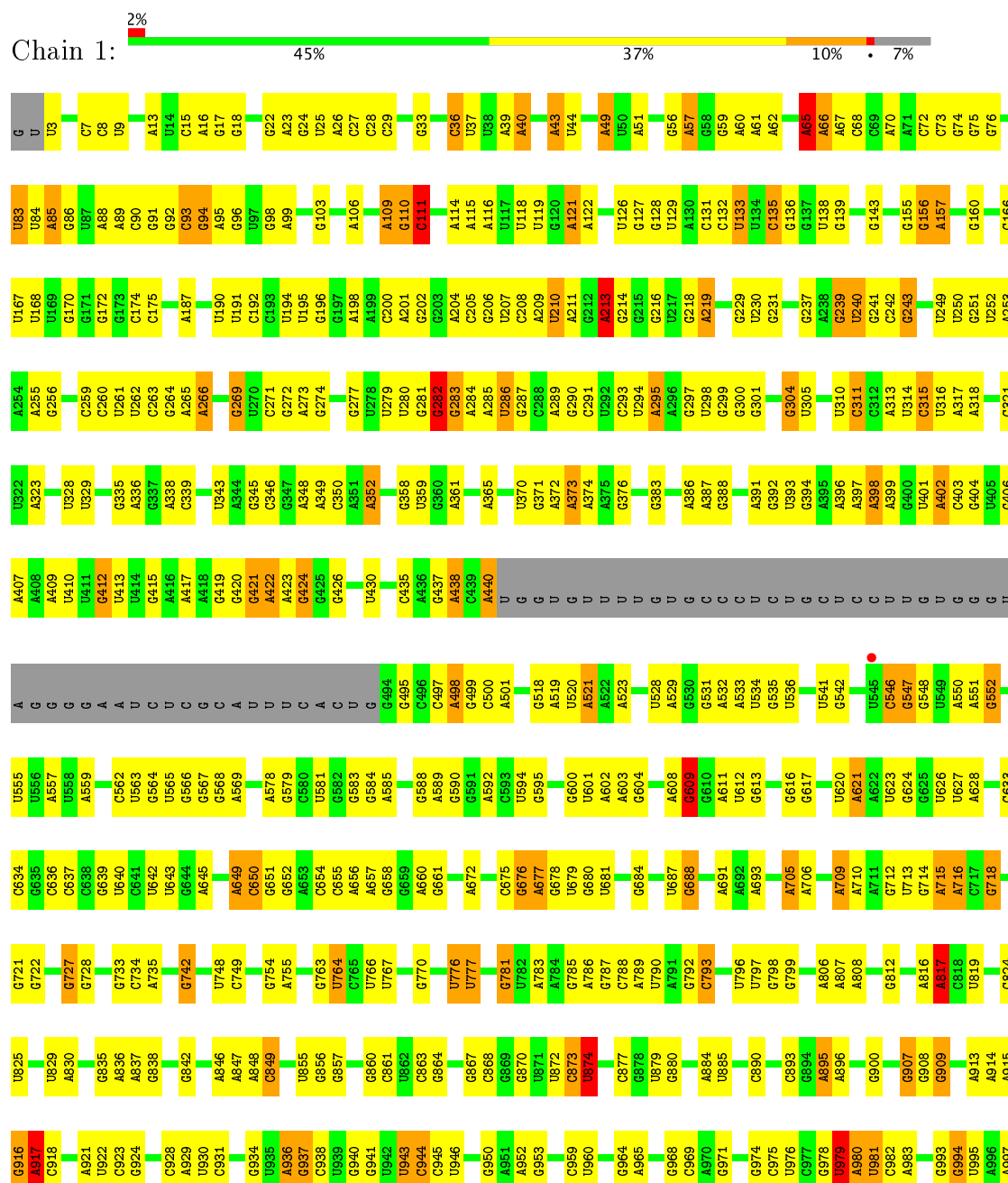
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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 87 | d9 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 87 | DR | 1 | Total 1 | Zn 1 | 0 | 0 |
| 87 | DO | 1 | Total 1 | Zn 1 | 0 | 0 |
| 87 | AN | 1 | Total 1 | Zn 1 | 0 | 0 |
| 87 | d7 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 87 | d6 | 1 | Total 1 | Zn 1 | 0 | 0 |

3 Residue-property plots

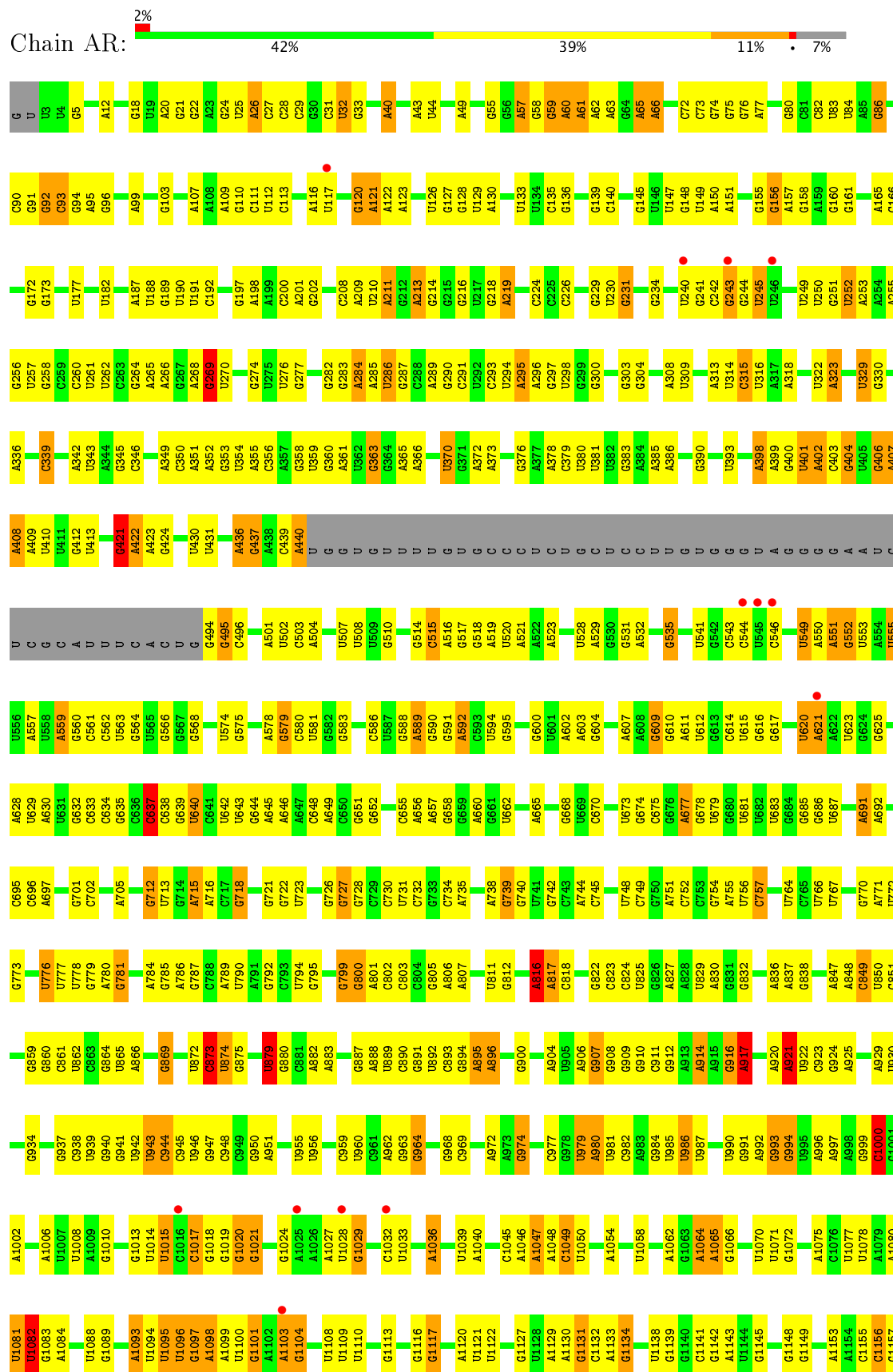
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: 25S ribosomal RNA

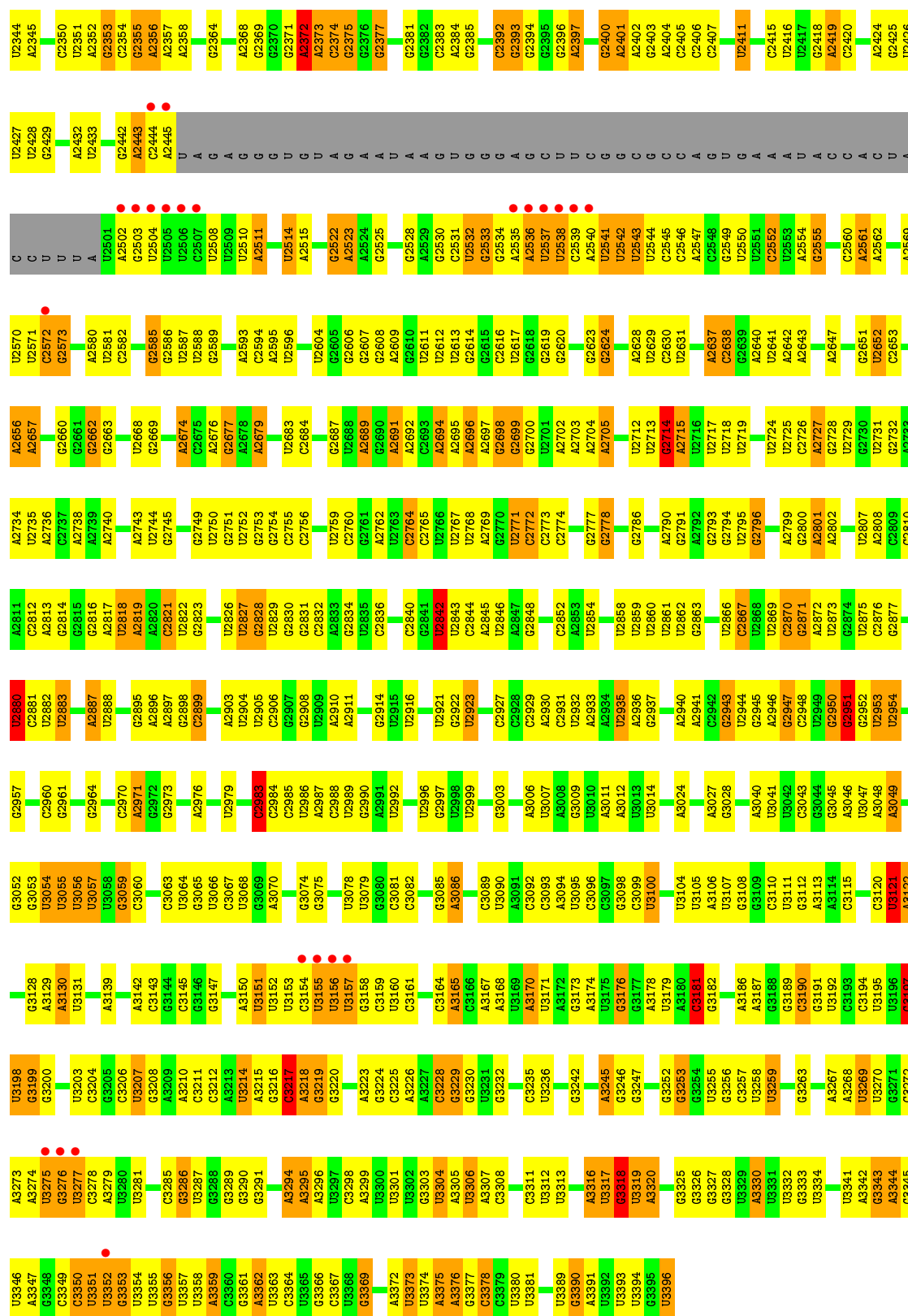


| | | | | | | | | | | | | |
|-------|---|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| C2128 | G | A1841 | C1767 | G1674 | C1582 | U1495 | U1415 | A1337 | A1245 | A1163 | U1073 | A998 |
| A2131 | U | A1842 | U1768 | G1675 | A1583 | C1496 | C1416 | C1338 | U1246 | G1164 | U1078 | G999 |
| U2137 | G | C1843 | G1769 | A1676 | G1586 | C1497 | A1418 | C1339 | G1248 | A1165 | U1081 | G1001 |
| A2138 | C | G1844 | G1770 | A1677 | A1587 | C1498 | A1419 | U1340 | G1249 | G1166 | U1087 | A1002 |
| U2140 | U | C1845 | G1780 | A1683 | A1588 | G1500 | C1420 | C1342 | G1250 | U1167 | U1087 | A1006 |
| U2141 | C | A1847 | G1784 | U1686 | A1589 | C1508 | G1421 | A1343 | A1251 | A1170 | U1007 | U1007 |
| U2142 | U | G1848 | U1785 | U1687 | G1591 | G1514 | U1425 | U1348 | C1254 | G1171 | A1090 | A1009 |
| A2143 | G | C1849 | U1786 | U1688 | G1592 | G1517 | U1426 | G1349 | G1255 | C1175 | C1092 | G1010 |
| A2144 | C | G1851 | A1787 | U1689 | A1593 | U1518 | U1427 | A1350 | C1257 | G1176 | A1099 | G1010 |
| U2149 | U | C1852 | C1788 | A1699 | U1595 | U1518 | A1428 | U1351 | U1258 | G1177 | U1094 | U1015 |
| A2149 | U | U1853 | G1789 | A1699 | U1595 | U1518 | U1428 | U1351 | U1258 | G1177 | U1094 | U1015 |
| G2155 | G | C1854 | G1790 | G1700 | C1596 | U1523 | U1429 | A1352 | G1261 | A1180 | U1095 | C1016 |
| C2156 | C | U1855 | C1791 | A1704 | C1597 | U1523 | U1430 | U1353 | G1262 | U1181 | U1096 | C1017 |
| G2157 | C | G1856 | C1792 | U1705 | G1598 | C1527 | G1431 | G1354 | U1181 | A1180 | G1097 | G1018 |
| A2158 | C | C1857 | G1793 | U1705 | G1599 | G1528 | A1432 | A1355 | A1263 | U1181 | A1098 | G1019 |
| U2158 | C | A1858 | G1794 | A1699 | U1600 | G1528 | A1433 | U1356 | G1264 | G1186 | A1099 | G1020 |
| G2165 | G | U1859 | U1795 | C1709 | A1603 | A1529 | A1434 | G1357 | U1269 | U1100 | U1100 | G1024 |
| G2165 | U | G1860 | U1796 | C1710 | G1604 | C1531 | U1435 | C1360 | U1270 | A1190 | A1102 | A1026 |
| C2169 | C | U1861 | A1797 | U1716 | A1605 | C1531 | U1436 | U1361 | A1271 | C1192 | A1103 | A1026 |
| U2172 | C | G1862 | A1798 | U1716 | U1606 | A1534 | U1437 | G1362 | C1272 | A1193 | G1104 | A1027 |
| C2173 | U | A1863 | A1799 | U1717 | U1607 | A1535 | U1438 | G1362 | A1273 | G1194 | A1105 | U1028 |
| U2173 | G | A1864 | C1802 | G1718 | U1607 | A1535 | U1439 | G1365 | A1274 | G1106 | G1029 | U1029 |
| G2174 | G | A1865 | C1802 | G1719 | U1607 | A1537 | U1440 | G1366 | C1201 | U1107 | A1030 | A1030 |
| G2174 | C | C1866 | C1805 | U1720 | A1613 | G1538 | G1441 | U1367 | A1278 | U1107 | U1108 | U1033 |
| A2178 | C | U1877 | A1806 | U1721 | C1614 | A1537 | A1446 | U1368 | C1279 | U1109 | U1109 | U1034 |
| C2179 | U | G1878 | G1807 | A1723 | C1615 | G1538 | G1446 | A1369 | A1204 | U1110 | U1110 | G1035 |
| U2186 | C | A1879 | G1808 | U1724 | U1616 | G1541 | G1450 | C1372 | G1209 | U1111 | U1111 | A1036 |
| C2181 | U | U1880 | A1809 | C1725 | U1620 | G1542 | A1456 | A1373 | U1210 | U1114 | U1114 | C1037 |
| U2186 | C | A1886 | A1810 | G1725 | A1621 | G1543 | A1456 | A1373 | U1211 | G1115 | G1115 | C1038 |
| G2187 | U | U1886 | G1812 | A1729 | U1629 | U1554 | A1460 | G1377 | G1288 | A1212 | G1116 | U1039 |
| A2188 | U | A1891 | A1813 | U1732 | U1630 | C1556 | A1461 | U1378 | G1289 | G1213 | G1117 | A1040 |
| C2189 | C | C1892 | A1814 | G1733 | C1631 | A1557 | G1464 | G1379 | U1214 | U1121 | U1121 | U1041 |
| U2190 | G | A1893 | U1815 | G1734 | G1634 | A1558 | A1465 | U1380 | G1295 | U1215 | U1042 | C1043 |
| A2095 | C | U1894 | A1816 | C1735 | G1635 | A1559 | G1466 | A1381 | C1296 | C1216 | U1042 | C1043 |
| C2096 | C | A1895 | G1817 | G1736 | U1636 | G1560 | G1466 | A1386 | G1297 | A1217 | G1127 | A1047 |
| U2097 | C | U1896 | U1818 | U1736 | A1637 | G1561 | U1471 | U1387 | G1298 | G1222 | A1128 | A1048 |
| C2098 | C | G1897 | U1819 | U1740 | U1637 | C1562 | U1472 | G1387 | G1300 | A1130 | A1129 | C1049 |
| C2101 | C | A1901 | U1820 | A1741 | A1638 | C1563 | U1472 | U1388 | G1300 | C1227 | G1131 | U1050 |
| U2102 | U | U1902 | U1821 | U1742 | G1639 | U1564 | G1473 | G1389 | A1301 | C1227 | C1132 | U1051 |
| A2107 | G | G1906 | C1822 | G1743 | C1640 | G1565 | A1477 | A1390 | A1302 | C1228 | A1133 | A1054 |
| C2108 | U | U1907 | A1823 | G1744 | A1643 | A1566 | C1478 | C1391 | G1230 | G1229 | G1134 | A1055 |
| U2203 | C | A1908 | U1824 | C1745 | U1643 | U1567 | U1479 | A1393 | U1309 | A1231 | A1135 | U1056 |
| U2205 | G | U1909 | C1826 | U1746 | G1650 | U1568 | G1480 | A1394 | G1232 | G1232 | A1136 | U1056 |
| C2111 | U | A1910 | U1827 | A1750 | G1650 | U1569 | A1481 | G1395 | G1233 | G1233 | U1061 | A1064 |
| U2112 | C | U1911 | A1828 | G1751 | C1657 | A1571 | A1482 | A1399 | C1313 | G1140 | G1140 | A1064 |
| A2113 | G | U1912 | G1829 | U1754 | U1659 | U1572 | G1483 | G1400 | G1234 | G1142 | G1142 | A1065 |
| C2114 | C | A1913 | U1830 | G1754 | U1659 | G1573 | U1484 | G1404 | G1236 | G1145 | G1145 | A1066 |
| A2120 | G | U1916 | G1833 | A1760 | G1661 | A1575 | G1486 | G1404 | C1237 | C1238 | G1145 | G1066 |
| G2121 | G | C1917 | U1834 | C1761 | G1662 | G1576 | G1487 | U1319 | G1239 | C1239 | U1067 | U1067 |
| C2122 | C | A1835 | A1835 | C1762 | G1662 | G1577 | G1488 | C1320 | A1153 | A1153 | C1088 | C1088 |
| G2123 | C | G1838 | U1838 | U1763 | G1666 | C1578 | U1492 | U1410 | U1241 | G1242 | A1158 | U1070 |
| A2125 | U | U1925 | G1838 | U1764 | A1667 | C1579 | G1492 | U1410 | U1329 | G1242 | U1071 | U1071 |
| C2126 | C | A1926 | U1839 | U1765 | G1668 | A1580 | U1493 | G1243 | A1330 | G1243 | C1160 | C1072 |

- Molecule 1: 25S ribosomal RNA



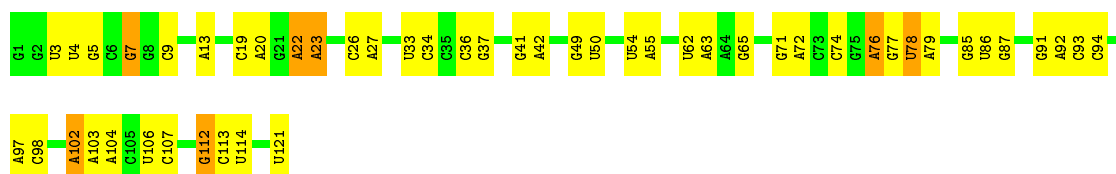
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|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| U2269 | A1158 | A1245 | G1412 | G1493 | A1866 | A1908 | A2104 | U2193 | A2269 | A2303 |
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| G2273 | G1161 | G1249 | U1415 | C1496 | U1659 | A1752 | U1912 | A2107 | U1912 | C2306 |
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| G2283 | | | U1348 | | G1669 | U1768 | A1922 | | A | C2245 |
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| U2286 | | G1263 | U1351 | C1508 | G1678 | C1771 | G1927 | G2122 | U | C2256 |
| C2287 | | A1264 | U1427 | C1509 | A1677 | | G | G2123 | G | U2257 |
| U2288 | C1187 | G1265 | A1428 | G1590 | A1679 | U1780 | A1932 | C2124 | C | U2258 |
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| A2295 | C1192 | | A1435 | U1522 | C1597 | U1786 | C | | U | G2216 |
| C2296 | A1193 | G1289 | U1436 | A1524 | G1598 | U1787 | A1839 | U2137 | A | A2220 |
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| | A1197 | C1292 | U1367 | C1527 | U1602 | U1692 | G1852 | | U | U2224 |
| | | U1293 | U1368 | | A1603 | A1696 | U1855 | U2148 | C | A2225 |
| A2303 | A1200 | U1298 | A1369 | U1533 | G1604 | C1790 | C1856 | A2149 | C | A2226 |
| C2304 | C1201 | U1299 | G1370 | G1536 | U1607 | C1791 | C1857 | | U | U2227 |
| G2305 | A1202 | G1300 | | G1537 | U1607 | U1702 | A1858 | A2152 | U | A2228 |
| C2306 | A1203 | U1298 | G1374 | G1538 | G1611 | U1703 | G1861 | A2153 | G | A2229 |
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| C2308 | A1205 | G1303 | U1380 | G1541 | C1613 | U1795 | A1868 | A2155 | A | A2233 |
| U2309 | G1209 | A1304 | G1382 | G1542 | C1614 | U1796 | C1869 | C2156 | G | |
| U2310 | U1210 | U1305 | G1383 | G1543 | C1615 | A1714 | U1797 | G2157 | A | |
| G2311 | U1211 | G1306 | U1384 | U1546 | U1620 | U1717 | A1798 | A2158 | C | |
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| A2313 | G1213 | A1308 | C1386 | C1548 | U1622 | G1719 | U1801 | A | G | |
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| C2333 | G1237 | A1326 | U1405 | G1483 | A1566 | G1734 | A1813 | A1895 | A | |
| U2334 | C1238 | U1329 | U1406 | U1484 | U1567 | G1735 | U1814 | U1896 | U | |
| G2335 | A1240 | U1330 | A1407 | G1485 | U1568 | G1736 | A1815 | G1897 | C | |
| U2336 | U1241 | U1331 | G1408 | G1486 | C1644 | U1737 | U1816 | U1898 | U | |
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| U2340 | | | | | U1572 | U1741 | U1820 | G1907 | G | |
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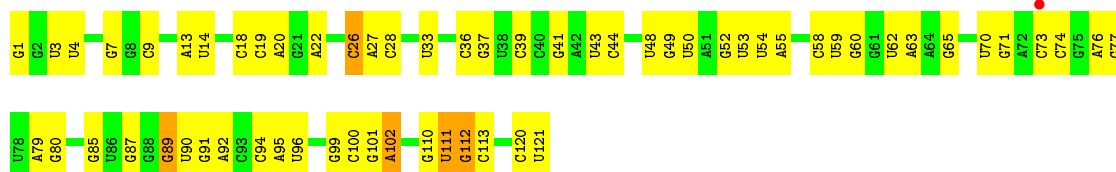
Molecule 2: 5S ribosomal RNA

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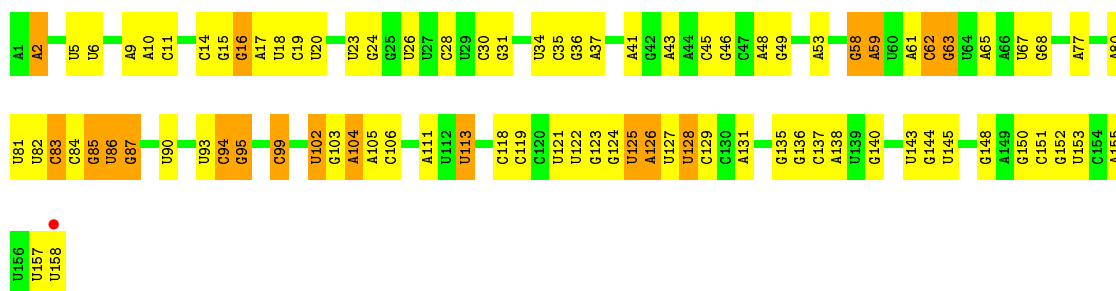
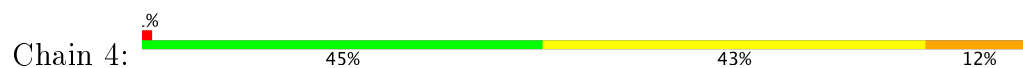




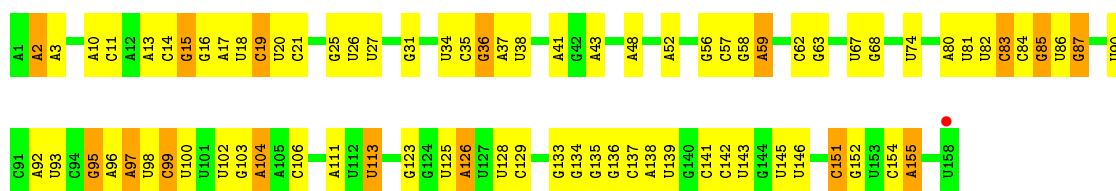
• Molecule 2: 5S ribosomal RNA



• Molecule 3: 5.8S ribosomal RNA



• Molecule 3: 5.8S ribosomal RNA

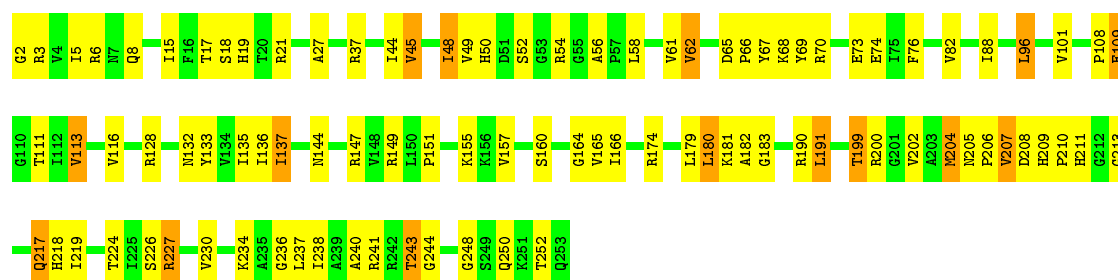


• Molecule 4: 60S ribosomal protein L2-A

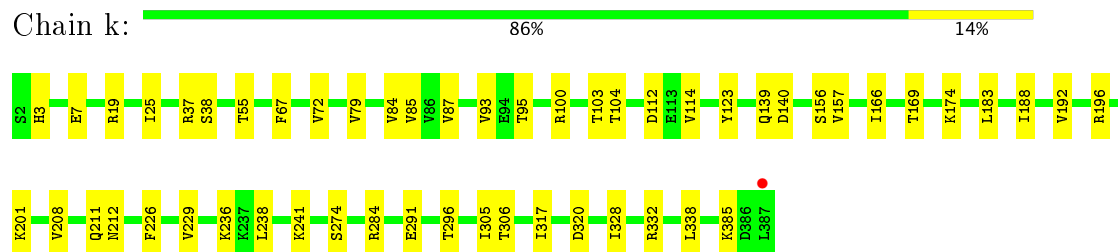


• Molecule 4: 60S ribosomal protein L2-A

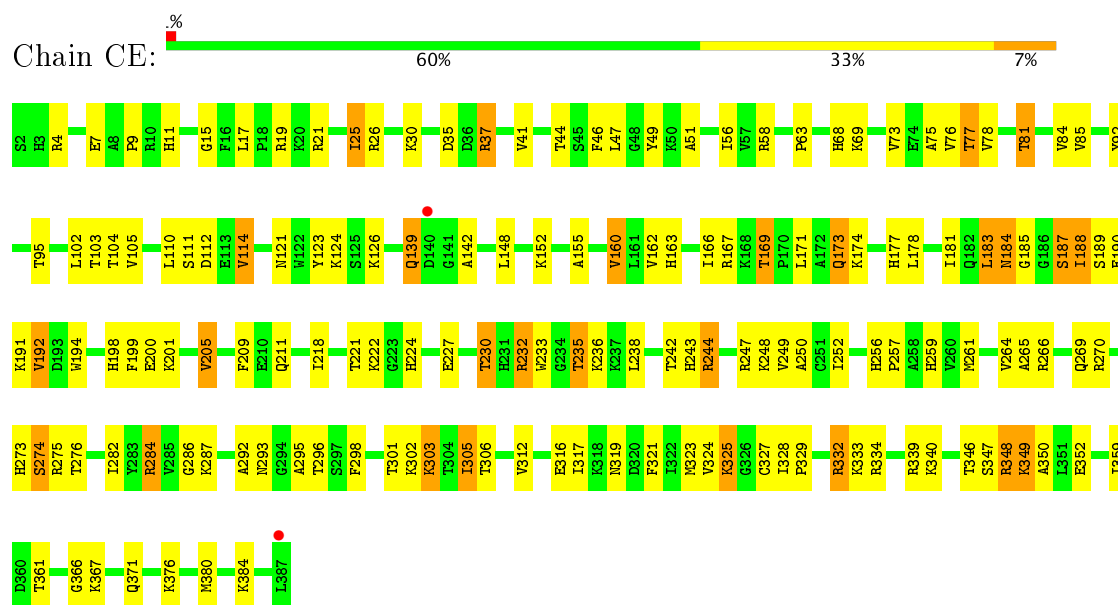




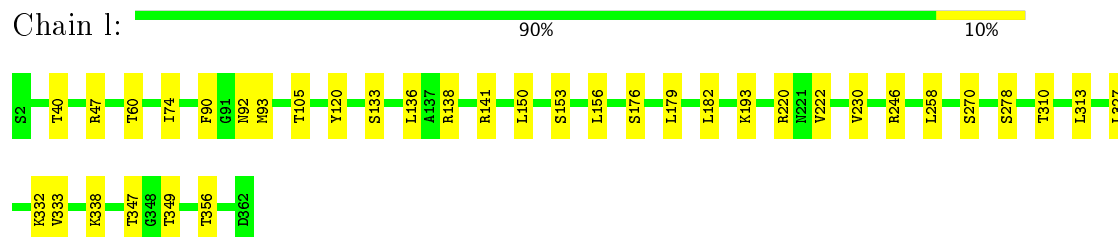
• Molecule 5: 60S ribosomal protein L3



• Molecule 5: 60S ribosomal protein L3

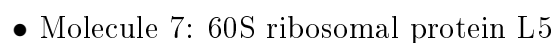


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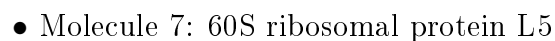


• Molecule 6: 60S ribosomal protein L4-A

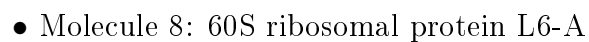
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|------------|------------|
| Yes | 63% |
| No | 33% |
| Don't know | 4% |



| Response | Percentage |
|------------|------------|
| Yes | 91% |
| No | 9% |
| Don't know | 0% |



| Frequency | Percentage |
|-----------|------------|
| Daily | 63% |
| Weekly | 31% |
| Monthly | 5% |




81% 7% 11%

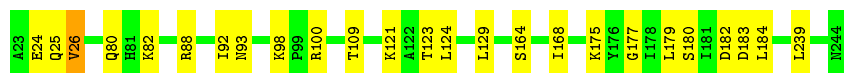


| Response | Percentage |
|------------------------------|------------|
| Best for the country | 61% |
| Not the best for the country | 23% |
| Don't know | 5% |
| Refuse to answer | 11% |



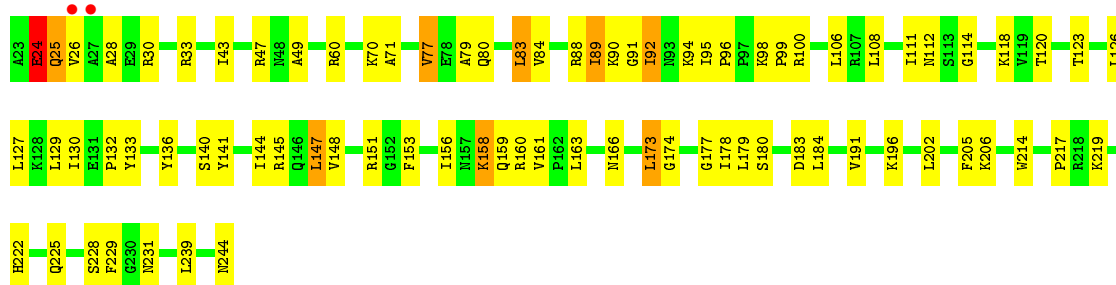
- Molecule 9: 60S ribosomal protein L7-A

Chain o:  89% 11%



- Molecule 9: 60S ribosomal protein L7-A

Chain CI:  64% 32%



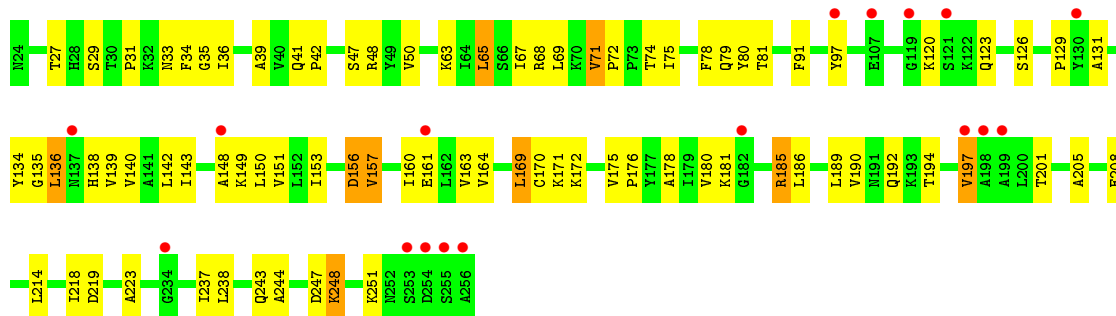
- Molecule 10: 60S ribosomal protein L8-A

Chain p:  91% 9%




- Molecule 10: 60S ribosomal protein L8-A

Chain CJ:  65% 31%

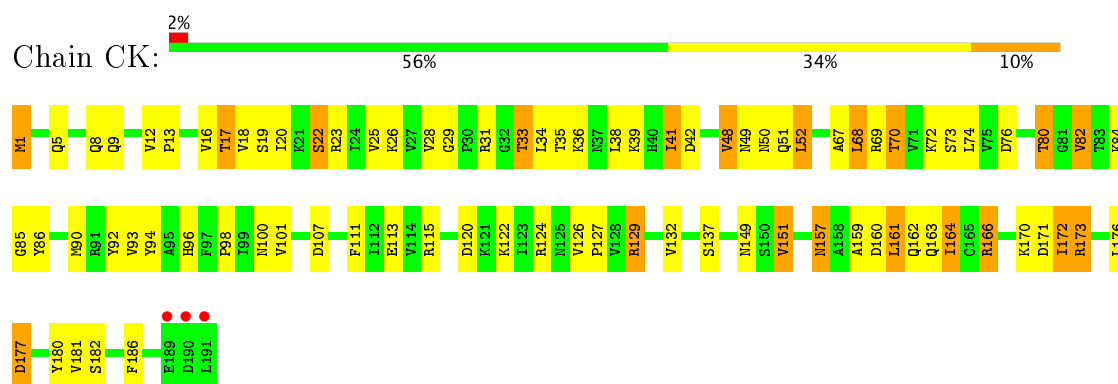


- Molecule 11: 60S ribosomal protein L9-A

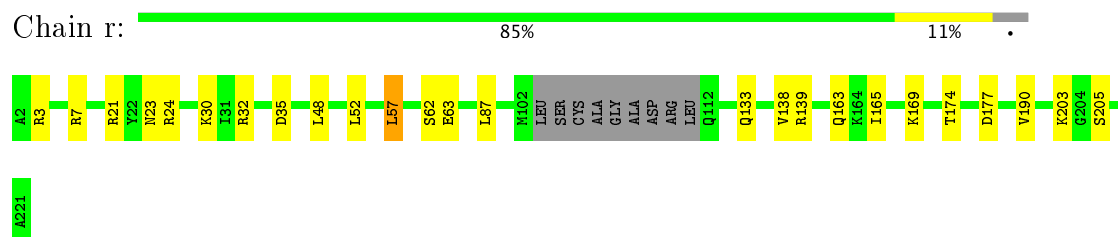
Chain q:  88% 12%



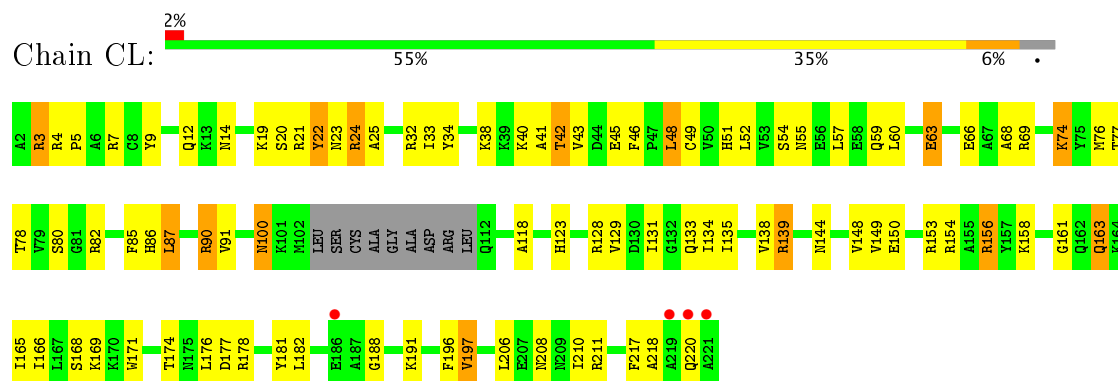
- Molecule 11: 60S ribosomal protein L9-A



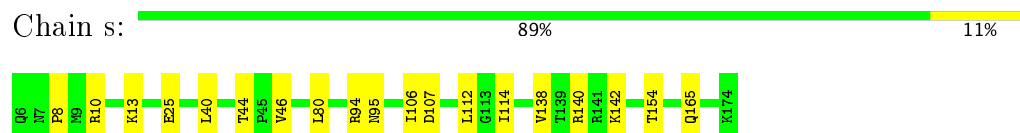
• Molecule 12: 60S ribosomal protein L10



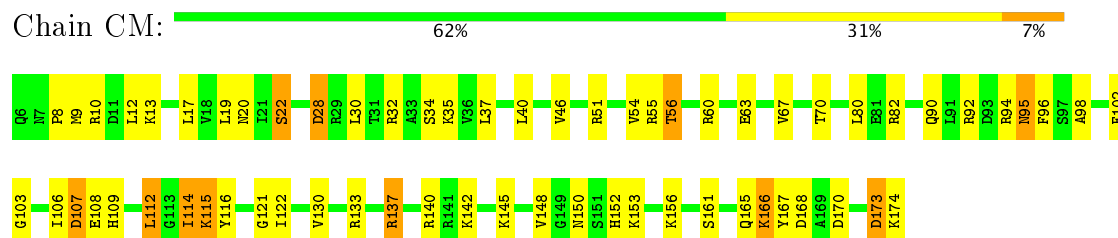
• Molecule 12: 60S ribosomal protein L10



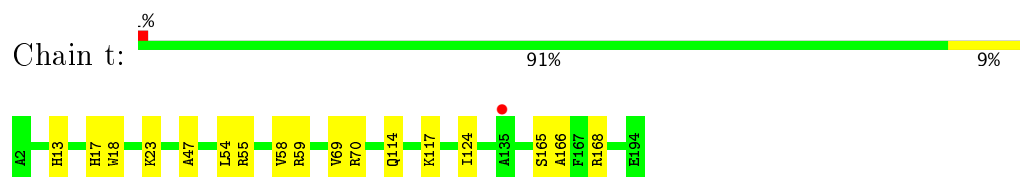
• Molecule 13: 60S ribosomal protein L11-B



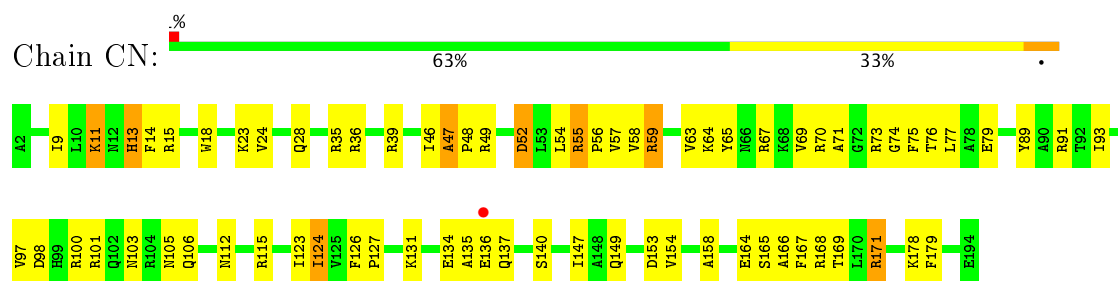
• Molecule 13: 60S ribosomal protein L11-B



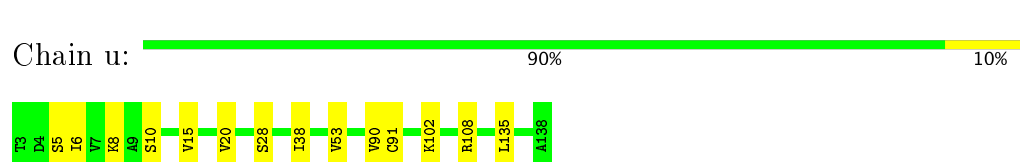
- Molecule 14: 60S ribosomal protein L13-A



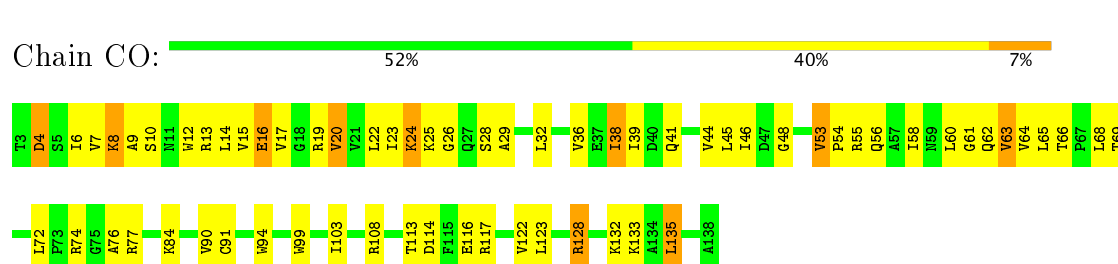
- Molecule 14: 60S ribosomal protein L13-A



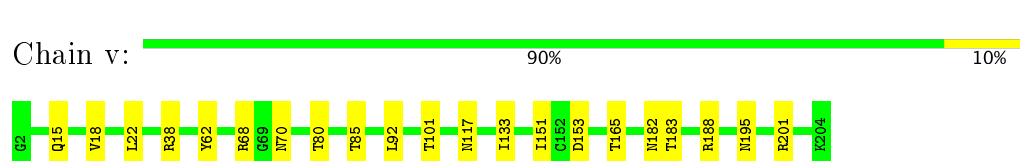
- Molecule 15: 60S ribosomal protein L14-A



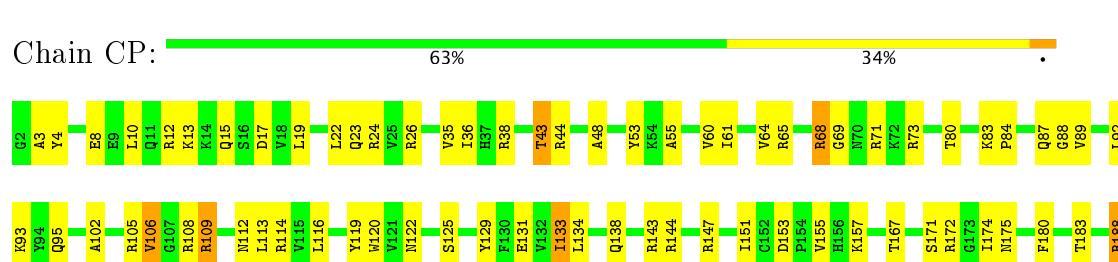
- Molecule 15: 60S ribosomal protein L14-A

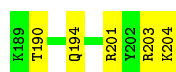


- Molecule 16: 60S ribosomal protein L15-A



- Molecule 16: 60S ribosomal protein L15-A





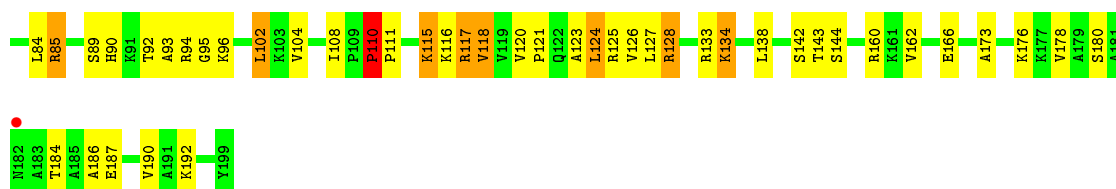
- Molecule 17: 60S ribosomal protein L16-A

Chain w: 87% 12%



- Molecule 17: 60S ribosomal protein L16-A

Chain CQ: 57% 37% 6%



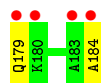
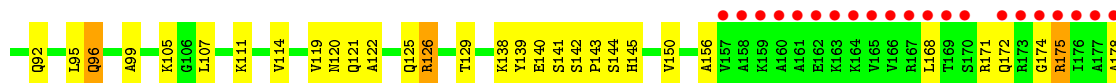
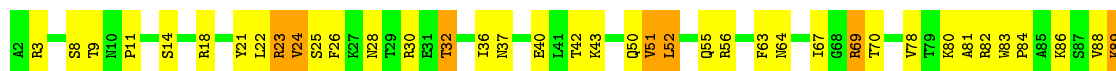
- Molecule 18: 60S ribosomal protein L17-A

Chain x: 4% 87% 13%



- Molecule 18: 60S ribosomal protein L17-A

Chain CR: 14% 61% 34% 5%

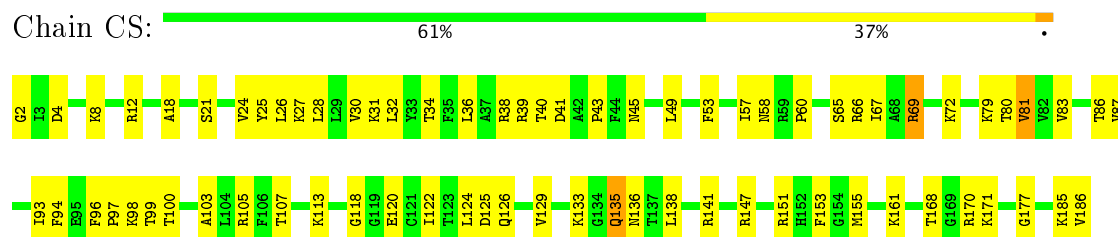


- Molecule 19: 60S ribosomal protein L18-A

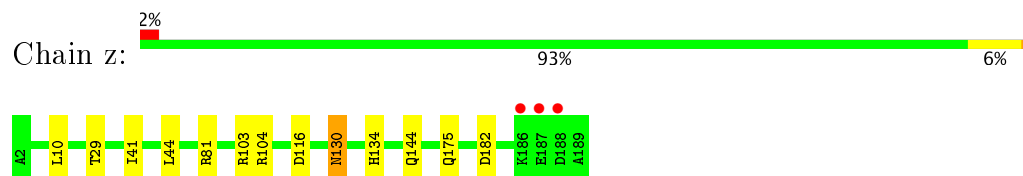
Chain y: 91% 9%



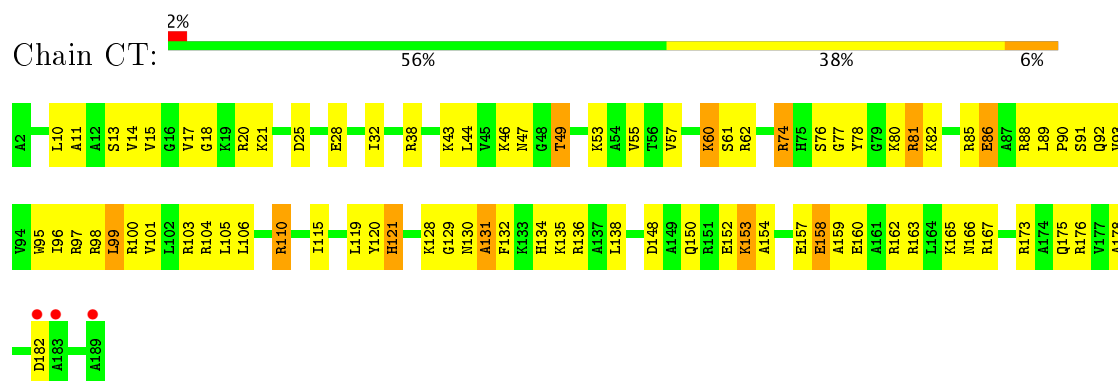
- Molecule 19: 60S ribosomal protein L18-A



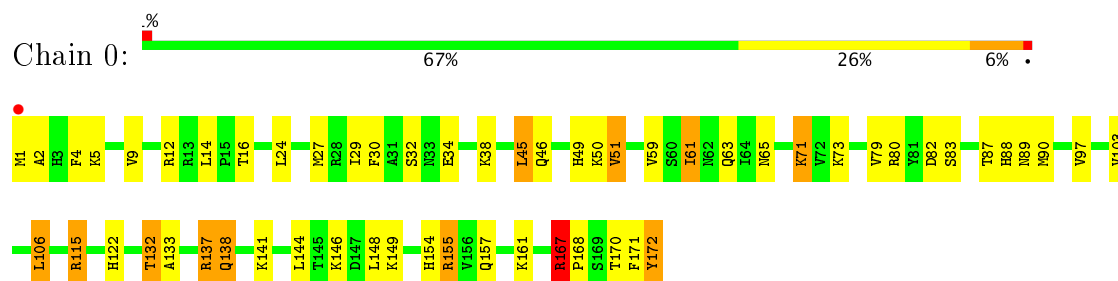
- Molecule 20: 60S ribosomal protein L19-A



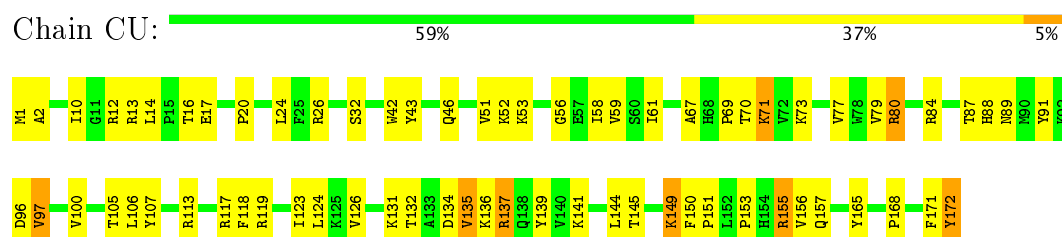
- Molecule 20: 60S ribosomal protein L19-A



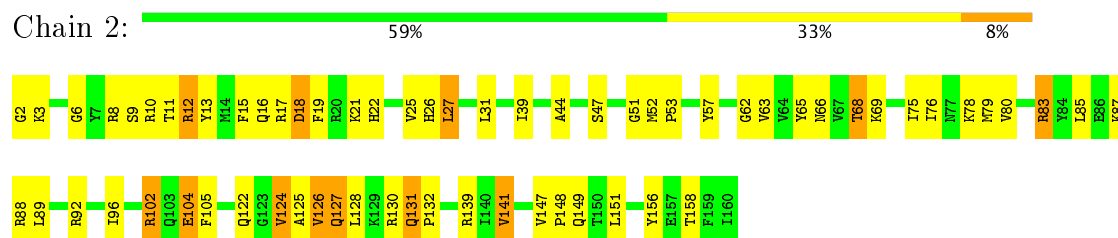
- Molecule 21: 60S ribosomal protein L20-A



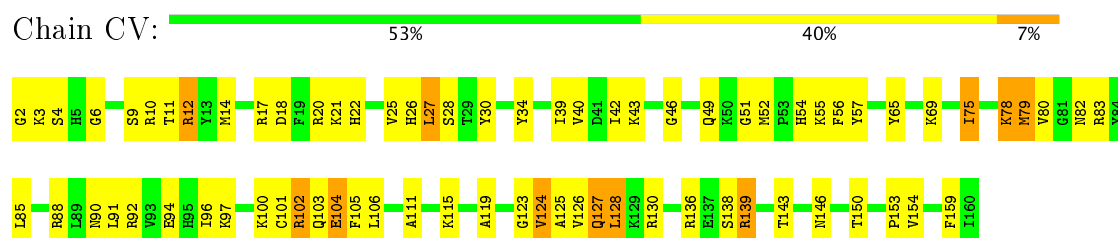
- Molecule 21: 60S ribosomal protein L20-A



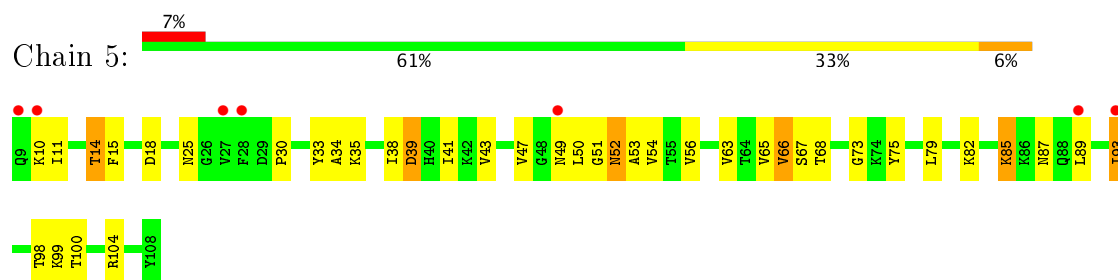
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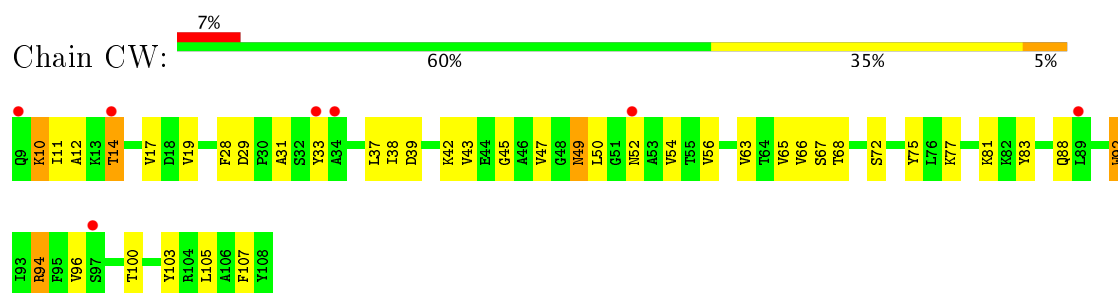
- Molecule 22: 60S ribosomal protein L21-A



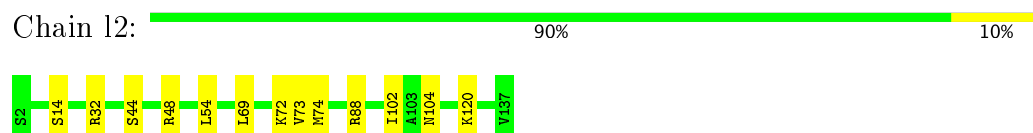
- Molecule 23: 60S ribosomal protein L22-A



- Molecule 23: 60S ribosomal protein L22-A

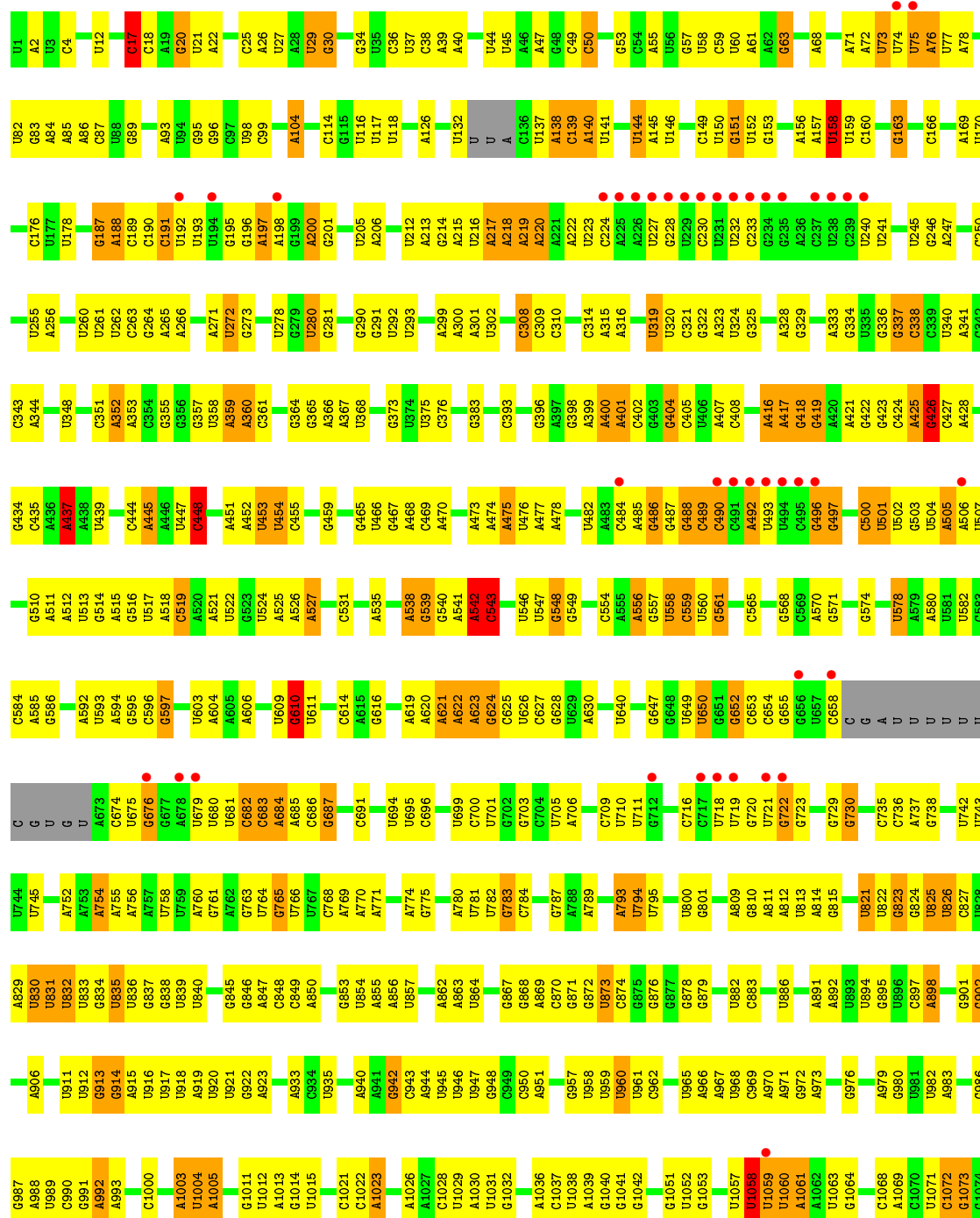


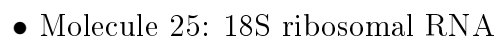
- Molecule 24: 60S ribosomal protein L23-A



- Molecule 24: 60S ribosomal protein L23-A

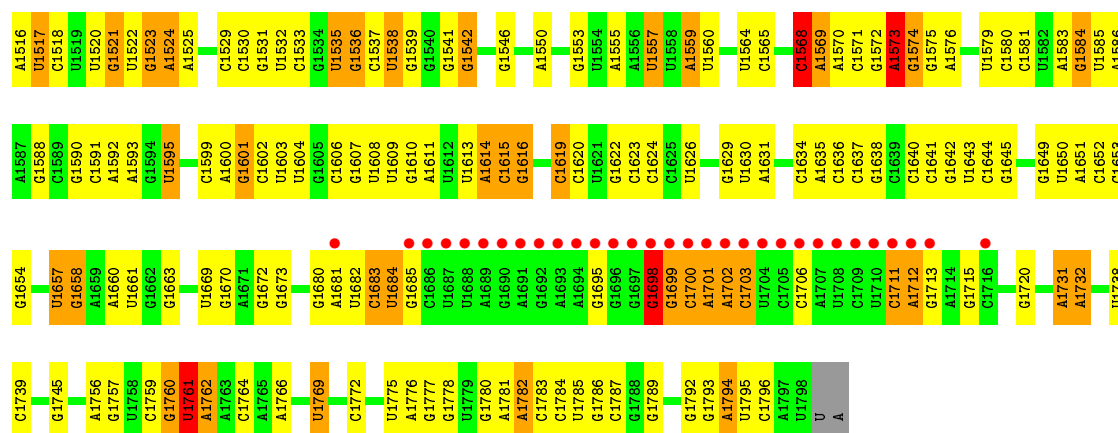




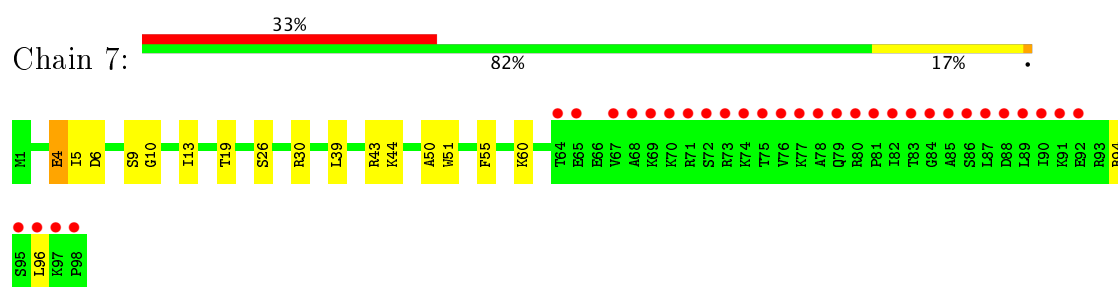


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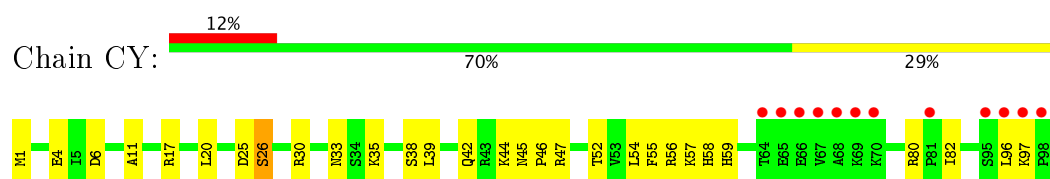
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| A1444 | U1363 | U1191 | U1017 | A940 | G867 | A799 | G722 | G658 | A579 | U507 | A445 | G373 |
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| G1446 | G1365 | G1193 | G1022 | G942 | A869 | G801 | G724 | G | U581 | G509 | U447 | A378 |
| C1447 | C1366 | C1194 | C943 | A944 | C870 | G802 | U725 | A | U582 | G510 | C448 | A379 |
| G1448 | C1367 | G1110 | A1025 | A951 | G872 | A806 | C726 | U | C583 | A511 | G449 | U380 |
| U1449 | G1368 | G1111 | A1026 | U873 | U872 | U807 | U727 | U | U585 | A512 | U450 | C381 |
| U1450 | U1369 | G1112 | U873 | C874 | U873 | U808 | U728 | U | G586 | U513 | A451 | C382 |
| C1451 | U1370 | A1113 | A1027 | G875 | C874 | U808 | G729 | U | U586 | G514 | A452 | G383 |
| U1452 | A1371 | G1114 | C1028 | G876 | G875 | U808 | G730 | U | U591 | A515 | U453 | G384 |
| C1456 | U1372 | G1119 | U1031 | G877 | G876 | U811 | C731 | U | A592 | G516 | G385 | G389 |
| G1459 | C1373 | A1124 | G1032 | G878 | G877 | A812 | G732 | C | U593 | G457 | A456 | A385 |
| A1460 | U1378 | A1201 | C1033 | G879 | G878 | A812 | A733 | G | U594 | A520 | G458 | A386 |
| C1461 | U1380 | A1203 | C1034 | G880 | G879 | A812 | A734 | U | A595 | A521 | A459 | A387 |
| G1464 | U1381 | G1130 | U1038 | G881 | G880 | G816 | C735 | G | C596 | U522 | U460 | G388 |
| A1469 | C1382 | C1207 | U1039 | A881 | U882 | A817 | C736 | U | U600 | G523 | G461 | G390 |
| C1470 | G1383 | A1208 | A1039 | U882 | U881 | G818 | A737 | A | U601 | U524 | G462 | A397 |
| A1471 | A1384 | G1213 | G1040 | G883 | U882 | C819 | G738 | C | A601 | A525 | U463 | A398 |
| G1472 | G1385 | A1217 | U1041 | G884 | U883 | U820 | G739 | U | U602 | A526 | A464 | A399 |
| C1473 | A1386 | G1218 | G1042 | U885 | U884 | U821 | C741 | G676 | U603 | A527 | U465 | A400 |
| A1474 | G1387 | A1219 | G1046 | U886 | U885 | U822 | U742 | G677 | U609 | U528 | G466 | A401 |
| U1475 | A1388 | C1220 | G1047 | U887 | U886 | U823 | U743 | A678 | U610 | A529 | G467 | A402 |
| G1479 | C1389 | U1303 | U1051 | U888 | U887 | G823 | U744 | U679 | U611 | U532 | A471 | A403 |
| A1480 | U1390 | G1226 | G1052 | U889 | U888 | U824 | G751 | U680 | U616 | U533 | U472 | A404 |
| C1481 | U1391 | A1227 | U1053 | A891 | U890 | U825 | A752 | A684 | G616 | C536 | A473 | C405 |
| A1482 | A1392 | U1228 | U1054 | U894 | U891 | U826 | A753 | A685 | U534 | G537 | U474 | U406 |
| G1483 | G1393 | G1229 | U1058 | G895 | U895 | C827 | A754 | G687 | A619 | A538 | A475 | A407 |
| A1484 | A1400 | U1231 | U1059 | U896 | U896 | U828 | A756 | G688 | A620 | G539 | A476 | C408 |
| C1485 | C1401 | U1232 | A1151 | A977 | C897 | A828 | U758 | G689 | A621 | A541 | A477 | U413 |
| G1486 | G1402 | G1233 | U1060 | A978 | U898 | U832 | U759 | U693 | A622 | A542 | A478 | C414 |
| A1487 | A1403 | A1234 | A1061 | A979 | G899 | U833 | A760 | U694 | A623 | C543 | C479 | C415 |
| G1488 | C1404 | U1235 | A1157 | G980 | A900 | U834 | A761 | U695 | A624 | A544 | A480 | A416 |
| U1489 | U1410 | G1237 | C1158 | G986 | U903 | U835 | G765 | C696 | G625 | A545 | U481 | A417 |
| C1490 | A1411 | A1238 | C1159 | G987 | U912 | U837 | U766 | C697 | U626 | U546 | U482 | C418 |
| U1491 | U1412 | U1239 | A1160 | A988 | G913 | U838 | U767 | U698 | U627 | U547 | A483 | G422 |
| A1492 | U1413 | G1242 | A1163 | G991 | G914 | U839 | C768 | G699 | U628 | G549 | A484 | G423 |
| C1493 | U1414 | A1243 | G1164 | A992 | A915 | U844 | A769 | U701 | A631 | A550 | A485 | C424 |
| G1494 | U1415 | U1244 | G1165 | A993 | U916 | G845 | U699 | G702 | U632 | G553 | G487 | A425 |
| U1495 | U1416 | G1245 | A1166 | G994 | U917 | C848 | C773 | G703 | U633 | C554 | C488 | A426 |
| A1496 | A1417 | U1246 | U1168 | A995 | U918 | C849 | G774 | C704 | A635 | A555 | C489 | C427 |
| G1498 | G1418 | U1247 | G1083 | U996 | U919 | A850 | G775 | A706 | U636 | A556 | C491 | A428 |
| C1499 | U1419 | A1248 | A1084 | U997 | U920 | U851 | G776 | A707 | U637 | G557 | A492 | G432 |
| U1500 | U1424 | U1249 | A1085 | G1002 | U921 | C852 | G777 | C708 | U640 | U558 | U493 | C433 |
| G1504 | A1427 | U1250 | A1086 | A1003 | G922 | U853 | G778 | C709 | G641 | C559 | U494 | G434 |
| A1505 | G1428 | U1251 | A1087 | U1004 | A923 | U854 | U781 | G710 | U642 | U560 | C495 | C435 |
| G1506 | U1429 | C1252 | A1091 | A1005 | G925 | U855 | U782 | U711 | G647 | G561 | G496 | A436 |
| C1507 | U1430 | U1253 | A1092 | G1008 | A926 | A856 | G783 | U712 | U648 | C565 | G497 | A437 |
| U1508 | A1344 | U1254 | A1093 | U1009 | C927 | U857 | C784 | A713 | U649 | U568 | U498 | A438 |
| G1509 | G1431 | G1172 | G1094 | C1010 | U928 | G858 | G787 | G714 | U650 | G568 | C500 | U439 |
| A1514 | U1432 | G1173 | U1095 | G1011 | U929 | A859 | G715 | U715 | G651 | U501 | U440 | U440 |
| U1515 | U1434 | U1262 | C1096 | U1012 | A933 | U861 | A788 | C717 | G652 | | | |
| | | G1263 | U1097 | A1013 | C934 | | | G717 | G653 | | | |



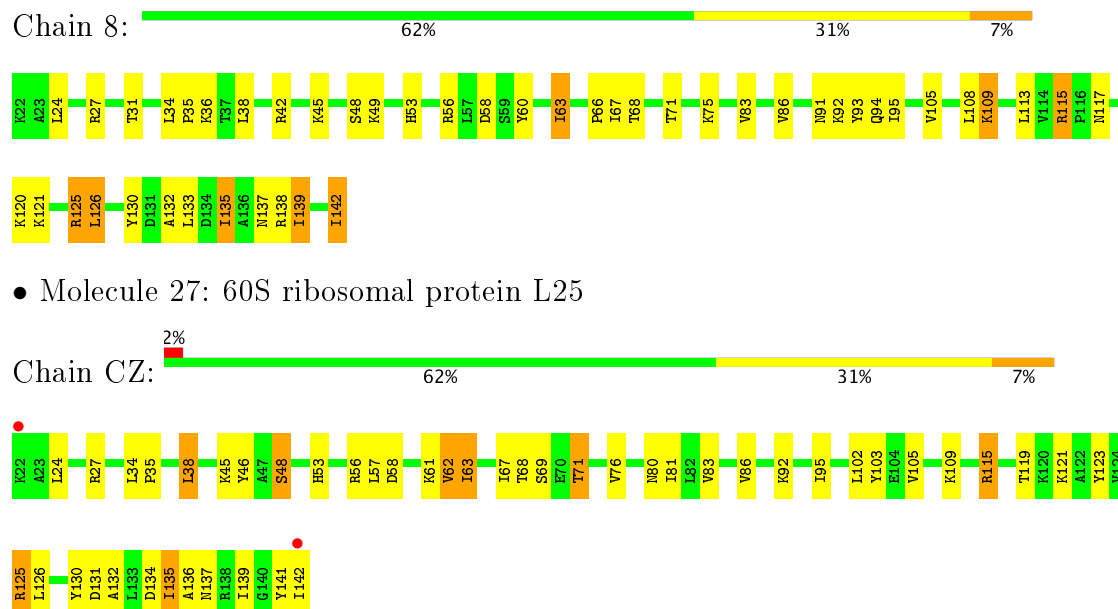
• Molecule 26: 60S ribosomal protein L24-A



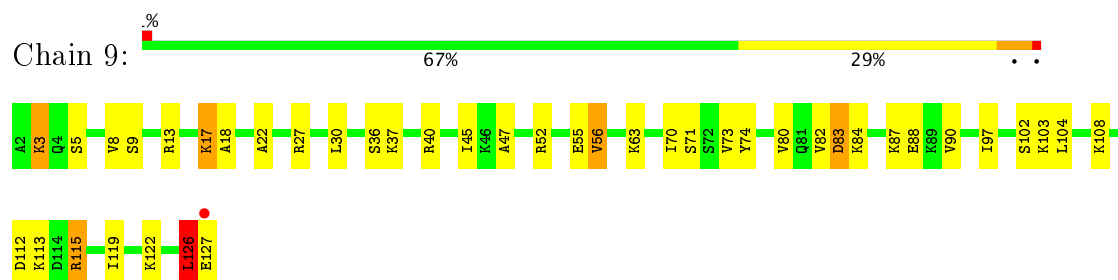
• Molecule 26: 60S ribosomal protein L24-A



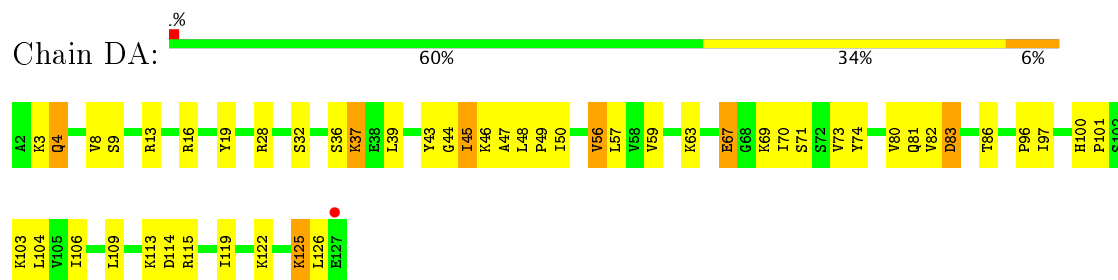
• Molecule 27: 60S ribosomal protein L25



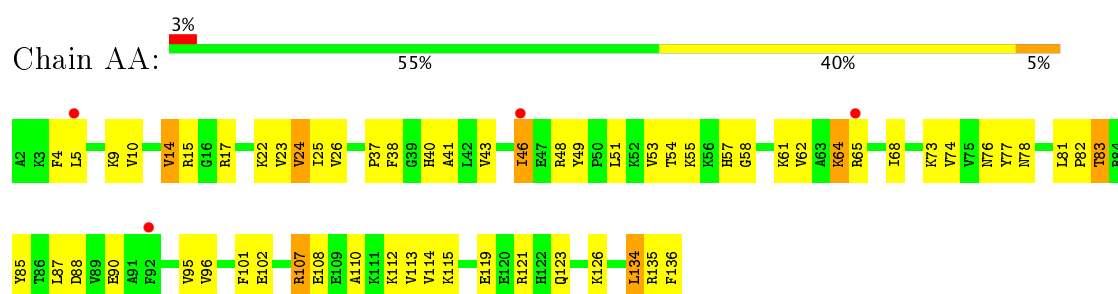
- Molecule 28: 60S ribosomal protein L26-A



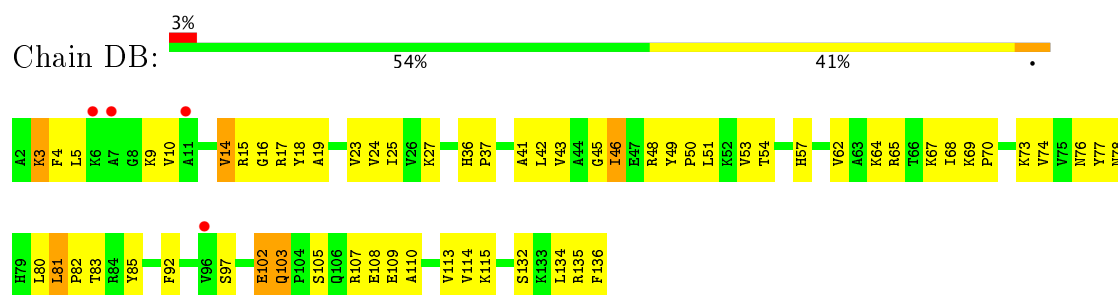
- Molecule 28: 60S ribosomal protein L26-A



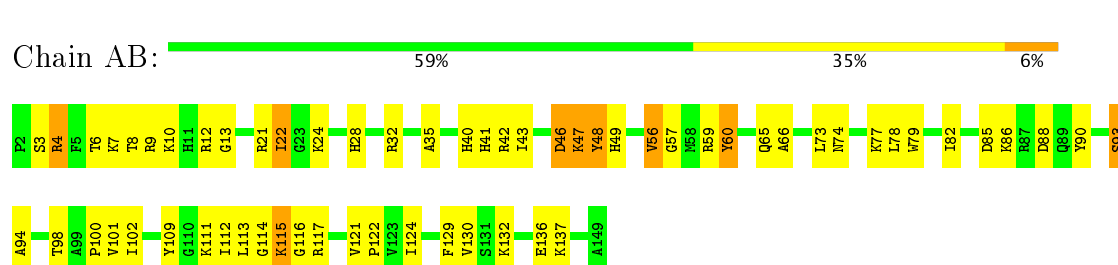
- Molecule 29: 60S ribosomal protein L27-A



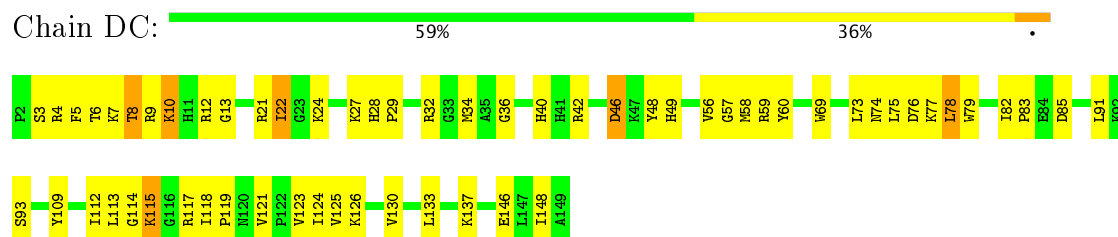
- Molecule 29: 60S ribosomal protein L27-A



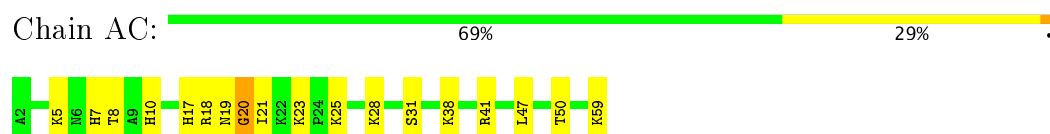
- Molecule 30: 60S ribosomal protein L28



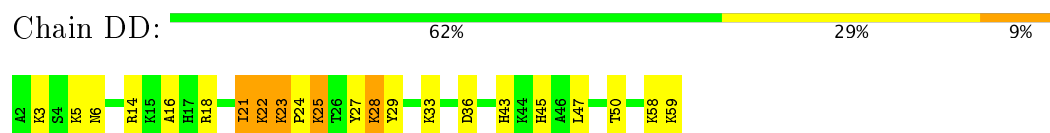
- Molecule 30: 60S ribosomal protein L28



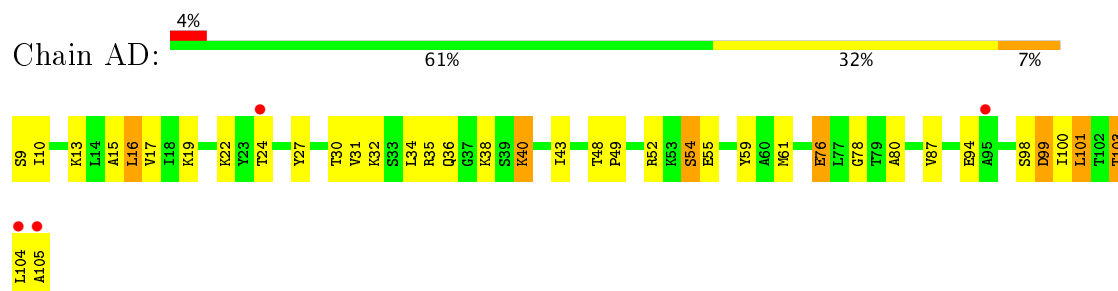
- Molecule 31: 60S ribosomal protein L29



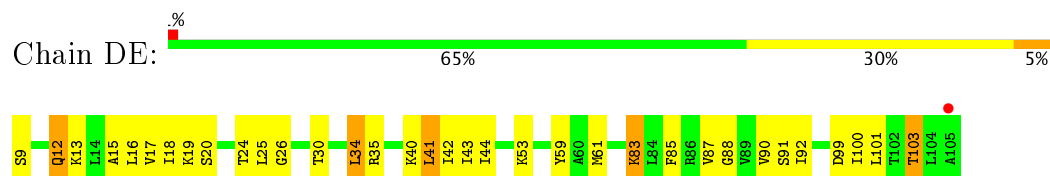
- Molecule 31: 60S ribosomal protein L29



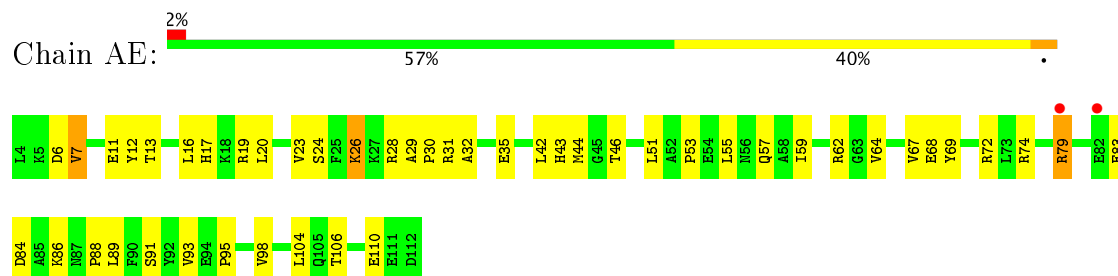
- Molecule 32: 60S ribosomal protein L30



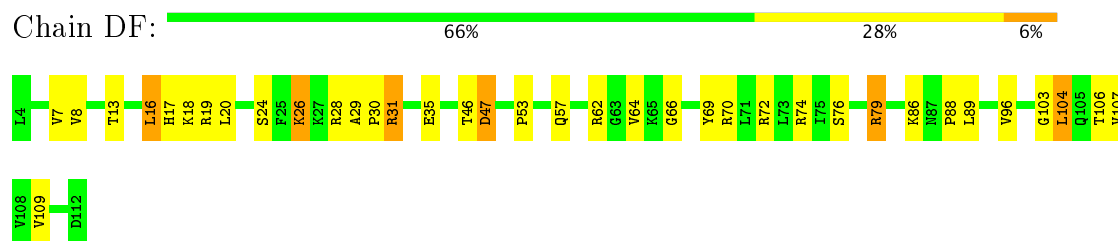
- Molecule 32: 60S ribosomal protein L30



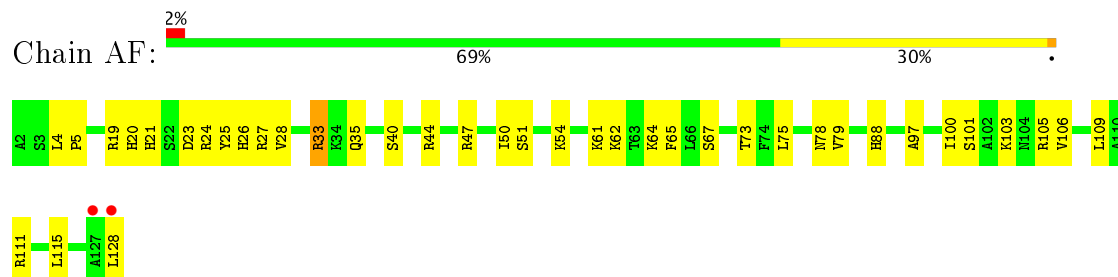
- Molecule 33: 60S ribosomal protein L31-A



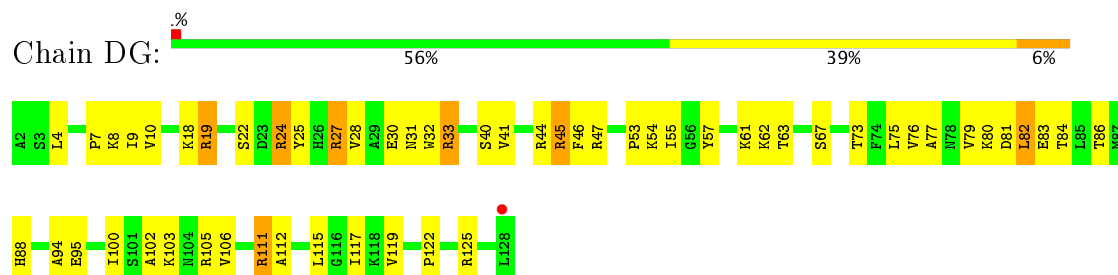
- Molecule 33: 60S ribosomal protein L31-A



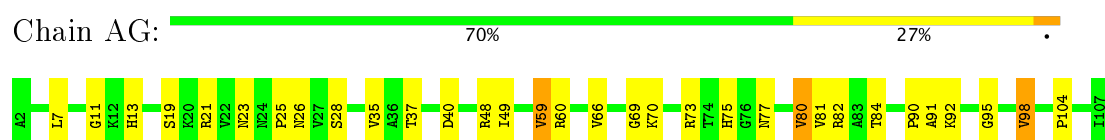
- Molecule 34: 60S ribosomal protein L32



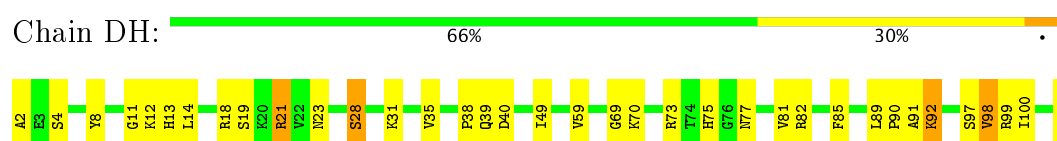
- Molecule 34: 60S ribosomal protein L32



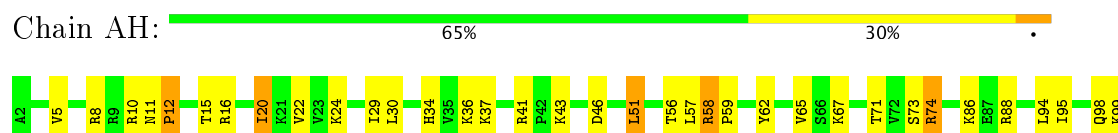
- Molecule 35: 60S ribosomal protein L33-A



- Molecule 35: 60S ribosomal protein L33-A



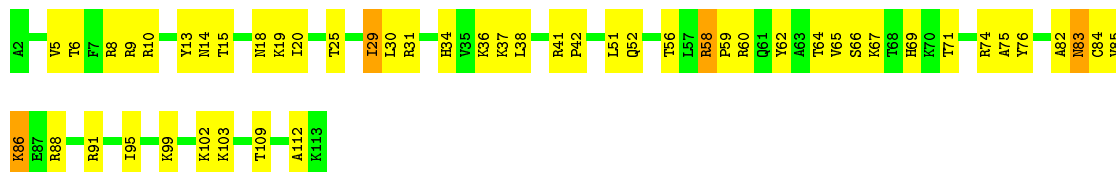
- Molecule 36: 60S ribosomal protein L34-A





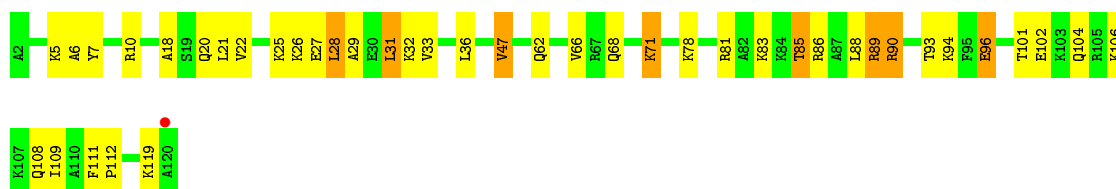
• Molecule 36: 60S ribosomal protein L34-A

Chain DI: 55% 41% .



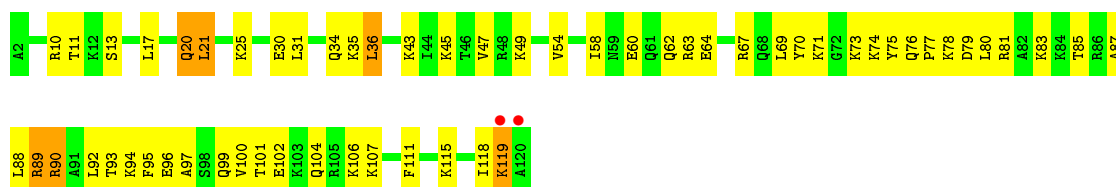
• Molecule 37: 60S ribosomal protein L35-A

Chain AI: .% 65% 29% 7%



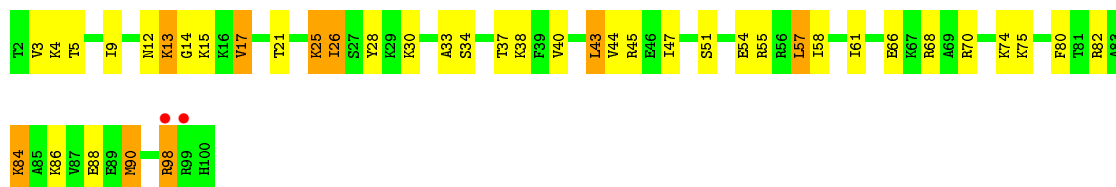
• Molecule 37: 60S ribosomal protein L35-A

Chain DJ: 2% 51% 44% 5%



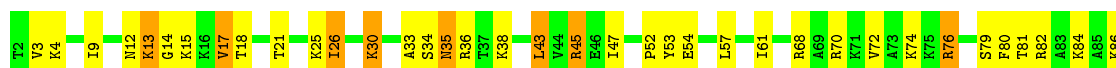
• Molecule 38: 60S ribosomal protein L36-A

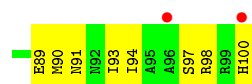
Chain AJ: 2% 59% 32% 9%



• Molecule 38: 60S ribosomal protein L36-A

Chain DK: 2% 55% 37% 8%





- Molecule 39: 60S ribosomal protein L37-A



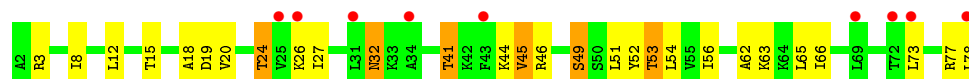
- Molecule 39: 60S ribosomal protein L37-A



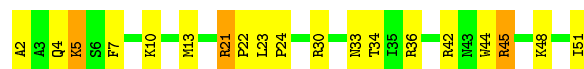
- Molecule 40: 60S ribosomal protein L38



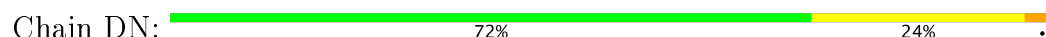
- Molecule 40: 60S ribosomal protein L38



- Molecule 41: 60S ribosomal protein L39

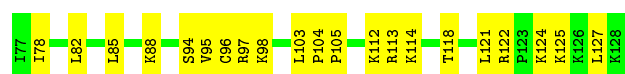


- Molecule 41: 60S ribosomal protein L39




- Molecule 42: Ubiquitin-60S ribosomal protein L40

Chain AN:  60% 40%



- Molecule 42: Ubiquitin-60S ribosomal protein L40

Chain DO:  73% 21% 6%



- Molecule 43: 60S ribosomal protein L41-B

Chain AO:  56% 32% 12%



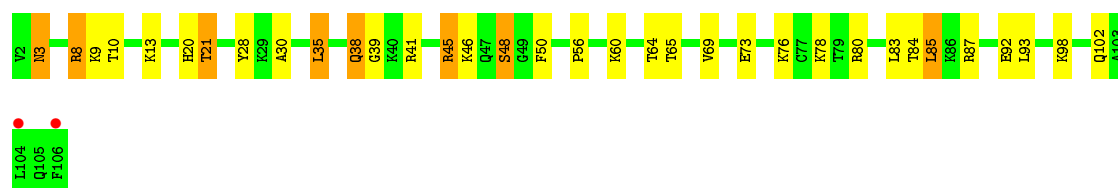
- Molecule 43: 60S ribosomal protein L41-B

Chain DP:  68% 20% 12%



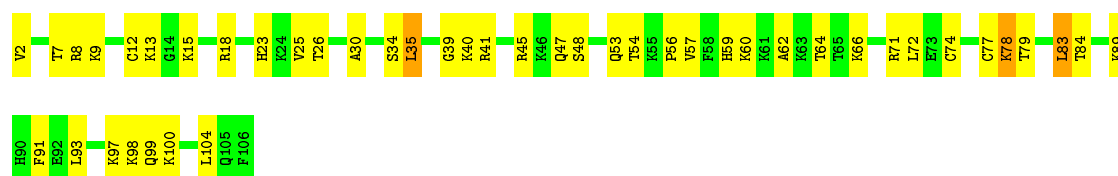
- Molecule 44: 60S ribosomal protein L42-A

Chain AP:  2% 68% 25% 8%



- Molecule 44: 60S ribosomal protein L42-A

Chain DQ:  57% 40% 3%



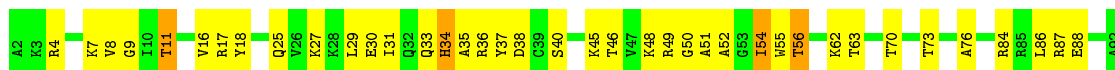
- Molecule 45: 60S ribosomal protein L43-A

Chain AQ:  67% 31% 2%

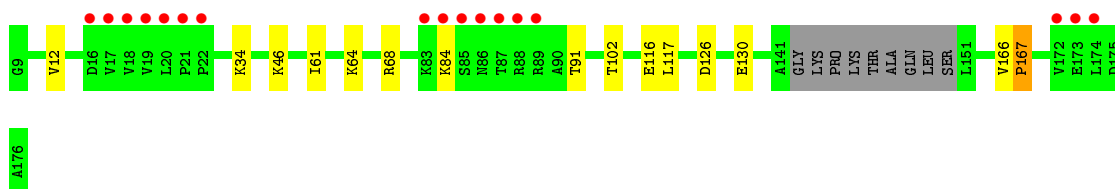
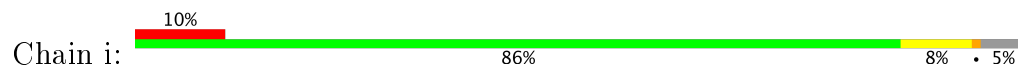




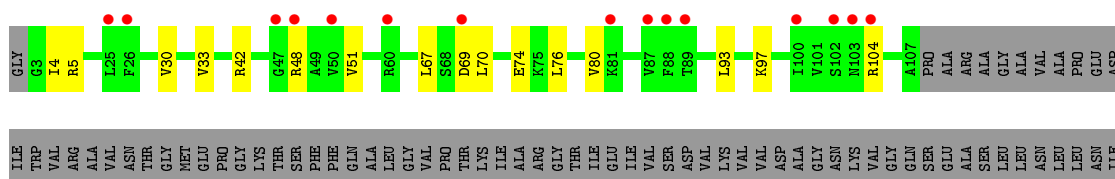
- Molecule 45: 60S ribosomal protein L43-A



- Molecule 46: Suppressor protein STM1



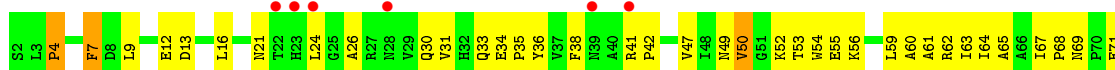
- Molecule 47: 60S acidic ribosomal protein P0

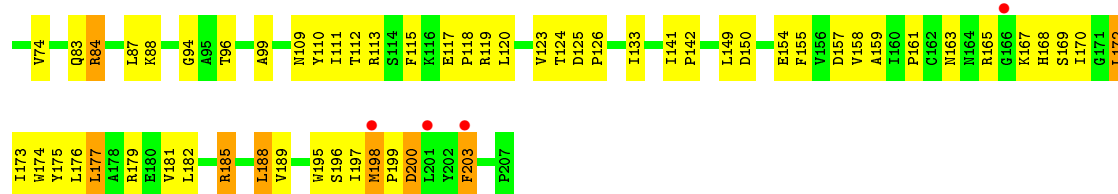


- Molecule 48: Suppressor protein STM1, Suppressor protein STM1, Suppressor protein Stm1 - Mol B



- Molecule 49: 40S ribosomal protein S0-A





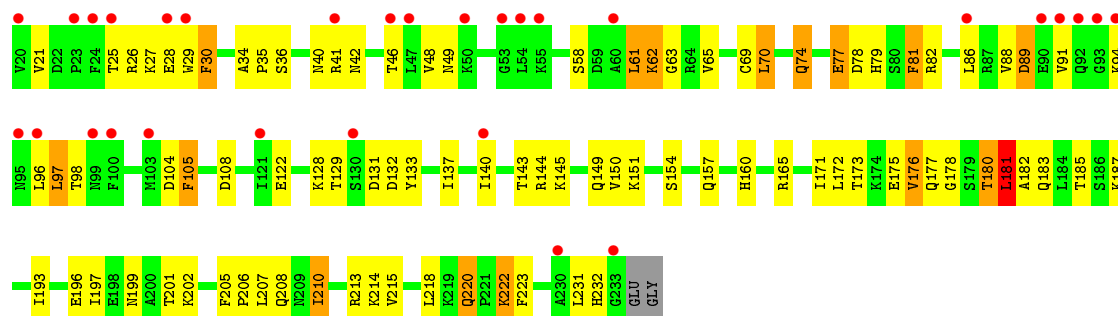
• Molecule 49: 40S ribosomal protein S0-A

Chain s0: 88% 12%



• Molecule 50: 40S ribosomal protein S1-A

Chain C: 14% 57% 35% 7%



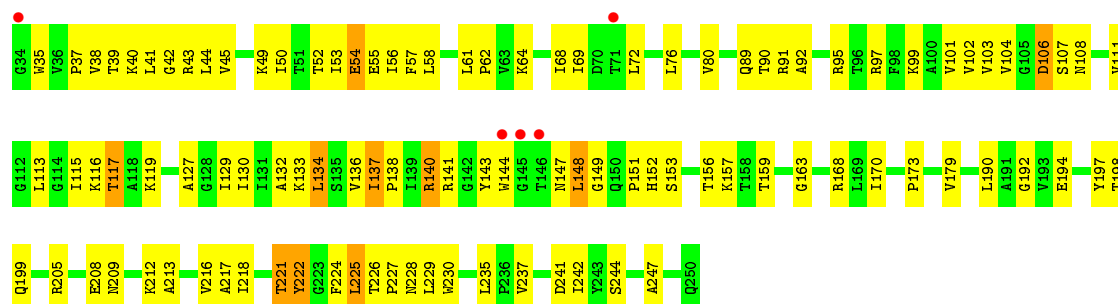
• Molecule 50: 40S ribosomal protein S1-A

Chain s1: 88% 11%

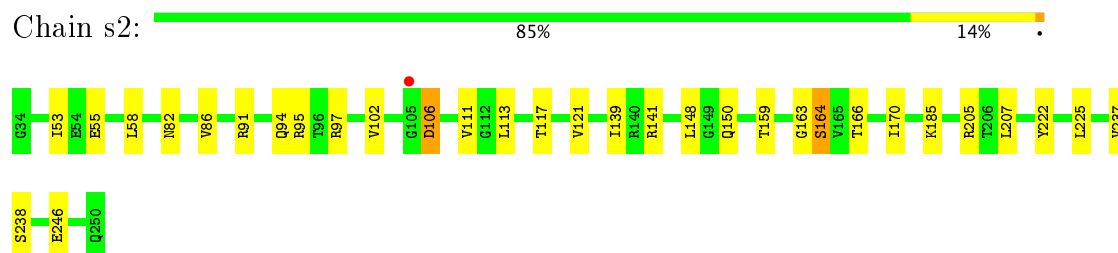


• Molecule 51: 40S ribosomal protein S2

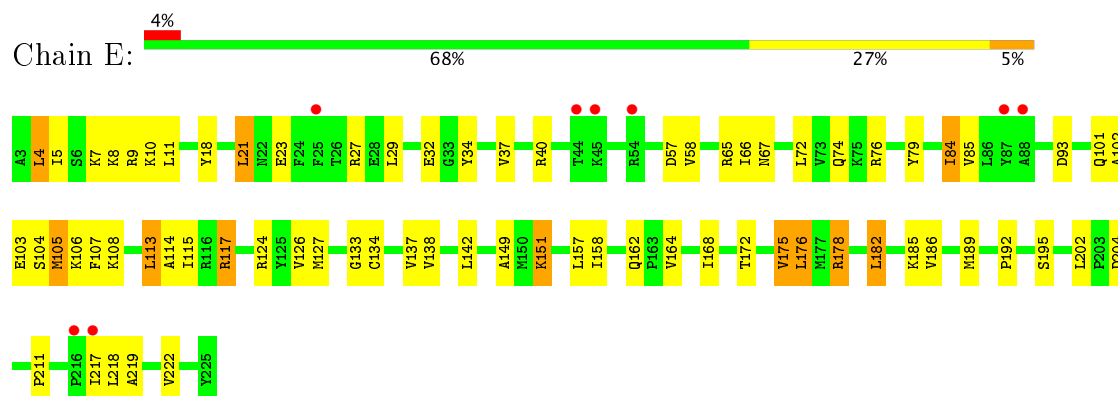
Chain D: 2% 53% 43% 5%



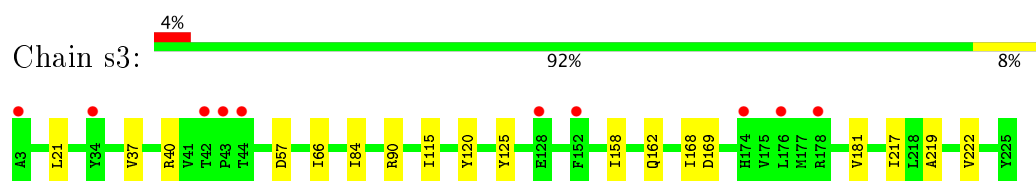
• Molecule 51: 40S ribosomal protein S2



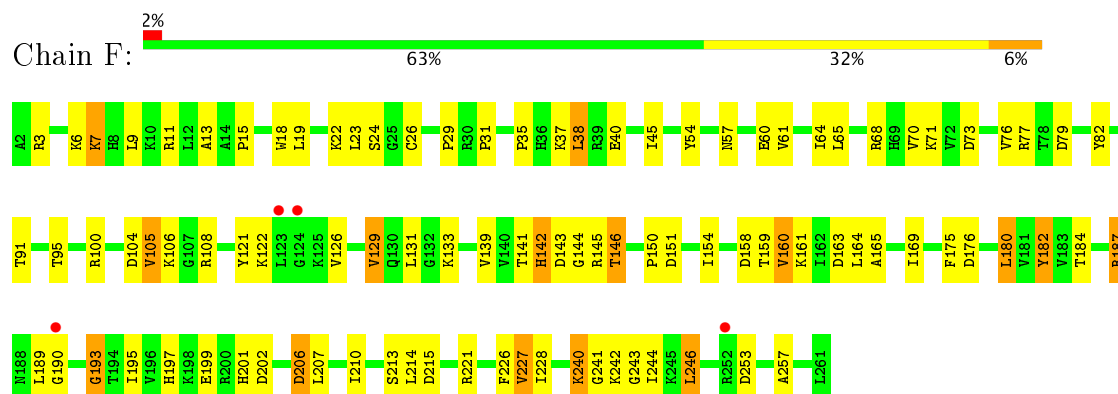
- Molecule 52: 40S ribosomal protein S3



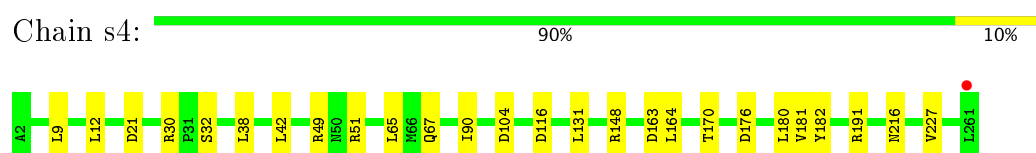
- Molecule 52: 40S ribosomal protein S3



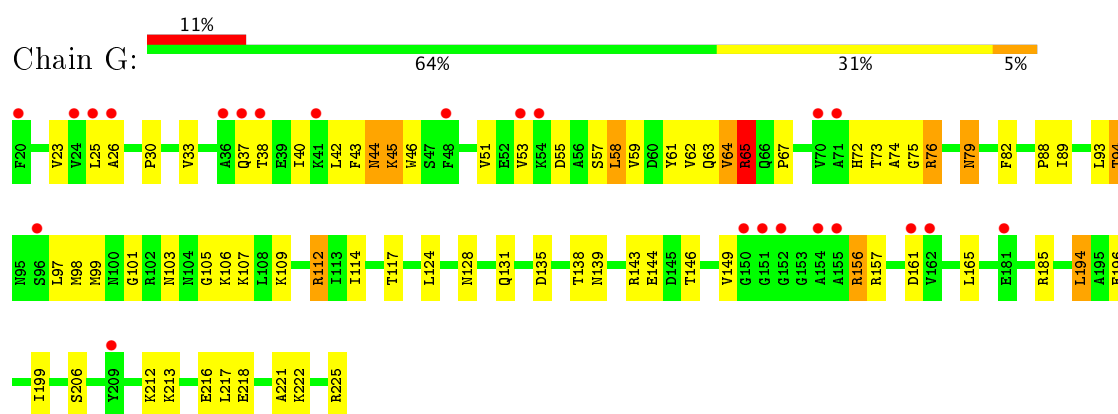
- Molecule 53: 40S ribosomal protein S4-A



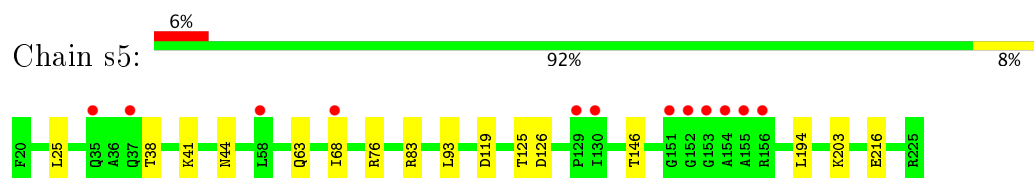
- Molecule 53: 40S ribosomal protein S4-A



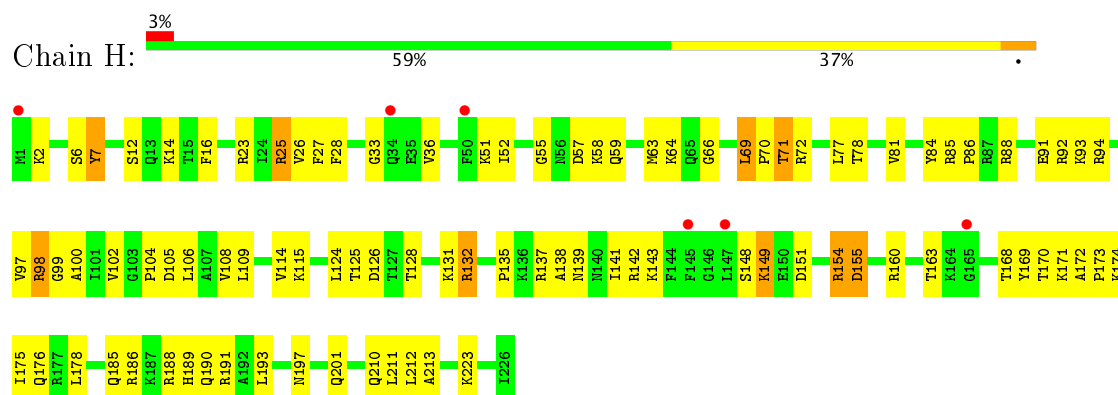
- Molecule 54: 40S ribosomal protein S5



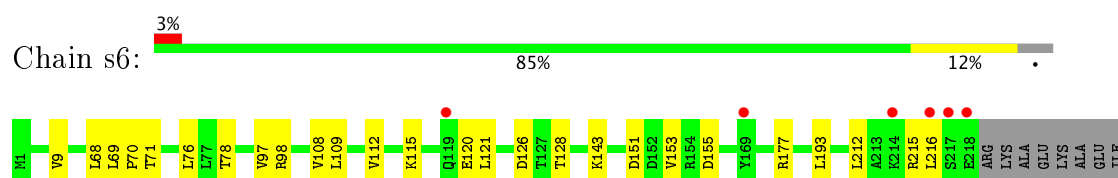
- Molecule 54: 40S ribosomal protein S5



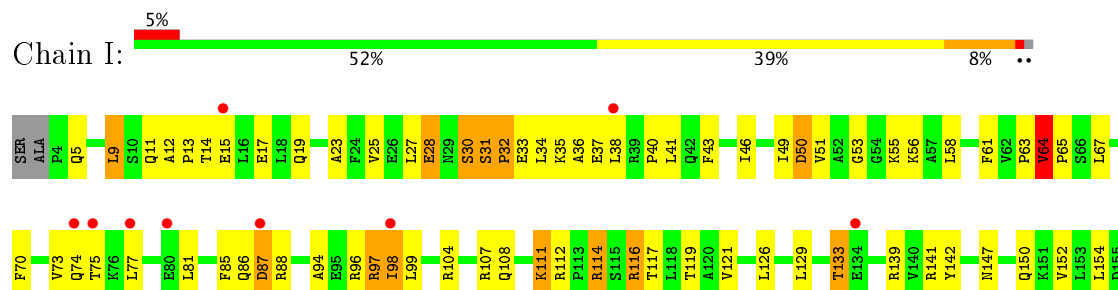
- Molecule 55: 40S ribosomal protein S6-A

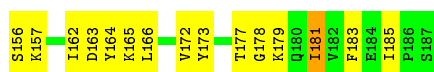


- Molecule 55: 40S ribosomal protein S6-A

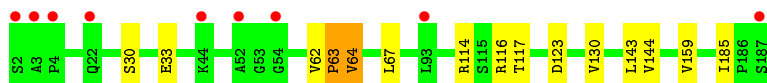
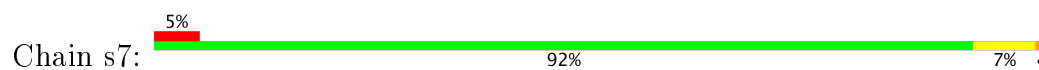


- Molecule 56: 40S ribosomal protein S7-A

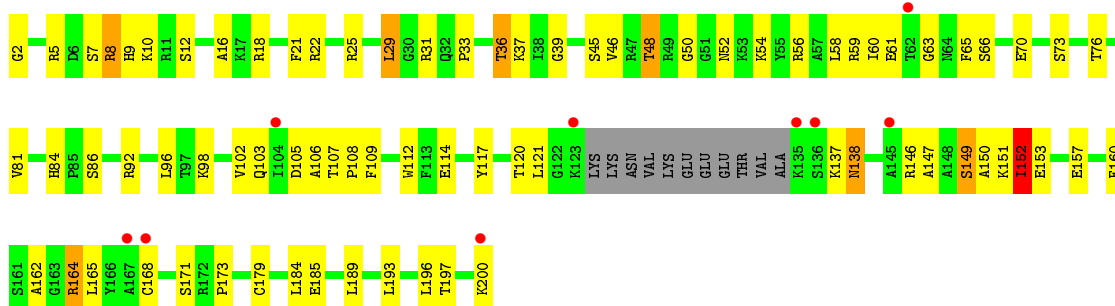




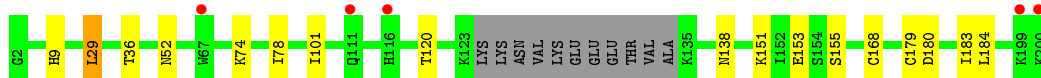
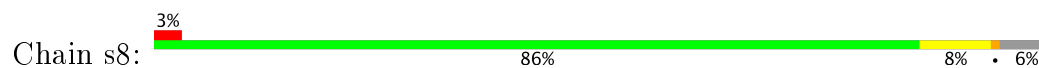
- Molecule 56: 40S ribosomal protein S7-A



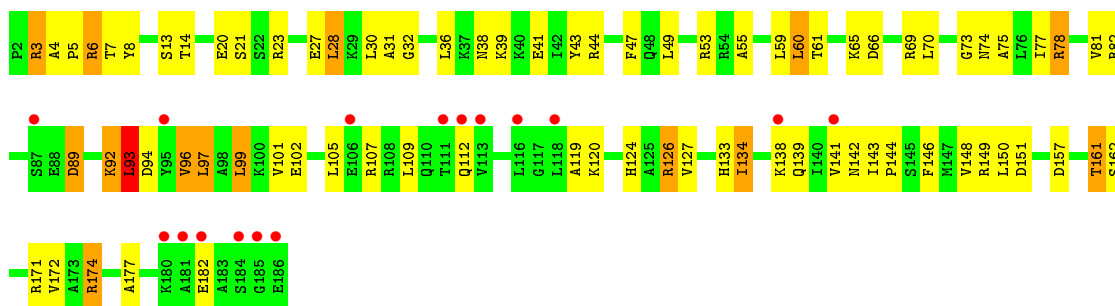
- Molecule 57: 40S ribosomal protein S8-A



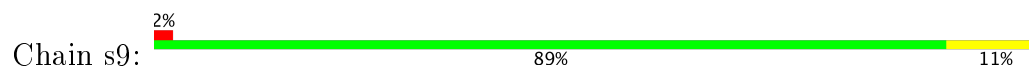
- Molecule 57: 40S ribosomal protein S8-A



- Molecule 58: 40S ribosomal protein S9-A

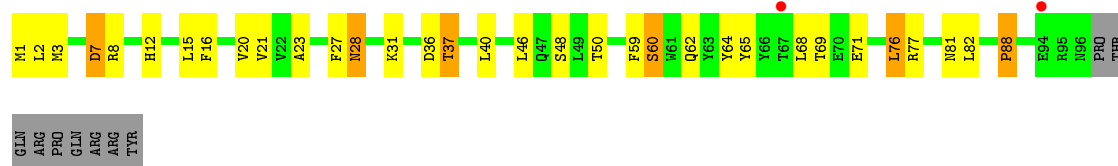


- Molecule 58: 40S ribosomal protein S9-A

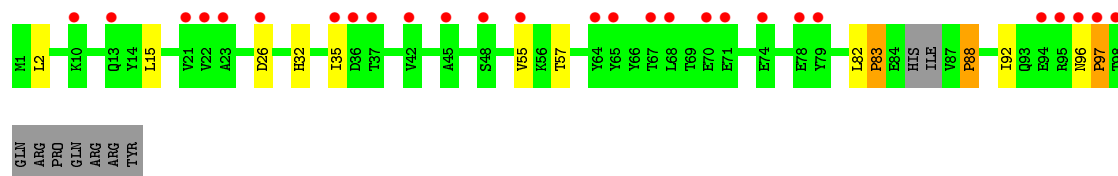
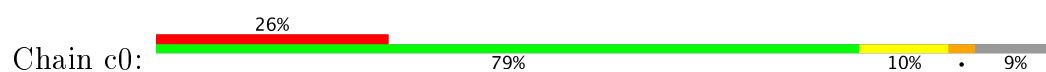




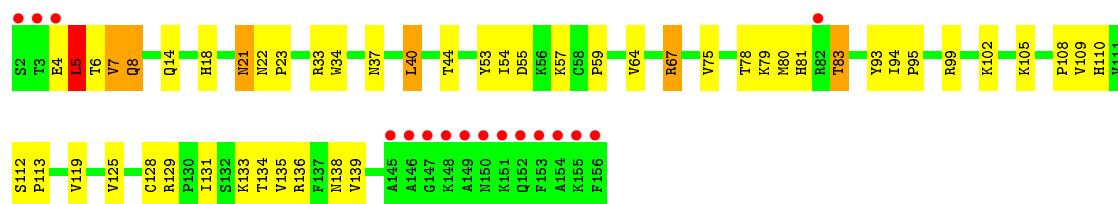
- Molecule 59: 40S ribosomal protein S10-A



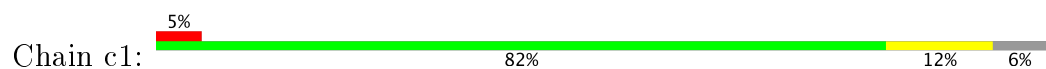
- Molecule 59: 40S ribosomal protein S10-A



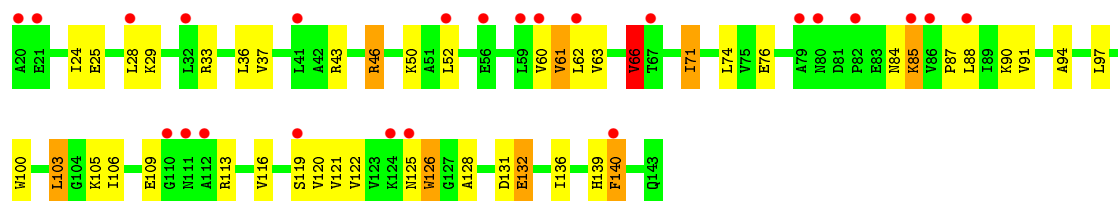
- Molecule 60: 40S ribosomal protein S11-A



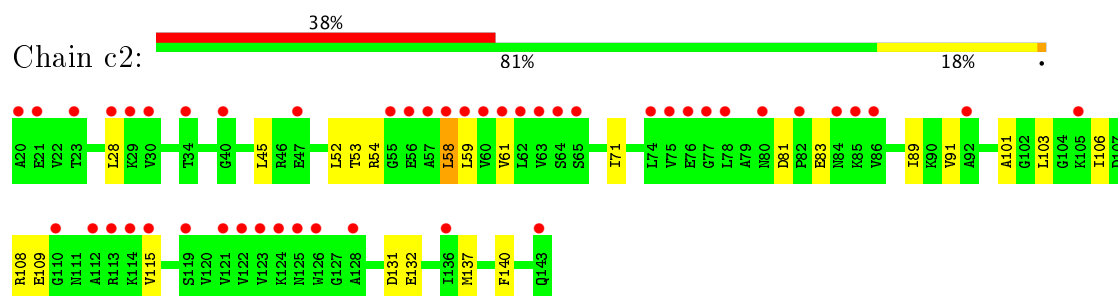
- Molecule 60: 40S ribosomal protein S11-A



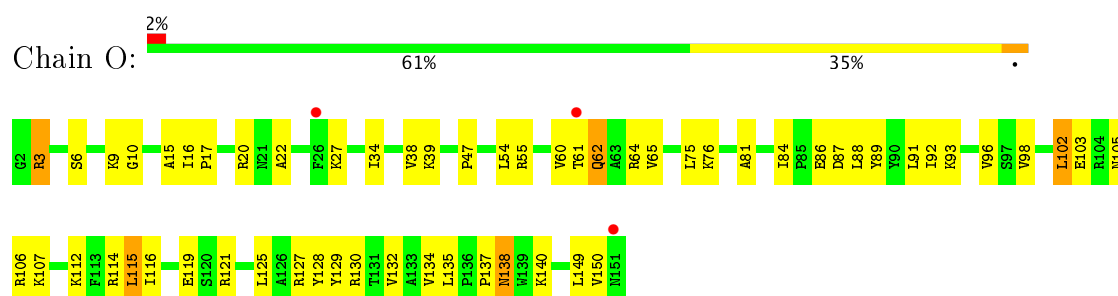
- Molecule 61: 40S ribosomal protein S12



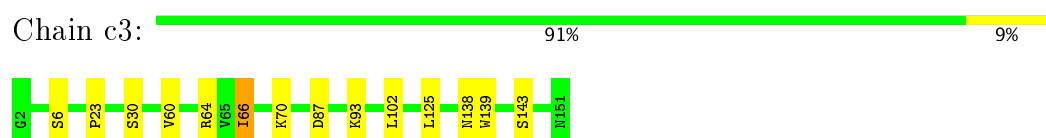
- Molecule 61: 40S ribosomal protein S12



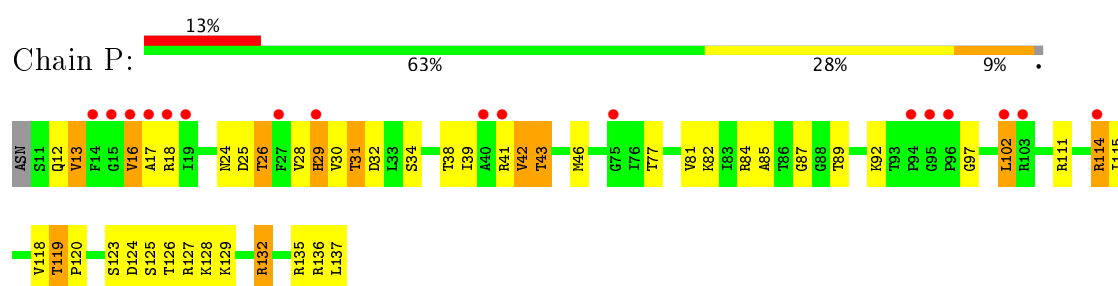
- Molecule 62: 40S ribosomal protein S13



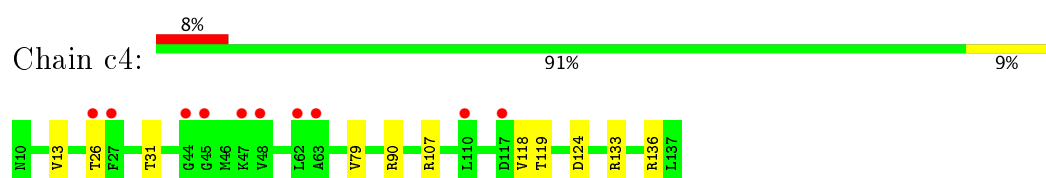
- Molecule 62: 40S ribosomal protein S13



- Molecule 63: 40S ribosomal protein S14-B

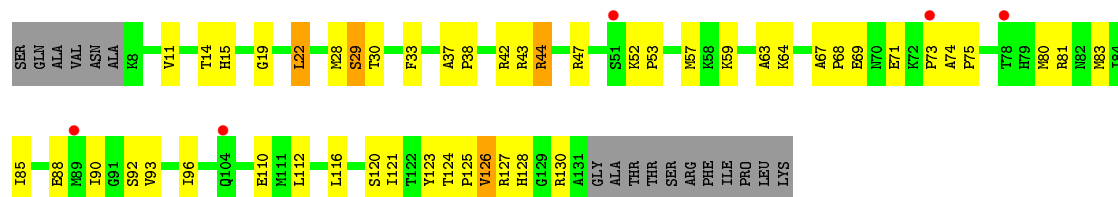


- Molecule 63: 40S ribosomal protein S14-B

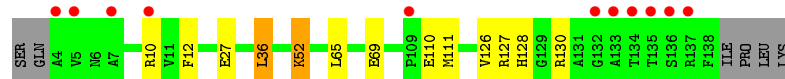
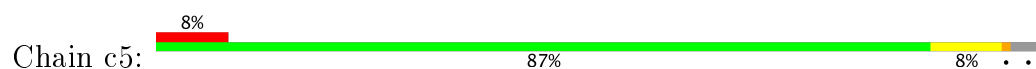


- Molecule 64: 40S ribosomal protein S15

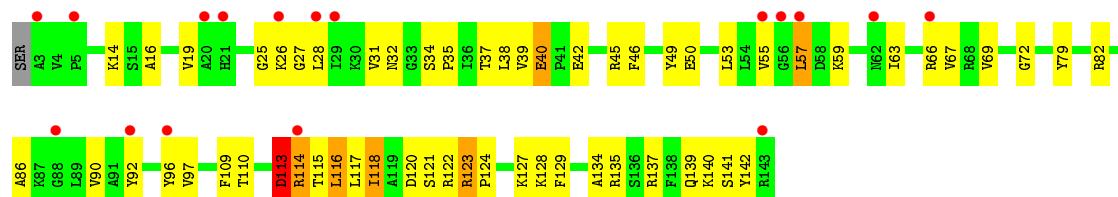




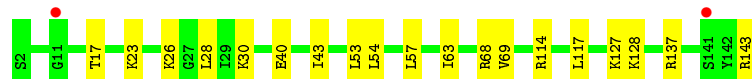
- Molecule 64: 40S ribosomal protein S15



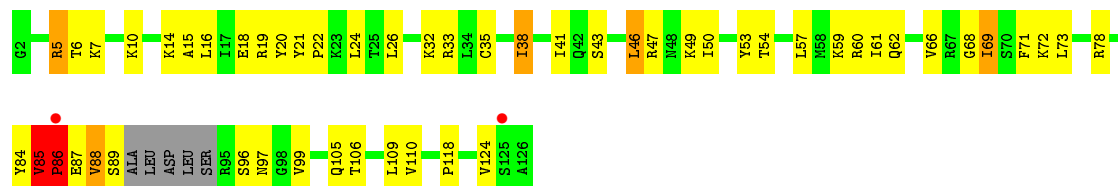
- Molecule 65: 40S ribosomal protein S16-A



- Molecule 65: 40S ribosomal protein S16-A



- Molecule 66: 40S ribosomal protein S17-B

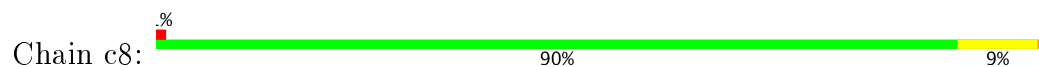


- Molecule 67: 40S ribosomal protein S18-A

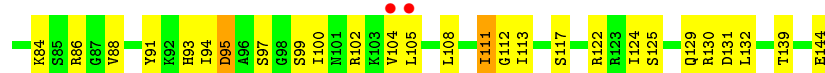
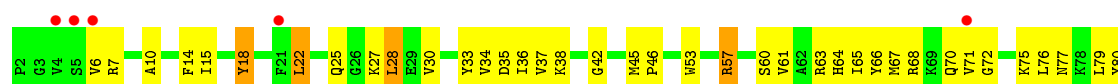




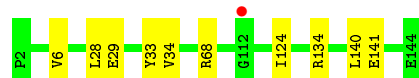
- Molecule 67: 40S ribosomal protein S18-A



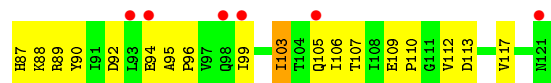
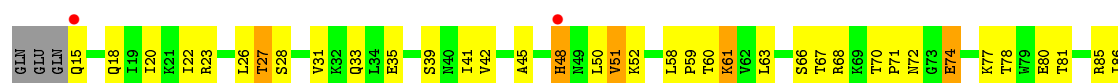
- Molecule 68: 40S ribosomal protein S19-A



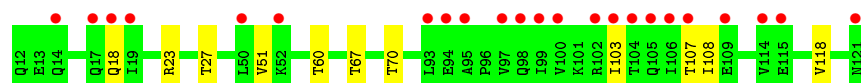
- Molecule 68: 40S ribosomal protein S19-A



- Molecule 69: 40S ribosomal protein S20

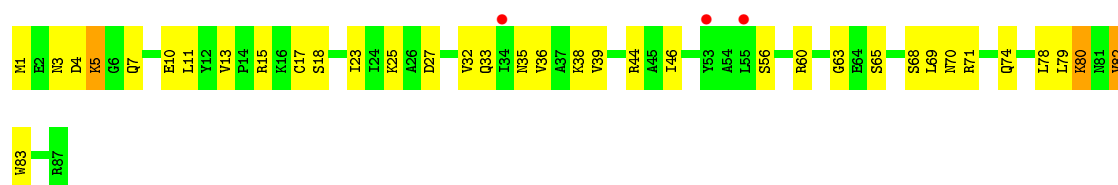


- Molecule 69: 40S ribosomal protein S20



- Molecule 70: 40S ribosomal protein S21-A





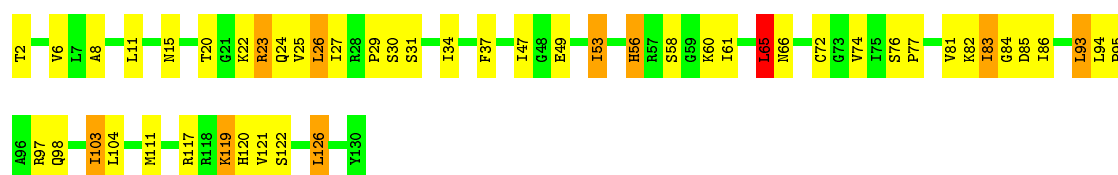
- Molecule 70: 40S ribosomal protein S21-A

Chain d1: 91% 9%



- Molecule 71: 40S ribosomal protein S22-A

Chain X: 61% 31% 7%



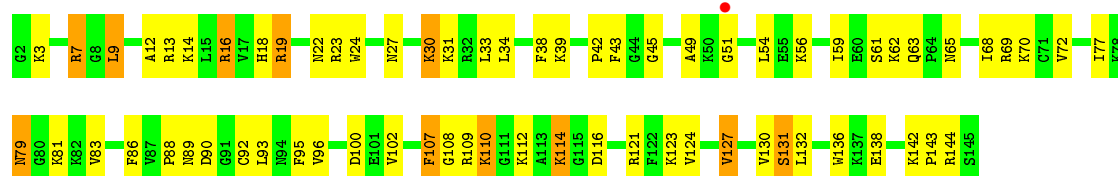
- Molecule 71: 40S ribosomal protein S22-A

Chain d2: 91% 9%



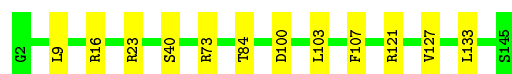
- Molecule 72: 40S ribosomal protein S23-A

Chain Y: 53% 40% 8%



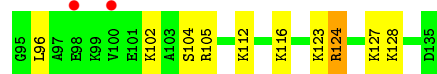
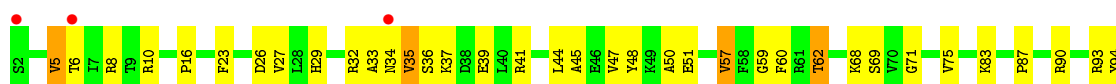
- Molecule 72: 40S ribosomal protein S23-A

Chain d3: 92% 8%

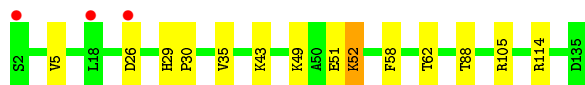
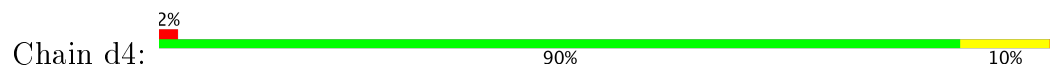


- Molecule 73: 40S ribosomal protein S24-A

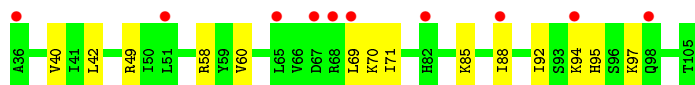
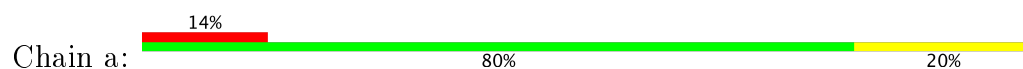
Chain Z: 4% 66% 31%



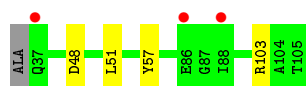
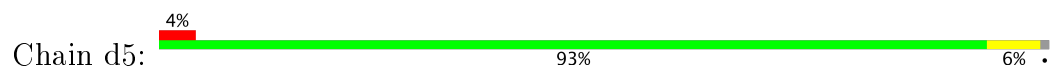
- Molecule 73: 40S ribosomal protein S24-A



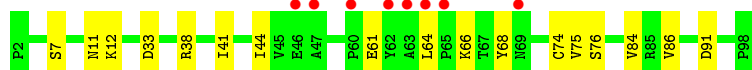
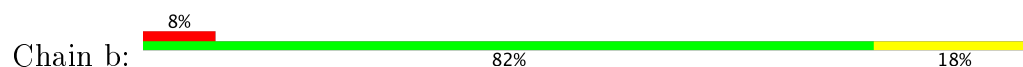
- Molecule 74: 40S ribosomal protein S25-A



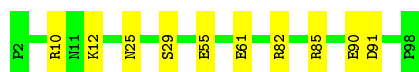
- Molecule 74: 40S ribosomal protein S25-A



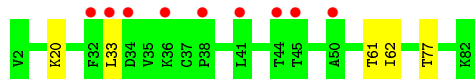
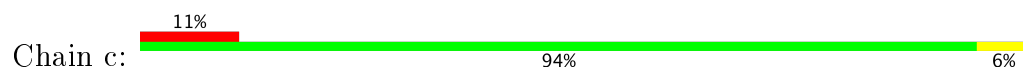
- Molecule 75: 40S ribosomal protein S26-B



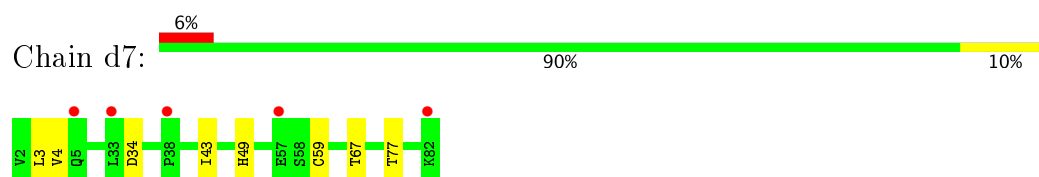
- Molecule 75: 40S ribosomal protein S26-B



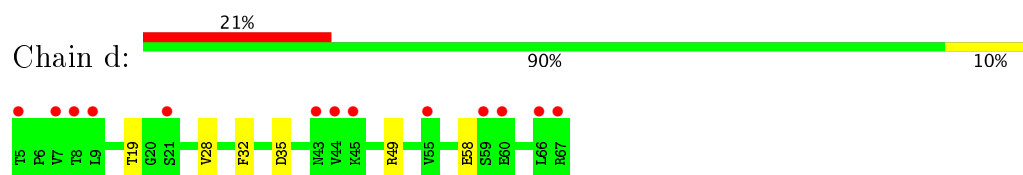
- Molecule 76: 40S ribosomal protein S27-A



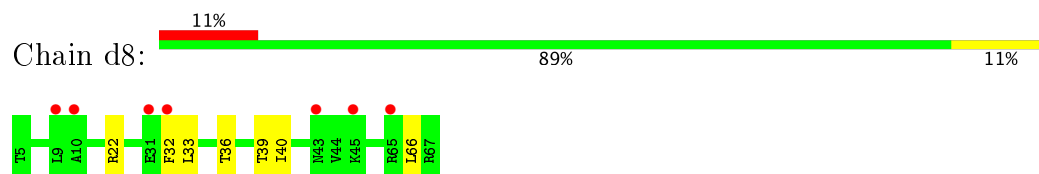
- Molecule 76: 40S ribosomal protein S27-A



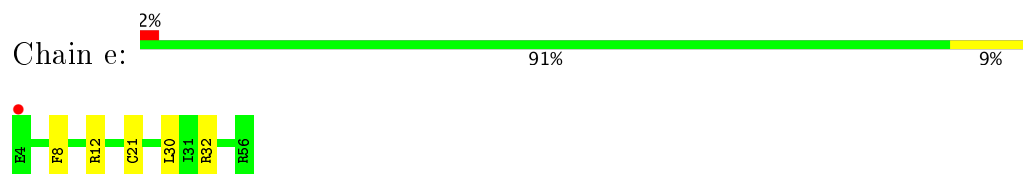
- Molecule 77: 40S ribosomal protein S28-A



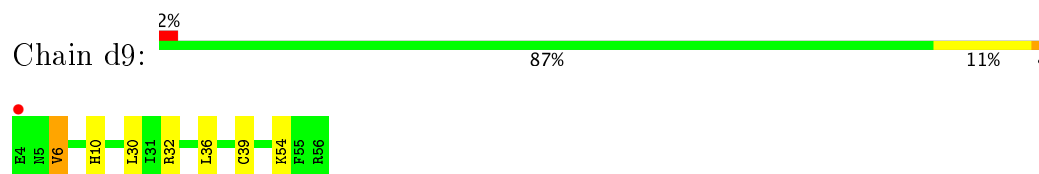
- Molecule 77: 40S ribosomal protein S28-A



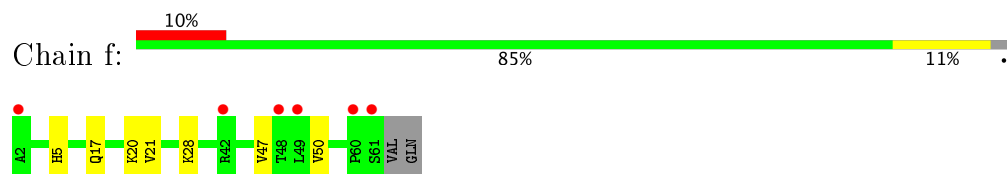
- Molecule 78: 40S ribosomal protein S29-A



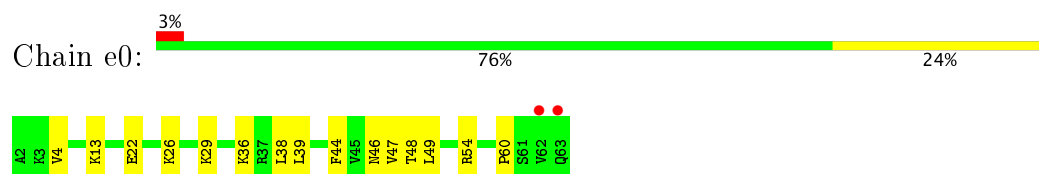
- Molecule 78: 40S ribosomal protein S29-A



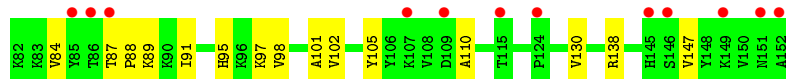
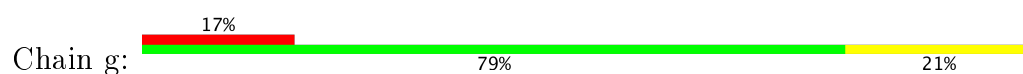
- Molecule 79: 40S ribosomal protein S30-A



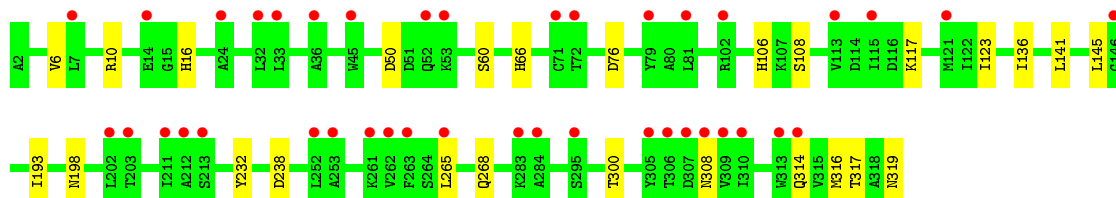
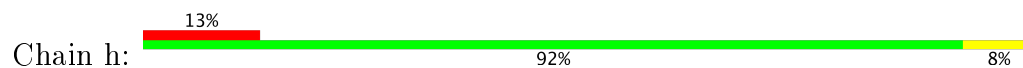
- Molecule 79: 40S ribosomal protein S30-A



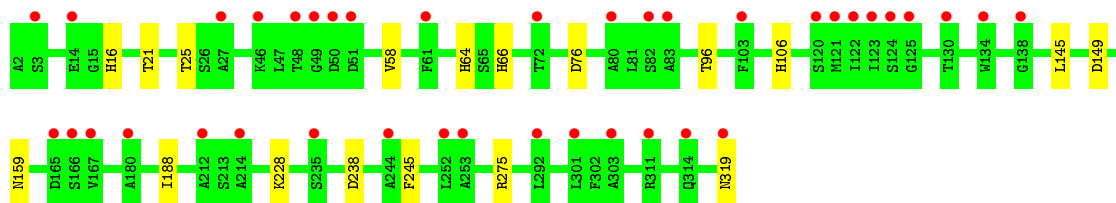
- Molecule 80: Ubiquitin-40S ribosomal protein S31



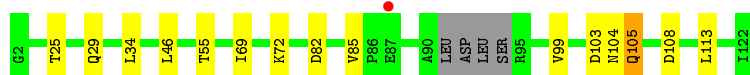
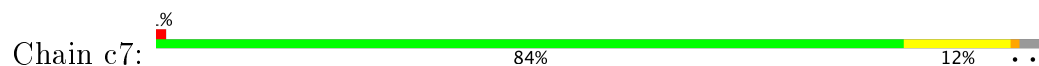
- Molecule 81: Guanine nucleotide-binding protein subunit beta-like protein



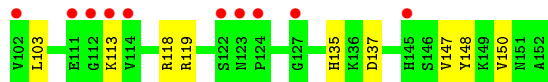
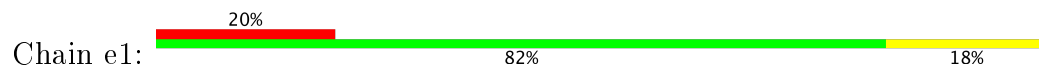
- Molecule 81: Guanine nucleotide-binding protein subunit beta-like protein



- Molecule 82: 40S ribosomal protein S17-A



- Molecule 83: Ubiquitin-40S ribosomal protein S31



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 304.08Å 286.55Å 436.55Å 90.00° 99.05° 90.00° | Depositor |
| Resolution (Å) | 98.38 – 3.50 98.38 – 3.50 | Depositor EDS |
| % Data completeness (in resolution range) | 100.0 (98.38-3.50) 100.0 (98.38-3.50) | Depositor EDS |
| R_{merge} | 0.57 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.30 (at 3.49Å) | Xtriage |
| Refinement program | PHENIX | Depositor |
| R, R_{free} | 0.195 , 0.239 0.195 , 0.239 | Depositor DCC |
| R_{free} test set | 18327 reflections (1.98%) | DCC |
| Wilson B-factor (Å ²) | 71.3 | Xtriage |
| Anisotropy | 0.145 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.29 , 84.2 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.91 | EDS |
| Total number of atoms | 409590 | wwPDB-VP |
| Average B, all atoms (Å ²) | 79.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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 | 0.68 | 3/75394 (0.0%) | 1.16 | 271/117545 (0.2%) |
| 1 | AR | 0.72 | 2/75394 (0.0%) | 1.19 | 322/117545 (0.3%) |
| 2 | 3 | 0.63 | 0/2883 | 1.06 | 5/4491 (0.1%) |
| 2 | AS | 0.68 | 0/2883 | 1.09 | 3/4491 (0.1%) |
| 3 | 4 | 0.62 | 0/3746 | 1.11 | 7/5832 (0.1%) |
| 3 | AT | 0.61 | 0/3746 | 1.07 | 7/5832 (0.1%) |
| 4 | CD | 0.46 | 0/1948 | 0.67 | 0/2617 |
| 4 | j | 0.47 | 0/1948 | 0.66 | 1/2617 (0.0%) |
| 5 | CE | 0.56 | 0/3146 | 0.69 | 0/4228 |
| 5 | k | 0.51 | 0/3146 | 0.65 | 0/4228 |
| 6 | CF | 0.49 | 0/2800 | 0.71 | 3/3790 (0.1%) |
| 6 | l | 0.50 | 0/2800 | 0.70 | 1/3790 (0.0%) |
| 7 | CG | 0.50 | 0/2425 | 0.62 | 0/3271 |
| 7 | m | 0.41 | 0/2425 | 0.58 | 0/3271 |
| 8 | CH | 0.51 | 0/1260 | 0.64 | 0/1694 |
| 8 | n | 0.50 | 0/1260 | 0.64 | 0/1694 |
| 9 | CI | 0.53 | 0/1821 | 0.67 | 0/2451 |
| 9 | o | 0.52 | 0/1821 | 0.66 | 1/2451 (0.0%) |
| 10 | CJ | 0.38 | 0/1836 | 0.57 | 1/2481 (0.0%) |
| 10 | p | 0.38 | 0/1836 | 0.56 | 0/2481 |
| 11 | CK | 0.52 | 0/1539 | 0.65 | 0/2073 |
| 11 | q | 0.46 | 0/1539 | 0.59 | 0/2073 |
| 12 | CL | 0.50 | 0/1741 | 0.64 | 0/2335 |
| 12 | r | 0.49 | 0/1741 | 0.62 | 1/2335 (0.0%) |
| 13 | CM | 0.48 | 0/1374 | 0.64 | 0/1842 |
| 13 | s | 0.40 | 0/1374 | 0.60 | 0/1842 |
| 14 | CN | 0.47 | 0/1568 | 0.64 | 0/2106 |
| 14 | t | 0.49 | 0/1568 | 0.67 | 0/2106 |
| 15 | CO | 0.53 | 0/1068 | 0.64 | 0/1438 |
| 15 | u | 0.48 | 0/1068 | 0.64 | 0/1438 |
| 16 | CP | 0.47 | 0/1757 | 0.61 | 0/2354 |
| 16 | v | 0.52 | 0/1757 | 0.66 | 0/2354 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | CQ | 0.64 | 0/1585 | 0.70 | 1/2128 (0.0%) |
| 17 | w | 0.56 | 0/1585 | 0.67 | 0/2128 |
| 18 | CR | 0.54 | 0/1443 | 0.67 | 0/1944 |
| 18 | x | 0.52 | 0/1443 | 0.66 | 0/1944 |
| 19 | CS | 0.47 | 0/1465 | 0.67 | 0/1965 |
| 19 | y | 0.51 | 0/1465 | 0.68 | 0/1965 |
| 20 | CT | 0.45 | 0/1538 | 0.64 | 0/2050 |
| 20 | z | 0.37 | 0/1538 | 0.55 | 0/2050 |
| 21 | 0 | 0.51 | 0/1481 | 0.68 | 0/1990 |
| 21 | CU | 0.55 | 0/1481 | 0.69 | 0/1990 |
| 22 | 2 | 0.52 | 0/1300 | 0.64 | 0/1743 |
| 22 | CV | 0.52 | 0/1300 | 0.64 | 0/1743 |
| 23 | 5 | 0.36 | 0/812 | 0.55 | 0/1099 |
| 23 | CW | 0.39 | 0/812 | 0.59 | 0/1099 |
| 24 | CX | 0.58 | 0/1018 | 0.69 | 0/1369 |
| 24 | l2 | 0.47 | 0/1018 | 0.63 | 0/1369 |
| 25 | 6 | 0.57 | 0/42490 | 1.06 | 96/66207 (0.1%) |
| 25 | A | 0.47 | 0/42443 | 0.97 | 50/66134 (0.1%) |
| 26 | 7 | 0.39 | 0/712 | 0.55 | 0/958 |
| 26 | CY | 0.48 | 0/712 | 0.66 | 0/958 |
| 27 | 8 | 0.43 | 0/979 | 0.63 | 0/1321 |
| 27 | CZ | 0.45 | 0/979 | 0.63 | 1/1321 (0.1%) |
| 28 | 9 | 0.45 | 0/1004 | 0.69 | 1/1341 (0.1%) |
| 28 | DA | 0.44 | 0/1004 | 0.67 | 0/1341 |
| 29 | AA | 0.36 | 0/1118 | 0.53 | 0/1497 |
| 29 | DB | 0.36 | 0/1118 | 0.56 | 0/1497 |
| 30 | AB | 0.48 | 0/1204 | 0.70 | 0/1612 |
| 30 | DC | 0.49 | 0/1204 | 0.74 | 0/1612 |
| 31 | AC | 0.43 | 0/473 | 0.65 | 1/629 (0.2%) |
| 31 | DD | 0.48 | 0/473 | 0.64 | 0/629 |
| 32 | AD | 0.33 | 0/751 | 0.51 | 0/1008 |
| 32 | DE | 0.38 | 0/751 | 0.55 | 0/1008 |
| 33 | AE | 0.42 | 0/890 | 0.58 | 0/1196 |
| 33 | DF | 0.49 | 0/890 | 0.65 | 0/1196 |
| 34 | AF | 0.55 | 0/1041 | 0.66 | 0/1394 |
| 34 | DG | 0.55 | 0/1041 | 0.64 | 0/1394 |
| 35 | AG | 0.55 | 0/868 | 0.70 | 0/1168 |
| 35 | DH | 0.55 | 0/868 | 0.67 | 0/1168 |
| 36 | AH | 0.40 | 0/890 | 0.57 | 0/1189 |
| 36 | DI | 0.39 | 0/890 | 0.60 | 0/1189 |
| 37 | AI | 0.44 | 0/978 | 0.58 | 0/1301 |
| 37 | DJ | 0.42 | 0/978 | 0.53 | 0/1301 |
| 38 | AJ | 0.44 | 0/778 | 0.61 | 0/1034 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 38 | DK | 0.41 | 0/778 | 0.58 | 0/1034 |
| 39 | AK | 0.49 | 0/696 | 0.72 | 0/923 |
| 39 | DL | 0.44 | 0/696 | 0.63 | 0/923 |
| 40 | AL | 0.36 | 0/618 | 0.52 | 0/826 |
| 40 | DM | 0.38 | 0/618 | 0.55 | 0/826 |
| 41 | AM | 0.46 | 0/443 | 0.67 | 0/588 |
| 41 | DN | 0.44 | 0/443 | 0.63 | 0/588 |
| 42 | AN | 0.50 | 0/423 | 0.67 | 0/562 |
| 42 | DO | 0.56 | 0/423 | 0.73 | 1/562 (0.2%) |
| 43 | AO | 0.42 | 0/234 | 0.64 | 0/300 |
| 43 | DP | 0.49 | 0/234 | 0.58 | 0/300 |
| 44 | AP | 0.48 | 0/860 | 0.72 | 1/1136 (0.1%) |
| 44 | DQ | 0.48 | 0/860 | 0.68 | 0/1136 |
| 45 | AQ | 0.44 | 0/701 | 0.61 | 0/934 |
| 45 | DR | 0.48 | 0/701 | 0.71 | 1/934 (0.1%) |
| 46 | i | 0.37 | 0/1113 | 0.57 | 1/1502 (0.1%) |
| 47 | p0 | 0.36 | 0/1092 | 0.53 | 0/1474 |
| 48 | sM | 0.41 | 0/480 | 0.64 | 0/642 |
| 49 | B | 0.37 | 0/1617 | 0.59 | 0/2215 |
| 49 | s0 | 0.39 | 0/1623 | 0.59 | 0/2222 |
| 50 | C | 0.32 | 0/1735 | 0.57 | 1/2335 (0.0%) |
| 50 | s1 | 0.36 | 0/1748 | 0.60 | 1/2352 (0.0%) |
| 51 | D | 0.36 | 0/1665 | 0.57 | 0/2263 |
| 51 | s2 | 0.43 | 0/1665 | 0.62 | 0/2263 |
| 52 | E | 0.35 | 0/1759 | 0.56 | 0/2368 |
| 52 | s3 | 0.33 | 0/1759 | 0.53 | 0/2368 |
| 53 | F | 0.36 | 0/2109 | 0.61 | 1/2839 (0.0%) |
| 53 | s4 | 0.41 | 0/2109 | 0.63 | 0/2839 |
| 54 | G | 0.32 | 0/1629 | 0.52 | 0/2202 |
| 54 | s5 | 0.36 | 0/1629 | 0.56 | 0/2202 |
| 55 | H | 0.34 | 0/1823 | 0.53 | 0/2439 |
| 55 | s6 | 0.40 | 0/1779 | 0.54 | 0/2379 |
| 56 | I | 0.33 | 0/1506 | 0.59 | 0/2028 |
| 56 | s7 | 0.35 | 0/1516 | 0.57 | 0/2043 |
| 57 | J | 0.40 | 0/1514 | 0.60 | 0/2021 |
| 57 | s8 | 0.44 | 0/1514 | 0.65 | 1/2021 (0.0%) |
| 58 | K | 0.32 | 0/1519 | 0.58 | 0/2035 |
| 58 | s9 | 0.40 | 0/1519 | 0.58 | 0/2035 |
| 59 | L | 0.35 | 0/789 | 0.66 | 1/1067 (0.1%) |
| 59 | c0 | 0.33 | 0/776 | 0.64 | 3/1047 (0.3%) |
| 60 | M | 0.43 | 0/1239 | 0.62 | 1/1673 (0.1%) |
| 60 | c1 | 0.47 | 0/1194 | 0.62 | 0/1610 |
| 61 | N | 0.34 | 0/898 | 0.63 | 0/1220 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 61 | c2 | 0.29 | 0/898 | 0.59 | 1/1220 (0.1%) |
| 62 | O | 0.35 | 0/1215 | 0.55 | 0/1638 |
| 62 | c3 | 0.41 | 0/1215 | 0.59 | 0/1638 |
| 63 | P | 0.34 | 0/901 | 0.61 | 0/1217 |
| 63 | c4 | 0.40 | 0/960 | 0.66 | 0/1290 |
| 64 | Q | 0.34 | 0/998 | 0.59 | 0/1341 |
| 64 | c5 | 0.38 | 0/1060 | 0.62 | 1/1426 (0.1%) |
| 65 | R | 0.35 | 0/1125 | 0.58 | 0/1510 |
| 65 | c6 | 0.39 | 0/1131 | 0.57 | 0/1518 |
| 66 | S | 0.37 | 0/935 | 0.65 | 2/1254 (0.2%) |
| 67 | T | 0.35 | 0/1211 | 0.55 | 0/1628 |
| 67 | c8 | 0.39 | 0/1211 | 0.59 | 0/1628 |
| 68 | U | 0.33 | 0/1130 | 0.53 | 0/1517 |
| 68 | c9 | 0.36 | 0/1130 | 0.53 | 0/1517 |
| 69 | V | 0.37 | 0/865 | 0.60 | 0/1169 |
| 69 | d0 | 0.37 | 0/892 | 0.58 | 0/1205 |
| 70 | W | 0.35 | 0/693 | 0.53 | 0/935 |
| 70 | d1 | 0.38 | 0/693 | 0.60 | 0/935 |
| 71 | X | 0.36 | 0/1038 | 0.67 | 2/1395 (0.1%) |
| 71 | d2 | 0.45 | 0/1038 | 0.62 | 0/1395 |
| 72 | Y | 0.44 | 0/1139 | 0.64 | 0/1518 |
| 72 | d3 | 0.51 | 0/1139 | 0.67 | 0/1518 |
| 73 | Z | 0.34 | 0/1087 | 0.50 | 0/1449 |
| 73 | d4 | 0.40 | 0/1087 | 0.61 | 0/1449 |
| 74 | a | 0.33 | 0/571 | 0.60 | 0/768 |
| 74 | d5 | 0.34 | 0/566 | 0.56 | 0/761 |
| 75 | b | 0.37 | 0/782 | 0.59 | 0/1047 |
| 75 | d6 | 0.42 | 0/782 | 0.60 | 0/1047 |
| 76 | c | 0.33 | 0/620 | 0.56 | 0/838 |
| 76 | d7 | 0.36 | 0/620 | 0.58 | 0/838 |
| 77 | d | 0.29 | 0/499 | 0.52 | 0/670 |
| 77 | d8 | 0.32 | 0/499 | 0.54 | 0/670 |
| 78 | d9 | 0.40 | 0/452 | 0.57 | 0/600 |
| 78 | e | 0.42 | 0/452 | 0.61 | 0/600 |
| 79 | e0 | 0.41 | 0/499 | 0.70 | 0/665 |
| 79 | f | 0.36 | 0/483 | 0.60 | 0/643 |
| 80 | g | 0.41 | 0/577 | 0.73 | 0/770 |
| 81 | h | 0.31 | 0/2490 | 0.51 | 0/3389 |
| 81 | sR | 0.32 | 0/2495 | 0.51 | 0/3395 |
| 82 | c7 | 0.37 | 0/914 | 0.58 | 0/1224 |
| 83 | e1 | 0.33 | 0/404 | 0.67 | 0/542 |
| All | All | 0.56 | 5/429965 (0.0%) | 0.96 | 792/631328 (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 |
|-----|-------|---------------------|---------------------|
| 7 | CG | 0 | 1 |
| 10 | CJ | 0 | 1 |
| 12 | CL | 0 | 1 |
| 15 | u | 0 | 1 |
| 17 | CQ | 0 | 1 |
| 17 | w | 0 | 1 |
| 20 | CT | 0 | 1 |
| 22 | 2 | 0 | 1 |
| 26 | 7 | 0 | 1 |
| 26 | CY | 0 | 2 |
| 28 | 9 | 0 | 1 |
| 28 | DA | 0 | 1 |
| 29 | DB | 0 | 1 |
| 30 | AB | 0 | 1 |
| 31 | AC | 0 | 1 |
| 48 | sM | 0 | 1 |
| 49 | B | 0 | 1 |
| 50 | s1 | 0 | 1 |
| 51 | D | 0 | 1 |
| 51 | s2 | 0 | 1 |
| 52 | E | 0 | 1 |
| 52 | s3 | 0 | 1 |
| 53 | F | 0 | 1 |
| 54 | G | 0 | 2 |
| 54 | s5 | 0 | 1 |
| 56 | I | 0 | 2 |
| 56 | s7 | 0 | 4 |
| 58 | K | 0 | 1 |
| 61 | c2 | 0 | 4 |
| 64 | Q | 0 | 1 |
| 64 | c5 | 0 | 1 |
| 65 | R | 0 | 2 |
| 65 | c6 | 0 | 1 |
| 66 | S | 0 | 2 |
| 73 | d4 | 0 | 2 |
| 74 | a | 0 | 1 |
| 80 | g | 0 | 2 |
| 82 | c7 | 0 | 1 |
| All | All | 0 | 51 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | AR | 895 | A | C5-C6 | -5.81 | 1.35 | 1.41 |
| 1 | 1 | 936 | A | N9-C4 | -5.30 | 1.34 | 1.37 |
| 1 | AR | 2911 | A | N9-C4 | -5.05 | 1.34 | 1.37 |
| 1 | 1 | 1865 | A | N9-C4 | -5.05 | 1.34 | 1.37 |
| 1 | 1 | 3180 | A | N9-C4 | -5.03 | 1.34 | 1.37 |

The worst 5 of 792 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | AR | 2821 | C | C6-N1-C2 | -9.74 | 116.40 | 120.30 |
| 1 | 1 | 637 | C | C6-N1-C2 | 9.70 | 124.18 | 120.30 |
| 3 | 4 | 94 | C | C6-N1-C2 | 9.68 | 124.17 | 120.30 |
| 1 | 1 | 2727 | A | N1-C6-N6 | -9.61 | 112.84 | 118.60 |
| 25 | 6 | 163 | G | N3-C4-N9 | -9.23 | 120.46 | 126.00 |

There are no chirality outliers.

5 of 51 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 22 | 2 | 122 | GLN | Peptide |
| 26 | 7 | 94 | ARG | Peptide |
| 28 | 9 | 83 | ASP | Peptide |
| 15 | u | 28 | SER | Peptide |
| 17 | w | 110 | PRO | Peptide |

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 1 | 67355 | 0 | 33846 | 1062 | 0 |
| 1 | AR | 67355 | 0 | 33843 | 1257 | 0 |
| 2 | 3 | 2579 | 0 | 1303 | 32 | 0 |
| 2 | AS | 2579 | 0 | 1304 | 48 | 0 |
| 3 | 4 | 3353 | 0 | 1695 | 64 | 0 |
| 3 | AT | 3353 | 0 | 1695 | 62 | 0 |
| 4 | CD | 1914 | 0 | 1981 | 78 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4 | j | 1914 | 0 | 1981 | 0 | 0 |
| 5 | CE | 3075 | 0 | 3142 | 128 | 0 |
| 5 | k | 3075 | 0 | 3142 | 0 | 0 |
| 6 | CF | 2748 | 0 | 2859 | 91 | 0 |
| 6 | l | 2748 | 0 | 2859 | 0 | 0 |
| 7 | CG | 2375 | 0 | 2325 | 78 | 0 |
| 7 | m | 2375 | 0 | 2325 | 0 | 0 |
| 8 | CH | 1239 | 0 | 1326 | 39 | 0 |
| 8 | n | 1239 | 0 | 1326 | 0 | 0 |
| 9 | CI | 1784 | 0 | 1862 | 59 | 0 |
| 9 | o | 1784 | 0 | 1862 | 0 | 0 |
| 10 | CJ | 1804 | 0 | 1877 | 47 | 0 |
| 10 | p | 1804 | 0 | 1877 | 0 | 0 |
| 11 | CK | 1518 | 0 | 1587 | 52 | 0 |
| 11 | q | 1518 | 0 | 1587 | 0 | 0 |
| 12 | CL | 1705 | 0 | 1736 | 63 | 0 |
| 12 | r | 1705 | 0 | 1736 | 0 | 0 |
| 13 | CM | 1353 | 0 | 1383 | 38 | 0 |
| 13 | s | 1353 | 0 | 1383 | 0 | 0 |
| 14 | CN | 1543 | 0 | 1608 | 58 | 0 |
| 14 | t | 1543 | 0 | 1608 | 0 | 0 |
| 15 | CO | 1053 | 0 | 1149 | 40 | 0 |
| 15 | u | 1053 | 0 | 1149 | 0 | 0 |
| 16 | CP | 1720 | 0 | 1779 | 53 | 0 |
| 16 | v | 1720 | 0 | 1778 | 0 | 0 |
| 17 | CQ | 1555 | 0 | 1659 | 53 | 0 |
| 17 | w | 1555 | 0 | 1659 | 0 | 0 |
| 18 | CR | 1420 | 0 | 1437 | 45 | 0 |
| 18 | x | 1420 | 0 | 1437 | 0 | 0 |
| 19 | CS | 1441 | 0 | 1543 | 54 | 0 |
| 19 | y | 1441 | 0 | 1543 | 0 | 0 |
| 20 | CT | 1521 | 0 | 1617 | 57 | 0 |
| 20 | z | 1521 | 0 | 1617 | 0 | 0 |
| 21 | 0 | 1445 | 0 | 1487 | 38 | 0 |
| 21 | CU | 1445 | 0 | 1487 | 48 | 0 |
| 22 | 2 | 1276 | 0 | 1323 | 45 | 0 |
| 22 | CV | 1276 | 0 | 1323 | 63 | 0 |
| 23 | 5 | 796 | 0 | 812 | 22 | 0 |
| 23 | CW | 796 | 0 | 812 | 20 | 0 |
| 24 | CX | 1003 | 0 | 1048 | 31 | 0 |
| 24 | l2 | 1003 | 0 | 1048 | 0 | 0 |
| 25 | 6 | 37990 | 0 | 19115 | 566 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 25 | A | 37948 | 0 | 19093 | 785 | 0 |
| 26 | 7 | 699 | 0 | 640 | 9 | 0 |
| 26 | CY | 699 | 0 | 640 | 14 | 0 |
| 27 | 8 | 964 | 0 | 1025 | 33 | 0 |
| 27 | CZ | 964 | 0 | 1025 | 33 | 0 |
| 28 | 9 | 993 | 0 | 1081 | 25 | 0 |
| 28 | DA | 993 | 0 | 1081 | 35 | 0 |
| 29 | AA | 1092 | 0 | 1155 | 49 | 0 |
| 29 | DB | 1092 | 0 | 1155 | 42 | 0 |
| 30 | AB | 1173 | 0 | 1214 | 52 | 0 |
| 30 | DC | 1173 | 0 | 1215 | 51 | 0 |
| 31 | AC | 462 | 0 | 491 | 8 | 0 |
| 31 | DD | 462 | 0 | 491 | 19 | 0 |
| 32 | AD | 743 | 0 | 797 | 25 | 0 |
| 32 | DE | 743 | 0 | 797 | 27 | 0 |
| 33 | AE | 876 | 0 | 912 | 28 | 0 |
| 33 | DF | 876 | 0 | 912 | 19 | 0 |
| 34 | AF | 1020 | 0 | 1090 | 22 | 0 |
| 34 | DG | 1020 | 0 | 1090 | 38 | 0 |
| 35 | AG | 850 | 0 | 880 | 22 | 0 |
| 35 | DH | 850 | 0 | 880 | 27 | 0 |
| 36 | AH | 880 | 0 | 945 | 27 | 0 |
| 36 | DI | 880 | 0 | 945 | 37 | 0 |
| 37 | AI | 969 | 0 | 1078 | 35 | 0 |
| 37 | DJ | 969 | 0 | 1078 | 40 | 0 |
| 38 | AJ | 771 | 0 | 849 | 31 | 0 |
| 38 | DK | 771 | 0 | 849 | 35 | 0 |
| 39 | AK | 681 | 0 | 683 | 24 | 0 |
| 39 | DL | 681 | 0 | 683 | 26 | 0 |
| 40 | AL | 612 | 0 | 682 | 12 | 0 |
| 40 | DM | 612 | 0 | 682 | 20 | 0 |
| 41 | AM | 436 | 0 | 475 | 19 | 0 |
| 41 | DN | 436 | 0 | 475 | 14 | 0 |
| 42 | AN | 417 | 0 | 455 | 11 | 0 |
| 42 | DO | 417 | 0 | 455 | 12 | 0 |
| 43 | AO | 233 | 0 | 284 | 8 | 0 |
| 43 | DP | 233 | 0 | 284 | 10 | 0 |
| 44 | AP | 847 | 0 | 917 | 23 | 0 |
| 44 | DQ | 847 | 0 | 918 | 27 | 0 |
| 45 | AQ | 694 | 0 | 736 | 17 | 0 |
| 45 | DR | 694 | 0 | 735 | 24 | 0 |
| 46 | i | 1104 | 0 | 996 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 47 | p0 | 1077 | 0 | 1041 | 0 | 0 |
| 48 | sM | 680 | 0 | 540 | 0 | 0 |
| 49 | B | 1577 | 0 | 1567 | 68 | 0 |
| 49 | s0 | 1583 | 0 | 1578 | 0 | 0 |
| 50 | C | 1709 | 0 | 1784 | 70 | 0 |
| 50 | s1 | 1722 | 0 | 1793 | 0 | 0 |
| 51 | D | 1635 | 0 | 1723 | 70 | 0 |
| 51 | s2 | 1635 | 0 | 1723 | 0 | 0 |
| 52 | E | 1734 | 0 | 1817 | 51 | 0 |
| 52 | s3 | 1734 | 0 | 1817 | 0 | 0 |
| 53 | F | 2068 | 0 | 2154 | 69 | 0 |
| 53 | s4 | 2068 | 0 | 2154 | 0 | 0 |
| 54 | G | 1609 | 0 | 1675 | 54 | 0 |
| 54 | s5 | 1609 | 0 | 1675 | 0 | 0 |
| 55 | H | 1799 | 0 | 1879 | 69 | 0 |
| 55 | s6 | 1755 | 0 | 1846 | 0 | 0 |
| 56 | I | 1481 | 0 | 1572 | 61 | 0 |
| 56 | s7 | 1491 | 0 | 1578 | 0 | 0 |
| 57 | J | 1489 | 0 | 1525 | 60 | 0 |
| 57 | s8 | 1489 | 0 | 1525 | 0 | 0 |
| 58 | K | 1494 | 0 | 1573 | 53 | 0 |
| 58 | s9 | 1494 | 0 | 1573 | 0 | 0 |
| 59 | L | 772 | 0 | 727 | 25 | 0 |
| 59 | c0 | 761 | 0 | 697 | 0 | 0 |
| 60 | M | 1213 | 0 | 1257 | 40 | 0 |
| 60 | c1 | 1168 | 0 | 1233 | 0 | 0 |
| 61 | N | 890 | 0 | 887 | 28 | 0 |
| 61 | c2 | 890 | 0 | 887 | 0 | 0 |
| 62 | O | 1192 | 0 | 1255 | 39 | 0 |
| 62 | c3 | 1192 | 0 | 1255 | 0 | 0 |
| 63 | P | 891 | 0 | 883 | 42 | 0 |
| 63 | c4 | 949 | 0 | 985 | 0 | 0 |
| 64 | Q | 977 | 0 | 1002 | 34 | 0 |
| 64 | c5 | 1039 | 0 | 1050 | 0 | 0 |
| 65 | R | 1105 | 0 | 1166 | 40 | 0 |
| 65 | c6 | 1111 | 0 | 1171 | 0 | 0 |
| 66 | S | 926 | 0 | 930 | 44 | 0 |
| 67 | T | 1192 | 0 | 1222 | 52 | 0 |
| 67 | c8 | 1192 | 0 | 1222 | 0 | 0 |
| 68 | U | 1112 | 0 | 1124 | 44 | 0 |
| 68 | c9 | 1112 | 0 | 1124 | 0 | 0 |
| 69 | V | 855 | 0 | 917 | 43 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 69 | d0 | 882 | 0 | 939 | 0 | 0 |
| 70 | W | 684 | 0 | 672 | 27 | 0 |
| 70 | d1 | 684 | 0 | 672 | 0 | 0 |
| 71 | X | 1021 | 0 | 1060 | 35 | 0 |
| 71 | d2 | 1021 | 0 | 1060 | 0 | 0 |
| 72 | Y | 1121 | 0 | 1196 | 47 | 0 |
| 72 | d3 | 1121 | 0 | 1196 | 0 | 0 |
| 73 | Z | 1073 | 0 | 1132 | 37 | 0 |
| 73 | d4 | 1073 | 0 | 1132 | 0 | 0 |
| 74 | a | 563 | 0 | 603 | 0 | 0 |
| 74 | d5 | 558 | 0 | 598 | 0 | 0 |
| 75 | b | 769 | 0 | 815 | 0 | 0 |
| 75 | d6 | 769 | 0 | 814 | 0 | 0 |
| 76 | c | 610 | 0 | 633 | 0 | 0 |
| 76 | d7 | 610 | 0 | 633 | 0 | 0 |
| 77 | d | 497 | 0 | 535 | 0 | 0 |
| 77 | d8 | 497 | 0 | 535 | 0 | 0 |
| 78 | d9 | 442 | 0 | 428 | 0 | 0 |
| 78 | e | 442 | 0 | 429 | 0 | 0 |
| 79 | e0 | 491 | 0 | 542 | 0 | 0 |
| 79 | f | 475 | 0 | 525 | 0 | 0 |
| 80 | g | 566 | 0 | 602 | 0 | 0 |
| 81 | h | 2437 | 0 | 2386 | 0 | 0 |
| 81 | sR | 2442 | 0 | 2392 | 0 | 0 |
| 82 | c7 | 906 | 0 | 909 | 0 | 0 |
| 83 | e1 | 397 | 0 | 396 | 0 | 0 |
| 84 | 1 | 2317 | 0 | 0 | 230 | 0 |
| 84 | 2 | 7 | 0 | 0 | 0 | 0 |
| 84 | 3 | 56 | 0 | 0 | 5 | 0 |
| 84 | 4 | 84 | 0 | 0 | 7 | 0 |
| 84 | 6 | 1099 | 0 | 0 | 105 | 0 |
| 84 | A | 994 | 0 | 0 | 120 | 0 |
| 84 | AC | 7 | 0 | 0 | 1 | 0 |
| 84 | AE | 7 | 0 | 0 | 4 | 0 |
| 84 | AG | 7 | 0 | 0 | 0 | 0 |
| 84 | AK | 14 | 0 | 0 | 2 | 0 |
| 84 | AP | 7 | 0 | 0 | 3 | 0 |
| 84 | AR | 2373 | 0 | 0 | 242 | 0 |
| 84 | AS | 70 | 0 | 0 | 7 | 0 |
| 84 | AT | 133 | 0 | 0 | 18 | 0 |
| 84 | CE | 14 | 0 | 0 | 2 | 0 |
| 84 | CF | 14 | 0 | 0 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 84 | CG | 21 | 0 | 0 | 4 | 0 |
| 84 | CK | 7 | 0 | 0 | 1 | 0 |
| 84 | CL | 14 | 0 | 0 | 2 | 0 |
| 84 | CM | 7 | 0 | 0 | 1 | 0 |
| 84 | CO | 7 | 0 | 0 | 0 | 0 |
| 84 | CP | 7 | 0 | 0 | 0 | 0 |
| 84 | CV | 7 | 0 | 0 | 1 | 0 |
| 84 | CX | 7 | 0 | 0 | 0 | 0 |
| 84 | CZ | 7 | 0 | 0 | 0 | 0 |
| 84 | DD | 7 | 0 | 0 | 0 | 0 |
| 84 | DG | 7 | 0 | 0 | 0 | 0 |
| 84 | DH | 7 | 0 | 0 | 0 | 0 |
| 84 | DI | 7 | 0 | 0 | 1 | 0 |
| 84 | DL | 14 | 0 | 0 | 2 | 0 |
| 84 | H | 7 | 0 | 0 | 0 | 0 |
| 84 | J | 7 | 0 | 0 | 0 | 0 |
| 84 | M | 7 | 0 | 0 | 2 | 0 |
| 84 | O | 7 | 0 | 0 | 1 | 0 |
| 84 | Q | 7 | 0 | 0 | 2 | 0 |
| 84 | T | 7 | 0 | 0 | 1 | 0 |
| 84 | c3 | 7 | 0 | 0 | 0 | 0 |
| 84 | c5 | 7 | 0 | 0 | 0 | 0 |
| 84 | c8 | 7 | 0 | 0 | 0 | 0 |
| 84 | d9 | 7 | 0 | 0 | 0 | 0 |
| 84 | e | 7 | 0 | 0 | 0 | 0 |
| 84 | h | 7 | 0 | 0 | 0 | 0 |
| 84 | k | 14 | 0 | 0 | 0 | 0 |
| 84 | l | 7 | 0 | 0 | 0 | 0 |
| 84 | r | 7 | 0 | 0 | 0 | 0 |
| 84 | s8 | 7 | 0 | 0 | 0 | 0 |
| 84 | sR | 7 | 0 | 0 | 0 | 0 |
| 84 | v | 7 | 0 | 0 | 0 | 0 |
| 84 | x | 14 | 0 | 0 | 0 | 0 |
| 84 | y | 7 | 0 | 0 | 0 | 0 |
| 84 | z | 7 | 0 | 0 | 0 | 0 |
| 85 | 1 | 490 | 0 | 0 | 0 | 0 |
| 85 | 3 | 12 | 0 | 0 | 0 | 0 |
| 85 | 4 | 21 | 0 | 0 | 0 | 0 |
| 85 | 6 | 141 | 0 | 0 | 0 | 0 |
| 85 | 9 | 1 | 0 | 0 | 0 | 0 |
| 85 | A | 111 | 0 | 0 | 0 | 0 |
| 85 | AB | 4 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 85 | AF | 2 | 0 | 0 | 0 | 0 |
| 85 | AH | 1 | 0 | 0 | 0 | 0 |
| 85 | AK | 1 | 0 | 0 | 0 | 0 |
| 85 | AP | 1 | 0 | 0 | 0 | 0 |
| 85 | AR | 504 | 0 | 0 | 0 | 0 |
| 85 | AS | 20 | 0 | 0 | 0 | 0 |
| 85 | AT | 12 | 0 | 0 | 0 | 0 |
| 85 | CD | 2 | 0 | 0 | 0 | 0 |
| 85 | CE | 4 | 0 | 0 | 0 | 0 |
| 85 | CF | 1 | 0 | 0 | 0 | 0 |
| 85 | CI | 1 | 0 | 0 | 0 | 0 |
| 85 | CK | 1 | 0 | 0 | 0 | 0 |
| 85 | CO | 2 | 0 | 0 | 0 | 0 |
| 85 | CP | 2 | 0 | 0 | 0 | 0 |
| 85 | CQ | 4 | 0 | 0 | 0 | 0 |
| 85 | CR | 6 | 0 | 0 | 0 | 0 |
| 85 | CU | 2 | 0 | 0 | 0 | 0 |
| 85 | CX | 2 | 0 | 0 | 0 | 0 |
| 85 | D | 1 | 0 | 0 | 0 | 0 |
| 85 | DA | 1 | 0 | 0 | 0 | 0 |
| 85 | DC | 4 | 0 | 0 | 0 | 0 |
| 85 | DD | 1 | 0 | 0 | 0 | 0 |
| 85 | DE | 1 | 0 | 0 | 0 | 0 |
| 85 | DF | 1 | 0 | 0 | 0 | 0 |
| 85 | DG | 1 | 0 | 0 | 0 | 0 |
| 85 | DH | 2 | 0 | 0 | 0 | 0 |
| 85 | DI | 1 | 0 | 0 | 0 | 0 |
| 85 | DO | 1 | 0 | 0 | 0 | 0 |
| 85 | DP | 1 | 0 | 0 | 0 | 0 |
| 85 | DR | 2 | 0 | 0 | 0 | 0 |
| 85 | F | 1 | 0 | 0 | 0 | 0 |
| 85 | Y | 1 | 0 | 0 | 0 | 0 |
| 85 | b | 1 | 0 | 0 | 0 | 0 |
| 85 | c6 | 1 | 0 | 0 | 0 | 0 |
| 85 | c9 | 1 | 0 | 0 | 0 | 0 |
| 85 | d3 | 3 | 0 | 0 | 0 | 0 |
| 85 | d5 | 1 | 0 | 0 | 0 | 0 |
| 85 | d6 | 1 | 0 | 0 | 0 | 0 |
| 85 | d9 | 1 | 0 | 0 | 0 | 0 |
| 85 | i | 1 | 0 | 0 | 0 | 0 |
| 85 | j | 2 | 0 | 0 | 0 | 0 |
| 85 | k | 2 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 85 | l | 2 | 0 | 0 | 0 | 0 |
| 85 | l2 | 2 | 0 | 0 | 0 | 0 |
| 85 | o | 3 | 0 | 0 | 0 | 0 |
| 85 | r | 1 | 0 | 0 | 0 | 0 |
| 85 | s | 1 | 0 | 0 | 0 | 0 |
| 85 | s1 | 1 | 0 | 0 | 0 | 0 |
| 85 | s2 | 1 | 0 | 0 | 0 | 0 |
| 85 | s6 | 1 | 0 | 0 | 0 | 0 |
| 85 | s8 | 1 | 0 | 0 | 0 | 0 |
| 85 | sM | 1 | 0 | 0 | 0 | 0 |
| 85 | t | 2 | 0 | 0 | 0 | 0 |
| 85 | v | 1 | 0 | 0 | 0 | 0 |
| 85 | w | 1 | 0 | 0 | 0 | 0 |
| 85 | x | 5 | 0 | 0 | 0 | 0 |
| 85 | z | 2 | 0 | 0 | 0 | 0 |
| 86 | 1 | 20 | 0 | 0 | 4 | 0 |
| 86 | AR | 20 | 0 | 0 | 3 | 0 |
| 87 | AK | 1 | 0 | 0 | 0 | 0 |
| 87 | AN | 1 | 0 | 0 | 0 | 0 |
| 87 | AP | 1 | 0 | 0 | 0 | 0 |
| 87 | AQ | 1 | 0 | 0 | 0 | 0 |
| 87 | DL | 1 | 0 | 0 | 0 | 0 |
| 87 | DO | 1 | 0 | 0 | 0 | 0 |
| 87 | DQ | 1 | 0 | 0 | 0 | 0 |
| 87 | DR | 1 | 0 | 0 | 0 | 0 |
| 87 | b | 1 | 0 | 0 | 0 | 0 |
| 87 | c | 1 | 0 | 0 | 0 | 0 |
| 87 | d6 | 1 | 0 | 0 | 0 | 0 |
| 87 | d7 | 1 | 0 | 0 | 0 | 0 |
| 87 | d9 | 1 | 0 | 0 | 0 | 0 |
| 87 | e | 1 | 0 | 0 | 0 | 0 |
| 87 | e1 | 1 | 0 | 0 | 0 | 0 |
| 87 | g | 1 | 0 | 0 | 0 | 0 |
| All | All | 409590 | 0 | 296688 | 6489 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 6489 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-------------------|--------------------------|-------------------|
| 1:1:1171:G:N7 | 84:1:3496:OHX:N2 | 2.13 | 0.96 |
| 25:6:1726:G:N7 | 84:6:2005:OHX:N2 | 2.12 | 0.95 |
| 1:AR:1481:A:O2' | 1:AR:1858:A:N3 | 2.00 | 0.95 |
| 25:6:1588:G:H1 | 25:6:1608:U:H3 | 1.15 | 0.95 |
| 1:AR:1878:G:OP1 | 84:AR:3457:OHX:N5 | 2.01 | 0.94 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%) | 238 (95%) | 12 (5%) | 0 | 100 | 100 |
| 4 | j | 250/252 (99%) | 232 (93%) | 18 (7%) | 0 | 100 | 100 |
| 5 | CE | 384/386 (100%) | 355 (92%) | 27 (7%) | 2 (0%) | 32 | 73 |
| 5 | k | 384/386 (100%) | 351 (91%) | 31 (8%) | 2 (0%) | 32 | 73 |
| 6 | CF | 359/361 (99%) | 331 (92%) | 28 (8%) | 0 | 100 | 100 |
| 6 | l | 359/361 (99%) | 326 (91%) | 32 (9%) | 1 (0%) | 44 | 80 |
| 7 | CG | 294/296 (99%) | 272 (92%) | 22 (8%) | 0 | 100 | 100 |
| 7 | m | 294/296 (99%) | 271 (92%) | 23 (8%) | 0 | 100 | 100 |
| 8 | CH | 152/175 (87%) | 144 (95%) | 6 (4%) | 2 (1%) | 14 | 55 |
| 8 | n | 152/175 (87%) | 145 (95%) | 6 (4%) | 1 (1%) | 25 | 68 |
| 9 | CI | 220/222 (99%) | 202 (92%) | 15 (7%) | 3 (1%) | 13 | 53 |
| 9 | o | 220/222 (99%) | 204 (93%) | 13 (6%) | 3 (1%) | 13 | 53 |
| 10 | CJ | 231/233 (99%) | 207 (90%) | 21 (9%) | 3 (1%) | 14 | 55 |
| 10 | p | 231/233 (99%) | 209 (90%) | 18 (8%) | 4 (2%) | 11 | 49 |
| 11 | CK | 189/191 (99%) | 178 (94%) | 11 (6%) | 0 | 100 | 100 |
| 11 | q | 189/191 (99%) | 176 (93%) | 12 (6%) | 1 (0%) | 32 | 73 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 12 | CL | 207/220 (94%) | 195 (94%) | 10 (5%) | 2 (1%) | 18 | 61 |
| 12 | r | 207/220 (94%) | 199 (96%) | 8 (4%) | 0 | 100 | 100 |
| 13 | CM | 167/169 (99%) | 146 (87%) | 18 (11%) | 3 (2%) | 10 | 48 |
| 13 | s | 167/169 (99%) | 149 (89%) | 15 (9%) | 3 (2%) | 10 | 48 |
| 14 | CN | 191/193 (99%) | 172 (90%) | 18 (9%) | 1 (0%) | 32 | 73 |
| 14 | t | 191/193 (99%) | 173 (91%) | 15 (8%) | 3 (2%) | 11 | 50 |
| 15 | CO | 134/136 (98%) | 125 (93%) | 7 (5%) | 2 (2%) | 12 | 52 |
| 15 | u | 134/136 (98%) | 122 (91%) | 10 (8%) | 2 (2%) | 12 | 52 |
| 16 | CP | 201/203 (99%) | 189 (94%) | 12 (6%) | 0 | 100 | 100 |
| 16 | v | 201/203 (99%) | 189 (94%) | 12 (6%) | 0 | 100 | 100 |
| 17 | CQ | 195/197 (99%) | 189 (97%) | 4 (2%) | 2 (1%) | 18 | 61 |
| 17 | w | 195/197 (99%) | 188 (96%) | 4 (2%) | 3 (2%) | 12 | 52 |
| 18 | CR | 181/183 (99%) | 166 (92%) | 14 (8%) | 1 (1%) | 28 | 70 |
| 18 | x | 181/183 (99%) | 170 (94%) | 10 (6%) | 1 (1%) | 28 | 70 |
| 19 | CS | 183/185 (99%) | 171 (93%) | 11 (6%) | 1 (0%) | 32 | 73 |
| 19 | y | 183/185 (99%) | 173 (94%) | 9 (5%) | 1 (0%) | 32 | 73 |
| 20 | CT | 186/188 (99%) | 172 (92%) | 13 (7%) | 1 (0%) | 32 | 73 |
| 20 | z | 186/188 (99%) | 178 (96%) | 7 (4%) | 1 (0%) | 32 | 73 |
| 21 | 0 | 170/172 (99%) | 154 (91%) | 15 (9%) | 1 (1%) | 28 | 70 |
| 21 | CU | 170/172 (99%) | 158 (93%) | 12 (7%) | 0 | 100 | 100 |
| 22 | 2 | 157/159 (99%) | 144 (92%) | 12 (8%) | 1 (1%) | 28 | 70 |
| 22 | CV | 157/159 (99%) | 147 (94%) | 9 (6%) | 1 (1%) | 28 | 70 |
| 23 | 5 | 98/100 (98%) | 88 (90%) | 9 (9%) | 1 (1%) | 18 | 61 |
| 23 | CW | 98/100 (98%) | 89 (91%) | 8 (8%) | 1 (1%) | 18 | 61 |
| 24 | CX | 134/136 (98%) | 132 (98%) | 2 (2%) | 0 | 100 | 100 |
| 24 | l2 | 134/136 (98%) | 131 (98%) | 3 (2%) | 0 | 100 | 100 |
| 26 | 7 | 96/98 (98%) | 85 (88%) | 10 (10%) | 1 (1%) | 18 | 61 |
| 26 | CY | 96/98 (98%) | 83 (86%) | 11 (12%) | 2 (2%) | 8 | 45 |
| 27 | 8 | 119/121 (98%) | 111 (93%) | 8 (7%) | 0 | 100 | 100 |
| 27 | CZ | 119/121 (98%) | 111 (93%) | 6 (5%) | 2 (2%) | 11 | 49 |
| 28 | 9 | 124/126 (98%) | 120 (97%) | 4 (3%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 28 | DA | 124/126 (98%) | 120 (97%) | 4 (3%) | 0 | 100 | 100 |
| 29 | AA | 133/135 (98%) | 123 (92%) | 10 (8%) | 0 | 100 | 100 |
| 29 | DB | 133/135 (98%) | 121 (91%) | 10 (8%) | 2 (2%) | 12 | 52 |
| 30 | AB | 146/148 (99%) | 127 (87%) | 17 (12%) | 2 (1%) | 13 | 53 |
| 30 | DC | 146/148 (99%) | 130 (89%) | 14 (10%) | 2 (1%) | 13 | 53 |
| 31 | AC | 56/58 (97%) | 51 (91%) | 4 (7%) | 1 (2%) | 10 | 48 |
| 31 | DD | 56/58 (97%) | 51 (91%) | 4 (7%) | 1 (2%) | 10 | 48 |
| 32 | AD | 95/97 (98%) | 92 (97%) | 3 (3%) | 0 | 100 | 100 |
| 32 | DE | 95/97 (98%) | 93 (98%) | 2 (2%) | 0 | 100 | 100 |
| 33 | AE | 107/109 (98%) | 101 (94%) | 5 (5%) | 1 (1%) | 20 | 63 |
| 33 | DF | 107/109 (98%) | 103 (96%) | 3 (3%) | 1 (1%) | 20 | 63 |
| 34 | AF | 125/127 (98%) | 122 (98%) | 3 (2%) | 0 | 100 | 100 |
| 34 | DG | 125/127 (98%) | 119 (95%) | 6 (5%) | 0 | 100 | 100 |
| 35 | AG | 104/106 (98%) | 98 (94%) | 4 (4%) | 2 (2%) | 9 | 47 |
| 35 | DH | 104/106 (98%) | 97 (93%) | 6 (6%) | 1 (1%) | 18 | 61 |
| 36 | AH | 110/112 (98%) | 104 (94%) | 4 (4%) | 2 (2%) | 10 | 48 |
| 36 | DI | 110/112 (98%) | 104 (94%) | 6 (6%) | 0 | 100 | 100 |
| 37 | AI | 117/119 (98%) | 111 (95%) | 6 (5%) | 0 | 100 | 100 |
| 37 | DJ | 117/119 (98%) | 111 (95%) | 6 (5%) | 0 | 100 | 100 |
| 38 | AJ | 97/99 (98%) | 83 (86%) | 13 (13%) | 1 (1%) | 18 | 61 |
| 38 | DK | 97/99 (98%) | 86 (89%) | 10 (10%) | 1 (1%) | 18 | 61 |
| 39 | AK | 85/87 (98%) | 77 (91%) | 8 (9%) | 0 | 100 | 100 |
| 39 | DL | 85/87 (98%) | 78 (92%) | 7 (8%) | 0 | 100 | 100 |
| 40 | AL | 75/77 (97%) | 74 (99%) | 1 (1%) | 0 | 100 | 100 |
| 40 | DM | 75/77 (97%) | 68 (91%) | 6 (8%) | 1 (1%) | 14 | 55 |
| 41 | AM | 48/50 (96%) | 46 (96%) | 2 (4%) | 0 | 100 | 100 |
| 41 | DN | 48/50 (96%) | 46 (96%) | 2 (4%) | 0 | 100 | 100 |
| 42 | AN | 50/52 (96%) | 45 (90%) | 5 (10%) | 0 | 100 | 100 |
| 42 | DO | 50/52 (96%) | 46 (92%) | 4 (8%) | 0 | 100 | 100 |
| 43 | AO | 23/25 (92%) | 22 (96%) | 1 (4%) | 0 | 100 | 100 |
| 43 | DP | 23/25 (92%) | 23 (100%) | 0 | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 44 | AP | 103/105 (98%) | 91 (88%) | 12 (12%) | 0 | 100 | 100 |
| 44 | DQ | 103/105 (98%) | 90 (87%) | 12 (12%) | 1 (1%) | 18 | 61 |
| 45 | AQ | 89/91 (98%) | 77 (86%) | 12 (14%) | 0 | 100 | 100 |
| 45 | DR | 89/91 (98%) | 83 (93%) | 6 (7%) | 0 | 100 | 100 |
| 46 | i | 155/168 (92%) | 129 (83%) | 23 (15%) | 3 (2%) | 9 | 47 |
| 47 | p0 | 139/220 (63%) | 130 (94%) | 8 (6%) | 1 (1%) | 25 | 68 |
| 48 | sM | 61/104 (59%) | 47 (77%) | 13 (21%) | 1 (2%) | 11 | 50 |
| 49 | B | 204/206 (99%) | 175 (86%) | 26 (13%) | 3 (2%) | 12 | 52 |
| 49 | s0 | 204/206 (99%) | 184 (90%) | 17 (8%) | 3 (2%) | 12 | 52 |
| 50 | C | 212/216 (98%) | 175 (82%) | 35 (16%) | 2 (1%) | 20 | 63 |
| 50 | s1 | 214/216 (99%) | 196 (92%) | 18 (8%) | 0 | 100 | 100 |
| 51 | D | 215/217 (99%) | 196 (91%) | 18 (8%) | 1 (0%) | 32 | 73 |
| 51 | s2 | 215/217 (99%) | 199 (93%) | 13 (6%) | 3 (1%) | 13 | 53 |
| 52 | E | 221/223 (99%) | 198 (90%) | 21 (10%) | 2 (1%) | 20 | 63 |
| 52 | s3 | 221/223 (99%) | 198 (90%) | 21 (10%) | 2 (1%) | 20 | 63 |
| 53 | F | 258/260 (99%) | 236 (92%) | 20 (8%) | 2 (1%) | 22 | 65 |
| 53 | s4 | 258/260 (99%) | 233 (90%) | 24 (9%) | 1 (0%) | 38 | 77 |
| 54 | G | 204/206 (99%) | 179 (88%) | 22 (11%) | 3 (2%) | 12 | 52 |
| 54 | s5 | 204/206 (99%) | 183 (90%) | 21 (10%) | 0 | 100 | 100 |
| 55 | H | 224/226 (99%) | 207 (92%) | 13 (6%) | 4 (2%) | 10 | 48 |
| 55 | s6 | 216/226 (96%) | 200 (93%) | 14 (6%) | 2 (1%) | 20 | 63 |
| 56 | I | 182/186 (98%) | 160 (88%) | 17 (9%) | 5 (3%) | 6 | 40 |
| 56 | s7 | 184/186 (99%) | 162 (88%) | 19 (10%) | 3 (2%) | 11 | 50 |
| 57 | J | 184/199 (92%) | 160 (87%) | 23 (12%) | 1 (0%) | 32 | 73 |
| 57 | s8 | 184/199 (92%) | 167 (91%) | 15 (8%) | 2 (1%) | 17 | 59 |
| 58 | K | 183/185 (99%) | 162 (88%) | 19 (10%) | 2 (1%) | 17 | 59 |
| 58 | s9 | 183/185 (99%) | 172 (94%) | 11 (6%) | 0 | 100 | 100 |
| 59 | L | 94/105 (90%) | 78 (83%) | 14 (15%) | 2 (2%) | 8 | 45 |
| 59 | c0 | 92/105 (88%) | 63 (68%) | 20 (22%) | 9 (10%) | 1 | 9 |
| 60 | M | 153/155 (99%) | 138 (90%) | 12 (8%) | 3 (2%) | 9 | 46 |
| 60 | c1 | 144/155 (93%) | 133 (92%) | 10 (7%) | 1 (1%) | 25 | 68 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 61 | N | 122/124 (98%) | 86 (70%) | 30 (25%) | 6 (5%) | 2 | 24 |
| 61 | c2 | 122/124 (98%) | 91 (75%) | 28 (23%) | 3 (2%) | 6 | 41 |
| 62 | O | 148/150 (99%) | 134 (90%) | 13 (9%) | 1 (1%) | 25 | 68 |
| 62 | c3 | 148/150 (99%) | 132 (89%) | 15 (10%) | 1 (1%) | 25 | 68 |
| 63 | P | 125/128 (98%) | 111 (89%) | 13 (10%) | 1 (1%) | 22 | 65 |
| 63 | c4 | 126/128 (98%) | 114 (90%) | 12 (10%) | 0 | 100 | 100 |
| 64 | Q | 122/141 (86%) | 107 (88%) | 13 (11%) | 2 (2%) | 11 | 50 |
| 64 | c5 | 133/141 (94%) | 107 (80%) | 24 (18%) | 2 (2%) | 12 | 52 |
| 65 | R | 139/142 (98%) | 122 (88%) | 14 (10%) | 3 (2%) | 8 | 44 |
| 65 | c6 | 140/142 (99%) | 132 (94%) | 8 (6%) | 0 | 100 | 100 |
| 66 | S | 116/125 (93%) | 99 (85%) | 13 (11%) | 4 (3%) | 4 | 35 |
| 67 | T | 143/145 (99%) | 127 (89%) | 13 (9%) | 3 (2%) | 8 | 45 |
| 67 | c8 | 143/145 (99%) | 121 (85%) | 18 (13%) | 4 (3%) | 6 | 39 |
| 68 | U | 141/143 (99%) | 129 (92%) | 12 (8%) | 0 | 100 | 100 |
| 68 | c9 | 141/143 (99%) | 129 (92%) | 11 (8%) | 1 (1%) | 25 | 68 |
| 69 | V | 105/110 (96%) | 93 (89%) | 12 (11%) | 0 | 100 | 100 |
| 69 | d0 | 108/110 (98%) | 92 (85%) | 14 (13%) | 2 (2%) | 9 | 47 |
| 70 | W | 85/87 (98%) | 76 (89%) | 8 (9%) | 1 (1%) | 15 | 57 |
| 70 | d1 | 85/87 (98%) | 78 (92%) | 7 (8%) | 0 | 100 | 100 |
| 71 | X | 127/129 (98%) | 120 (94%) | 6 (5%) | 1 (1%) | 22 | 65 |
| 71 | d2 | 127/129 (98%) | 117 (92%) | 9 (7%) | 1 (1%) | 22 | 65 |
| 72 | Y | 142/144 (99%) | 119 (84%) | 21 (15%) | 2 (1%) | 13 | 53 |
| 72 | d3 | 142/144 (99%) | 131 (92%) | 11 (8%) | 0 | 100 | 100 |
| 73 | Z | 132/134 (98%) | 121 (92%) | 9 (7%) | 2 (2%) | 12 | 52 |
| 73 | d4 | 132/134 (98%) | 119 (90%) | 10 (8%) | 3 (2%) | 7 | 43 |
| 74 | a | 68/70 (97%) | 56 (82%) | 10 (15%) | 2 (3%) | 5 | 38 |
| 74 | d5 | 67/70 (96%) | 59 (88%) | 8 (12%) | 0 | 100 | 100 |
| 75 | b | 95/97 (98%) | 68 (72%) | 24 (25%) | 3 (3%) | 5 | 36 |
| 75 | d6 | 95/97 (98%) | 76 (80%) | 19 (20%) | 0 | 100 | 100 |
| 76 | c | 79/81 (98%) | 71 (90%) | 7 (9%) | 1 (1%) | 14 | 55 |
| 76 | d7 | 79/81 (98%) | 75 (95%) | 3 (4%) | 1 (1%) | 14 | 55 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|-----------|----------|-------------|-----|
| 77 | d | 61/63 (97%) | 50 (82%) | 11 (18%) | 0 | 100 | 100 |
| 77 | d8 | 61/63 (97%) | 50 (82%) | 11 (18%) | 0 | 100 | 100 |
| 78 | d9 | 51/53 (96%) | 46 (90%) | 4 (8%) | 1 (2%) | 9 | 46 |
| 78 | e | 51/53 (96%) | 45 (88%) | 6 (12%) | 0 | 100 | 100 |
| 79 | e0 | 60/62 (97%) | 50 (83%) | 8 (13%) | 2 (3%) | 4 | 35 |
| 79 | f | 58/62 (94%) | 50 (86%) | 7 (12%) | 1 (2%) | 11 | 49 |
| 80 | g | 69/71 (97%) | 44 (64%) | 19 (28%) | 6 (9%) | 1 | 10 |
| 81 | h | 316/318 (99%) | 292 (92%) | 23 (7%) | 1 (0%) | 44 | 80 |
| 81 | sR | 316/318 (99%) | 292 (92%) | 24 (8%) | 0 | 100 | 100 |
| 82 | c7 | 113/121 (93%) | 102 (90%) | 8 (7%) | 3 (3%) | 6 | 40 |
| 83 | e1 | 49/51 (96%) | 40 (82%) | 9 (18%) | 0 | 100 | 100 |
| All | All | 22260/22868 (97%) | 20206 (91%) | 1851 (8%) | 203 (1%) | 20 | 63 |

5 of 203 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | n | 98 | VAL |
| 10 | p | 36 | ILE |
| 11 | q | 50 | ASN |
| 30 | AB | 48 | TYR |
| 46 | i | 167 | PRO |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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%) | 4 | 21 |
| 4 | j | 193/194 (100%) | 174 (90%) | 19 (10%) | 9 | 38 |
| 5 | CE | 319/322 (99%) | 273 (86%) | 46 (14%) | 4 | 21 |
| 5 | k | 319/322 (99%) | 268 (84%) | 51 (16%) | 3 | 16 |
| 6 | CF | 288/288 (100%) | 255 (88%) | 33 (12%) | 6 | 30 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 6 | l | 288/288 (100%) | 254 (88%) | 34 (12%) | 6 | 29 |
| 7 | CG | 244/244 (100%) | 209 (86%) | 35 (14%) | 4 | 22 |
| 7 | m | 244/244 (100%) | 216 (88%) | 28 (12%) | 6 | 30 |
| 8 | CH | 134/152 (88%) | 119 (89%) | 15 (11%) | 7 | 32 |
| 8 | n | 134/152 (88%) | 120 (90%) | 14 (10%) | 8 | 36 |
| 9 | CI | 186/186 (100%) | 171 (92%) | 15 (8%) | 14 | 48 |
| 9 | o | 186/186 (100%) | 164 (88%) | 22 (12%) | 6 | 29 |
| 10 | CJ | 187/191 (98%) | 170 (91%) | 17 (9%) | 11 | 42 |
| 10 | p | 187/191 (98%) | 170 (91%) | 17 (9%) | 11 | 42 |
| 11 | CK | 171/171 (100%) | 139 (81%) | 32 (19%) | 2 | 9 |
| 11 | q | 171/171 (100%) | 150 (88%) | 21 (12%) | 5 | 27 |
| 12 | CL | 177/186 (95%) | 154 (87%) | 23 (13%) | 5 | 25 |
| 12 | r | 177/186 (95%) | 152 (86%) | 25 (14%) | 4 | 22 |
| 13 | CM | 147/147 (100%) | 124 (84%) | 23 (16%) | 3 | 18 |
| 13 | s | 147/147 (100%) | 131 (89%) | 16 (11%) | 7 | 33 |
| 14 | CN | 154/154 (100%) | 134 (87%) | 20 (13%) | 5 | 25 |
| 14 | t | 154/154 (100%) | 140 (91%) | 14 (9%) | 11 | 42 |
| 15 | CO | 107/107 (100%) | 88 (82%) | 19 (18%) | 2 | 12 |
| 15 | u | 107/107 (100%) | 96 (90%) | 11 (10%) | 8 | 36 |
| 16 | CP | 175/175 (100%) | 155 (89%) | 20 (11%) | 7 | 31 |
| 16 | v | 175/175 (100%) | 154 (88%) | 21 (12%) | 6 | 28 |
| 17 | CQ | 160/160 (100%) | 138 (86%) | 22 (14%) | 4 | 23 |
| 17 | w | 160/160 (100%) | 137 (86%) | 23 (14%) | 4 | 21 |
| 18 | CR | 140/145 (97%) | 115 (82%) | 25 (18%) | 2 | 11 |
| 18 | x | 140/145 (97%) | 117 (84%) | 23 (16%) | 2 | 15 |
| 19 | CS | 150/150 (100%) | 141 (94%) | 9 (6%) | 22 | 60 |
| 19 | y | 150/150 (100%) | 134 (89%) | 16 (11%) | 8 | 34 |
| 20 | CT | 153/153 (100%) | 131 (86%) | 22 (14%) | 4 | 21 |
| 20 | z | 153/153 (100%) | 140 (92%) | 13 (8%) | 12 | 45 |
| 21 | 0 | 156/156 (100%) | 137 (88%) | 19 (12%) | 6 | 27 |
| 21 | CU | 156/156 (100%) | 133 (85%) | 23 (15%) | 3 | 20 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 22 | 2 | 136/136 (100%) | 113 (83%) | 23 (17%) | 2 | 14 |
| 22 | CV | 136/136 (100%) | 116 (85%) | 20 (15%) | 3 | 20 |
| 23 | 5 | 87/87 (100%) | 77 (88%) | 10 (12%) | 6 | 30 |
| 23 | CW | 87/87 (100%) | 75 (86%) | 12 (14%) | 4 | 23 |
| 24 | CX | 104/104 (100%) | 94 (90%) | 10 (10%) | 10 | 39 |
| 24 | l2 | 104/104 (100%) | 91 (88%) | 13 (12%) | 5 | 26 |
| 26 | 7 | 57/86 (66%) | 52 (91%) | 5 (9%) | 12 | 43 |
| 26 | CY | 57/86 (66%) | 53 (93%) | 4 (7%) | 18 | 55 |
| 27 | 8 | 104/105 (99%) | 87 (84%) | 17 (16%) | 3 | 15 |
| 27 | CZ | 104/105 (99%) | 92 (88%) | 12 (12%) | 6 | 30 |
| 28 | 9 | 109/109 (100%) | 99 (91%) | 10 (9%) | 11 | 41 |
| 28 | DA | 109/109 (100%) | 98 (90%) | 11 (10%) | 9 | 37 |
| 29 | AA | 115/115 (100%) | 104 (90%) | 11 (10%) | 10 | 39 |
| 29 | DB | 115/115 (100%) | 105 (91%) | 10 (9%) | 12 | 44 |
| 30 | AB | 118/118 (100%) | 106 (90%) | 12 (10%) | 8 | 36 |
| 30 | DC | 118/118 (100%) | 107 (91%) | 11 (9%) | 10 | 41 |
| 31 | AC | 46/46 (100%) | 41 (89%) | 5 (11%) | 7 | 33 |
| 31 | DD | 46/46 (100%) | 39 (85%) | 7 (15%) | 3 | 19 |
| 32 | AD | 81/81 (100%) | 70 (86%) | 11 (14%) | 4 | 23 |
| 32 | DE | 81/81 (100%) | 75 (93%) | 6 (7%) | 16 | 52 |
| 33 | AE | 92/96 (96%) | 81 (88%) | 11 (12%) | 6 | 28 |
| 33 | DF | 92/96 (96%) | 74 (80%) | 18 (20%) | 1 | 8 |
| 34 | AF | 109/109 (100%) | 95 (87%) | 14 (13%) | 5 | 25 |
| 34 | DG | 109/109 (100%) | 93 (85%) | 16 (15%) | 3 | 20 |
| 35 | AG | 90/90 (100%) | 83 (92%) | 7 (8%) | 15 | 49 |
| 35 | DH | 90/90 (100%) | 83 (92%) | 7 (8%) | 15 | 49 |
| 36 | AH | 95/95 (100%) | 85 (90%) | 10 (10%) | 8 | 35 |
| 36 | DI | 95/95 (100%) | 82 (86%) | 13 (14%) | 4 | 23 |
| 37 | AI | 104/104 (100%) | 90 (86%) | 14 (14%) | 4 | 24 |
| 37 | DJ | 104/104 (100%) | 87 (84%) | 17 (16%) | 3 | 15 |
| 38 | AJ | 81/81 (100%) | 69 (85%) | 12 (15%) | 3 | 20 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 38 | DK | 81/81 (100%) | 67 (83%) | 14 (17%) | 2 | 13 |
| 39 | AK | 70/70 (100%) | 63 (90%) | 7 (10%) | 9 | 37 |
| 39 | DL | 70/70 (100%) | 61 (87%) | 9 (13%) | 5 | 25 |
| 40 | AL | 68/68 (100%) | 58 (85%) | 10 (15%) | 3 | 20 |
| 40 | DM | 68/68 (100%) | 60 (88%) | 8 (12%) | 6 | 29 |
| 41 | AM | 45/45 (100%) | 40 (89%) | 5 (11%) | 7 | 32 |
| 41 | DN | 45/45 (100%) | 42 (93%) | 3 (7%) | 19 | 57 |
| 42 | AN | 47/47 (100%) | 42 (89%) | 5 (11%) | 8 | 35 |
| 42 | DO | 47/47 (100%) | 43 (92%) | 4 (8%) | 12 | 45 |
| 43 | AO | 23/23 (100%) | 16 (70%) | 7 (30%) | 0 | 3 |
| 43 | DP | 23/23 (100%) | 19 (83%) | 4 (17%) | 2 | 13 |
| 44 | AP | 90/90 (100%) | 75 (83%) | 15 (17%) | 2 | 14 |
| 44 | DQ | 90/90 (100%) | 78 (87%) | 12 (13%) | 4 | 24 |
| 45 | AQ | 71/71 (100%) | 62 (87%) | 9 (13%) | 5 | 25 |
| 45 | DR | 71/71 (100%) | 60 (84%) | 11 (16%) | 3 | 18 |
| 46 | i | 97/137 (71%) | 85 (88%) | 12 (12%) | 5 | 27 |
| 47 | p0 | 105/186 (56%) | 89 (85%) | 16 (15%) | 3 | 19 |
| 48 | sM | 54/54 (100%) | 47 (87%) | 7 (13%) | 5 | 25 |
| 49 | B | 164/173 (95%) | 148 (90%) | 16 (10%) | 9 | 38 |
| 49 | s0 | 165/173 (95%) | 144 (87%) | 21 (13%) | 5 | 25 |
| 50 | C | 191/192 (100%) | 167 (87%) | 24 (13%) | 5 | 26 |
| 50 | s1 | 192/192 (100%) | 166 (86%) | 26 (14%) | 4 | 24 |
| 51 | D | 176/176 (100%) | 151 (86%) | 25 (14%) | 4 | 22 |
| 51 | s2 | 176/176 (100%) | 146 (83%) | 30 (17%) | 2 | 14 |
| 52 | E | 182/182 (100%) | 160 (88%) | 22 (12%) | 6 | 27 |
| 52 | s3 | 182/182 (100%) | 167 (92%) | 15 (8%) | 13 | 47 |
| 53 | F | 221/221 (100%) | 195 (88%) | 26 (12%) | 6 | 29 |
| 53 | s4 | 221/221 (100%) | 196 (89%) | 25 (11%) | 7 | 31 |
| 54 | G | 173/173 (100%) | 158 (91%) | 15 (9%) | 12 | 44 |
| 54 | s5 | 173/173 (100%) | 158 (91%) | 15 (9%) | 12 | 44 |
| 55 | H | 188/193 (97%) | 171 (91%) | 17 (9%) | 11 | 42 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 55 | s6 | 187/193 (97%) | 163 (87%) | 24 (13%) | 5 | 25 |
| 56 | I | 165/166 (99%) | 146 (88%) | 19 (12%) | 6 | 30 |
| 56 | s7 | 165/166 (99%) | 155 (94%) | 10 (6%) | 22 | 60 |
| 57 | J | 150/160 (94%) | 132 (88%) | 18 (12%) | 6 | 28 |
| 57 | s8 | 150/160 (94%) | 135 (90%) | 15 (10%) | 9 | 37 |
| 58 | K | 158/158 (100%) | 132 (84%) | 26 (16%) | 2 | 15 |
| 58 | s9 | 158/158 (100%) | 138 (87%) | 20 (13%) | 5 | 25 |
| 59 | L | 77/98 (79%) | 71 (92%) | 6 (8%) | 15 | 49 |
| 59 | c0 | 73/98 (74%) | 69 (94%) | 4 (6%) | 25 | 62 |
| 60 | M | 129/136 (95%) | 120 (93%) | 9 (7%) | 18 | 55 |
| 60 | c1 | 129/136 (95%) | 111 (86%) | 18 (14%) | 4 | 22 |
| 61 | N | 88/100 (88%) | 72 (82%) | 16 (18%) | 2 | 11 |
| 61 | c2 | 88/100 (88%) | 72 (82%) | 16 (18%) | 2 | 11 |
| 62 | O | 127/127 (100%) | 114 (90%) | 13 (10%) | 8 | 36 |
| 62 | c3 | 127/127 (100%) | 113 (89%) | 14 (11%) | 7 | 33 |
| 63 | P | 81/97 (84%) | 67 (83%) | 14 (17%) | 2 | 13 |
| 63 | c4 | 97/97 (100%) | 86 (89%) | 11 (11%) | 7 | 31 |
| 64 | Q | 101/117 (86%) | 93 (92%) | 8 (8%) | 14 | 49 |
| 64 | c5 | 103/117 (88%) | 92 (89%) | 11 (11%) | 8 | 34 |
| 65 | R | 117/118 (99%) | 102 (87%) | 15 (13%) | 5 | 25 |
| 65 | c6 | 118/118 (100%) | 100 (85%) | 18 (15%) | 3 | 19 |
| 66 | S | 94/113 (83%) | 84 (89%) | 10 (11%) | 8 | 35 |
| 67 | T | 128/128 (100%) | 113 (88%) | 15 (12%) | 6 | 29 |
| 67 | c8 | 128/128 (100%) | 117 (91%) | 11 (9%) | 12 | 45 |
| 68 | U | 115/115 (100%) | 96 (84%) | 19 (16%) | 2 | 15 |
| 68 | c9 | 115/115 (100%) | 106 (92%) | 9 (8%) | 15 | 49 |
| 69 | V | 100/103 (97%) | 89 (89%) | 11 (11%) | 7 | 33 |
| 69 | d0 | 103/103 (100%) | 94 (91%) | 9 (9%) | 12 | 44 |
| 70 | W | 74/74 (100%) | 64 (86%) | 10 (14%) | 4 | 24 |
| 70 | d1 | 74/74 (100%) | 66 (89%) | 8 (11%) | 7 | 34 |
| 71 | X | 110/110 (100%) | 96 (87%) | 14 (13%) | 5 | 25 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|------------|-------------|----|
| 71 | d2 | 110/110 (100%) | 100 (91%) | 10 (9%) | 11 | 42 |
| 72 | Y | 119/119 (100%) | 102 (86%) | 17 (14%) | 4 | 22 |
| 72 | d3 | 119/119 (100%) | 107 (90%) | 12 (10%) | 9 | 37 |
| 73 | Z | 112/112 (100%) | 106 (95%) | 6 (5%) | 26 | 63 |
| 73 | d4 | 112/112 (100%) | 102 (91%) | 10 (9%) | 11 | 43 |
| 74 | a | 61/61 (100%) | 50 (82%) | 11 (18%) | 2 | 11 |
| 74 | d5 | 61/61 (100%) | 57 (93%) | 4 (7%) | 19 | 57 |
| 75 | b | 83/83 (100%) | 69 (83%) | 14 (17%) | 2 | 14 |
| 75 | d6 | 83/83 (100%) | 73 (88%) | 10 (12%) | 6 | 28 |
| 76 | c | 70/70 (100%) | 66 (94%) | 4 (6%) | 24 | 61 |
| 76 | d7 | 70/70 (100%) | 63 (90%) | 7 (10%) | 9 | 37 |
| 77 | d | 56/56 (100%) | 50 (89%) | 6 (11%) | 8 | 34 |
| 77 | d8 | 56/56 (100%) | 49 (88%) | 7 (12%) | 5 | 26 |
| 78 | d9 | 47/47 (100%) | 40 (85%) | 7 (15%) | 3 | 20 |
| 78 | e | 47/47 (100%) | 42 (89%) | 5 (11%) | 8 | 35 |
| 79 | e0 | 53/53 (100%) | 40 (76%) | 13 (24%) | 1 | 4 |
| 79 | f | 51/53 (96%) | 45 (88%) | 6 (12%) | 6 | 29 |
| 80 | g | 62/62 (100%) | 55 (89%) | 7 (11%) | 7 | 31 |
| 81 | h | 259/261 (99%) | 234 (90%) | 25 (10%) | 9 | 38 |
| 81 | sR | 260/261 (100%) | 242 (93%) | 18 (7%) | 18 | 55 |
| 82 | c7 | 92/110 (84%) | 80 (87%) | 12 (13%) | 5 | 25 |
| 83 | e1 | 43/43 (100%) | 34 (79%) | 9 (21%) | 1 | 7 |
| All | All | 18681/19177 (97%) | 16432 (88%) | 2249 (12%) | 6 | 28 |

5 of 2249 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19 | CS | 41 | ASP |
| 39 | DL | 17 | THR |
| 65 | c6 | 28 | LEU |
| 21 | CU | 51 | VAL |
| 29 | DB | 92 | PHE |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | CT | 92 | GLN |
| 37 | DJ | 59 | ASN |
| 67 | c8 | 25 | ASN |
| 29 | DB | 36 | HIS |
| 41 | DN | 33 | ASN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------------|-------------------|-----------------|
| 1 | 1 | 3145/3396 (92%) | 563 (17%) | 51 (1%) |
| 1 | AR | 3145/3396 (92%) | 581 (18%) | 51 (1%) |
| 2 | 3 | 120/121 (99%) | 16 (13%) | 0 |
| 2 | AS | 120/121 (99%) | 15 (12%) | 2 (1%) |
| 25 | 6 | 1780/1800 (98%) | 383 (21%) | 30 (1%) |
| 25 | A | 1778/1800 (98%) | 409 (23%) | 47 (2%) |
| 3 | 4 | 157/158 (99%) | 32 (20%) | 2 (1%) |
| 3 | AT | 157/158 (99%) | 28 (17%) | 3 (1%) |
| All | All | 10402/10950 (94%) | 2027 (19%) | 186 (1%) |

5 of 2027 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 1 | 26 | A |
| 1 | 1 | 40 | A |
| 1 | 1 | 49 | A |
| 1 | 1 | 57 | A |
| 1 | 1 | 59 | G |

5 of 186 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AR | 588 | G |
| 1 | AR | 1481 | A |
| 25 | A | 1196 | A |
| 1 | AR | 715 | A |
| 1 | AR | 1103 | A |

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2494 ligands modelled in this entry, 1422 are monoatomic - leaving 1072 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 | 3401 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3402 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3403 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3404 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3405 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3406 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3407 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3408 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3409 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3410 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3411 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3412 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3413 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3414 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3415 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3416 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3417 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3418 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3419 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3420 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3421 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3422 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3423 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3424 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3425 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3426 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3427 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | 1 | 3428 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3429 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3430 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3431 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3432 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3433 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3434 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3435 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3436 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3437 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3438 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3439 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3440 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3441 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3442 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3443 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3444 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3445 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3446 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3447 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3448 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3449 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3450 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3451 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3452 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3453 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3454 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3455 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3456 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3457 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3458 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3459 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3460 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3461 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3462 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3463 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3464 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3465 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3466 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3467 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3468 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3469 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3470 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | 1 | 3471 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3472 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3473 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3474 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3475 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3476 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3477 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3478 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3479 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3480 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3481 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3482 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3483 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3484 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3485 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3486 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3487 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3488 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3489 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3490 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3491 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3492 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3493 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3494 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3495 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3496 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3497 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3498 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3499 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3500 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3501 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3502 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3503 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3504 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3505 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3506 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3507 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3508 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3509 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3510 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3511 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3512 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3513 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | 1 | 3514 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3515 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3516 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3517 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3518 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3519 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3520 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3521 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3522 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3523 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3524 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3525 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3526 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3527 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3528 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3529 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3530 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3531 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3532 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3533 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3534 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3535 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3536 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3537 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3538 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3539 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3540 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3541 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3542 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3543 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3544 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3545 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3546 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3547 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3548 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3549 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3550 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3551 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3552 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3553 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3554 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3555 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3556 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | 1 | 3557 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3558 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3559 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3560 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3561 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3562 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3563 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3564 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3565 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3566 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3567 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3568 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3569 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3570 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3571 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3572 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3573 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3574 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3575 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3576 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3577 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3578 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3579 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3580 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3581 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3582 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3583 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3584 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3585 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3586 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3587 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3588 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3589 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3590 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3591 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3592 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3593 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3594 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3595 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3596 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3597 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3598 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3599 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | 1 | 3600 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3601 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3602 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3603 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3604 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3605 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3606 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3607 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3608 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3609 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3610 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3611 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3612 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3613 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3614 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3615 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3616 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3617 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3618 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3619 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3620 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3621 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3622 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3623 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3624 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3625 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3626 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3627 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3628 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3629 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3630 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3631 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3632 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3633 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3634 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3635 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3636 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3637 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3638 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3639 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3640 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3641 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3642 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | 1 | 3643 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3644 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3645 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3646 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3647 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3648 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3649 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3650 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3651 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3652 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3653 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3654 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3655 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3656 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3657 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3658 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3659 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3660 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3661 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3662 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3663 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3664 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3665 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3666 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3667 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3668 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3669 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3670 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3671 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3672 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3673 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3674 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3675 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3676 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3677 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3678 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3679 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3680 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3681 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3682 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3683 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3684 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3685 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | 1 | 3686 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3687 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3688 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3689 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3690 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3691 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3692 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3693 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3694 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3695 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3696 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3697 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3698 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3699 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3700 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3701 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3702 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3703 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3704 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3705 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3706 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3707 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3708 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3709 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3710 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3711 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3712 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3713 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3714 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3715 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3716 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3717 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3718 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3719 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3720 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3721 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3722 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3723 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3724 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3725 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3726 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3727 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3728 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | 1 | 3729 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3730 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 1 | 3731 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | 7MB | 1 | 4216 | - | 16,23,23 | 1.33 | 3 (18%) | 6,38,38 | 2.02 | 2 (33%) |
| 84 | OHX | 2 | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 3 | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 3 | 202 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 3 | 203 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 3 | 204 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 3 | 205 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 3 | 206 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 3 | 207 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 3 | 208 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 4 | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 4 | 202 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 4 | 203 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 4 | 204 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 4 | 205 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 4 | 206 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 4 | 207 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 4 | 208 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 4 | 209 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 4 | 210 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 4 | 211 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 4 | 212 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1901 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1902 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1903 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1904 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1905 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1906 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1907 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1908 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1909 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1910 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1911 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1912 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1913 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1914 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1915 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1916 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1917 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1918 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | 6 | 1919 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1920 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1921 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1922 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1923 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1924 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1925 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1926 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1927 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1928 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1929 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1930 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1931 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1932 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1933 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1934 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1935 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1936 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1937 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1938 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1939 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1940 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1941 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1942 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1943 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1944 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1945 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1946 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1947 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1948 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1949 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1950 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1951 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1952 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1953 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1954 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1955 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1956 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1957 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1958 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1959 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1960 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1961 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | 6 | 1962 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1963 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1964 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1965 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1966 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1967 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1968 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1969 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1970 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1971 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1972 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1973 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1974 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1975 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1976 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1977 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1978 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1979 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1980 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1981 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1982 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1983 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1984 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1985 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1986 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1987 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1988 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1989 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1990 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1991 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1992 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1993 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1994 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1995 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1996 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1997 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1998 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 1999 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2000 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2001 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2002 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2003 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2004 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | 6 | 2005 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2006 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2007 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2008 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2009 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2010 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2011 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2012 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2013 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2014 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2015 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2016 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2017 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2018 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2019 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2020 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2021 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2022 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2023 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2024 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2025 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2026 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2027 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2028 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2029 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2030 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2031 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2032 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2033 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2034 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2035 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2036 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2037 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2038 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2039 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2040 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2041 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2042 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2043 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2044 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2045 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2046 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2047 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | 6 | 2048 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2049 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2050 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2051 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2052 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2053 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2054 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2055 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2056 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | 6 | 2057 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1901 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1902 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1903 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1904 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1905 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1906 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1907 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1908 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1909 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1910 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1911 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1912 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1913 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1914 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1915 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1916 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1917 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1918 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1919 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1920 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1921 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1922 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1923 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1924 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1925 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1926 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1927 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1928 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1929 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1930 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1931 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1932 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1933 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | A | 1934 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1935 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1936 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1937 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1938 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1939 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1940 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1941 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1942 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1943 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1944 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1945 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1946 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1947 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1948 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1949 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1950 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1951 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1952 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1953 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1954 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1955 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1956 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1957 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1958 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1959 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1960 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1961 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1962 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1963 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1964 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1965 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1966 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1967 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1968 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1969 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1970 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1971 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1972 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1973 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1974 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1975 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1976 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | A | 1977 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1978 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1979 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1980 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1981 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1982 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1983 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1984 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1985 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1986 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1987 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1988 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1989 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1990 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1991 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1992 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1993 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1994 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1995 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1996 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1997 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1998 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 1999 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2000 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2001 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2002 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2003 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2004 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2005 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2006 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2007 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2008 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2009 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2010 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2011 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2012 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2013 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2014 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2015 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2016 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2017 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2018 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2019 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | A | 2020 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2021 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2022 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2023 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2024 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2025 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2026 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2027 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2028 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2029 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2030 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2031 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2032 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2033 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2034 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2035 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2036 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2037 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2038 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2039 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2040 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2041 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | A | 2042 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AC | 101 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AE | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AG | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AK | 102 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AK | 103 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AP | 502 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3401 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3402 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3403 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3404 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3405 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3406 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3407 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3408 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3409 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3410 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3411 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3412 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3413 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3414 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | AR | 3415 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3416 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3417 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3418 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3419 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3420 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3421 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3422 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3423 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3424 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3425 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3426 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3427 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3428 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3429 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3430 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3431 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3432 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3433 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3434 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3435 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3436 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3437 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3438 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3439 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3440 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3441 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3442 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3443 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3444 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3445 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3446 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3447 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3448 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3449 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3450 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3451 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3452 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3453 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3454 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3455 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3456 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3457 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | AR | 3458 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3459 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3460 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3461 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3462 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3463 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3464 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3465 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3466 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3467 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3468 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3469 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3470 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3471 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3472 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3473 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3474 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3475 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3476 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3477 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3478 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3479 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3480 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3481 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3482 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3483 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3484 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3485 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3486 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3487 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3488 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3489 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3490 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3491 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3492 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3493 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3494 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3495 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3496 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3497 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3498 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3499 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3500 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | AR | 3501 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3502 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3503 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3504 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3505 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3506 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3507 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3508 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3509 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3510 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3511 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3512 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3513 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3514 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3515 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3516 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3517 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3518 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3519 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3520 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3521 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3522 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3523 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3524 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3525 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3526 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3527 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3528 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3529 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3530 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3531 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3532 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3533 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3534 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3535 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3536 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3537 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3538 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3539 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3540 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3541 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3542 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3543 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | AR | 3544 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3545 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3546 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3547 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3548 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3549 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3550 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3551 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3552 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3553 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3554 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3555 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3556 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3557 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3558 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3559 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3560 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3561 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3562 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3563 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3564 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3565 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3566 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3567 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3568 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3569 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3570 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3571 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3572 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3573 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3574 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3575 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3576 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3577 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3578 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3579 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3580 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3581 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3582 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3583 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3584 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3585 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3586 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | AR | 3587 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3588 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3589 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3590 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3591 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3592 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3593 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3594 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3595 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3596 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3597 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3598 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3599 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3600 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3601 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3602 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3603 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3604 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3605 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3606 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3607 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3608 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3609 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3610 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3611 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3612 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3613 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3614 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3615 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3616 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3617 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3618 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3619 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3620 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3621 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3622 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3623 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3624 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3625 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3626 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3627 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3628 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3629 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | AR | 3630 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3631 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3632 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3633 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3634 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3635 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3636 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3637 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3638 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3639 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3640 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3641 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3642 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3643 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3644 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3645 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3646 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3647 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3648 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3649 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3650 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3651 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3652 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3653 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3654 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3655 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3656 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3657 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3658 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3659 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3660 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3661 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3662 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3663 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3664 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3665 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3666 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3667 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3668 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3669 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3670 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3671 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3672 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | AR | 3673 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3674 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3675 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3676 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3677 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3678 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3679 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3680 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3681 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3682 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3683 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3684 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3685 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3686 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3687 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3688 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3689 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3690 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3691 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3692 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3693 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3694 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3695 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3696 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3697 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3698 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3699 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3700 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3701 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3702 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3703 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3704 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3705 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3706 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3707 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3708 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3709 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3710 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3711 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3712 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3713 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3714 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3715 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | AR | 3716 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3717 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3718 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3719 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3720 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3721 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3722 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3723 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3724 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3725 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3726 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3727 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3728 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3729 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3730 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3731 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3732 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3733 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3734 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3735 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3736 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3737 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3738 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AR | 3739 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 86 | 7MB | AR | 4239 | - | 16,23,23 | 0.83 | 0 | 6,38,38 | 0.75 | 0 |
| 84 | OHX | AS | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AS | 202 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AS | 203 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AS | 204 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AS | 205 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AS | 206 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AS | 207 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AS | 208 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AS | 209 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AS | 210 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AT | 202 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AT | 203 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AT | 204 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AT | 205 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AT | 206 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AT | 207 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AT | 208 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AT | 209 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | AT | 210 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AT | 211 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AT | 212 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AT | 213 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AT | 214 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AT | 215 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AT | 216 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AT | 217 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AT | 218 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AT | 219 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | AT | 220 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | CE | 402 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | CE | 403 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | CF | 401 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | CF | 402 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | CG | 301 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | CG | 302 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | CG | 303 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | CK | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | CL | 301 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | CL | 302 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | CM | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | CO | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | CP | 501 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | CV | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | CX | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | CZ | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | DD | 102 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | DG | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | DH | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | DI | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | DL | 101 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | DL | 102 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | H | 301 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | J | 301 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | M | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | O | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | Q | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | T | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | c3 | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | c5 | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | c8 | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | d9 | 101 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 84 | OHX | e | 101 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | h | 401 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | k | 401 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | k | 402 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | l | 401 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | r | 301 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | s8 | 301 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | sR | 401 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | v | 301 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | x | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | x | 202 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | y | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |
| 84 | OHX | z | 201 | - | 0,6,6 | 0.00 | - | 0,15,15 | 0.00 | - |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 84 | OHX | 1 | 3401 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3402 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3403 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3404 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3405 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3406 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3407 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3408 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3409 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3410 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3411 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3412 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3413 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3414 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3415 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3416 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3417 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3418 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3419 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3420 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3421 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3422 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3423 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 84 | OHX | 1 | 3424 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3425 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3426 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3427 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3428 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3429 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3430 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3431 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3432 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3433 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3434 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3435 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3436 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3437 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3438 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3439 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3440 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3441 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3442 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3443 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3444 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3445 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3446 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3447 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3448 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3449 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3450 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3451 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3452 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3453 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3454 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3455 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3456 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3457 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3458 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3459 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3460 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3461 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3462 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3463 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3464 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3465 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 84 | OHX | 1 | 3466 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3467 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3468 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3469 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3470 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3471 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3472 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3473 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3474 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3475 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3476 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3477 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3478 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3479 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3480 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3481 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3482 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3483 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3484 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3485 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3486 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3487 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3488 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3489 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3490 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3491 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3492 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3493 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3494 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3495 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3496 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3497 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3498 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3499 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3500 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3501 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3502 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3503 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3504 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3505 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3506 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3507 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 84 | OHX | 1 | 3508 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3509 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3510 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3511 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3512 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3513 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3514 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3515 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3516 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3517 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3518 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3519 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3520 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3521 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3522 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3523 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3524 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3525 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3526 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3527 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3528 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3529 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3530 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3531 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3532 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3533 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3534 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3535 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3536 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3537 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3538 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3539 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3540 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3541 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3542 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3543 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3544 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3545 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3546 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3547 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3548 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3549 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 84 | OHX | 1 | 3550 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3551 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3552 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3553 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3554 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3555 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3556 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3557 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3558 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3559 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3560 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3561 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3562 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3563 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3564 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3565 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3566 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3567 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3568 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3569 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3570 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3571 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3572 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3573 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3574 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3575 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3576 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3577 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3578 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3579 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3580 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3581 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3582 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3583 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3584 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3585 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3586 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3587 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3588 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3589 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3590 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3591 | - | - | 0/0/0/0 | 0/0/0/0 |

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Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 84 | OHX | 1 | 3592 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3593 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3594 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3595 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3596 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3597 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3598 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3599 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3600 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3601 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3602 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3603 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3604 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3605 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3606 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3607 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3608 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3609 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3610 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3611 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3612 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3613 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3614 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3615 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3616 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3617 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3618 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3619 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3620 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3621 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3622 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3623 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3624 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3625 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3626 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3627 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3628 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3629 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3630 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3631 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3632 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3633 | - | - | 0/0/0/0 | 0/0/0/0 |

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Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 84 | OHX | 1 | 3634 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3635 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3636 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3637 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3638 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3639 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3640 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3641 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3642 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3643 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3644 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3645 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3646 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3647 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3648 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3649 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3650 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3651 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3652 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3653 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3654 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3655 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3656 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3657 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3658 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3659 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3660 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3661 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3662 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3663 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3664 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3665 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3666 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3667 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3668 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3669 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3670 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3671 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3672 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3673 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3674 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3675 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 84 | OHX | 1 | 3676 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3677 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3678 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3679 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3680 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3681 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3682 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3683 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3684 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3685 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3686 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3687 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3688 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3689 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3690 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3691 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3692 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3693 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3694 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3695 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3696 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3697 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3698 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3699 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3700 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3701 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3702 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3703 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3704 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3705 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3706 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3707 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3708 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3709 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3710 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3711 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3712 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3713 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3714 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3715 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3716 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3717 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 84 | OHX | 1 | 3718 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3719 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3720 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3721 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3722 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3723 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3724 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3725 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3726 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3727 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3728 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3729 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3730 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 1 | 3731 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | 7MB | 1 | 4216 | - | - | 0/0/45/45 | 0/3/4/4 |
| 84 | OHX | 2 | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 3 | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 3 | 202 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 3 | 203 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 3 | 204 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 3 | 205 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 3 | 206 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 3 | 207 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 3 | 208 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 4 | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 4 | 202 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 4 | 203 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 4 | 204 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 4 | 205 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 4 | 206 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 4 | 207 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 4 | 208 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 4 | 209 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 4 | 210 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 4 | 211 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 4 | 212 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1901 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1902 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1903 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1904 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1905 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1906 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 84 | OHX | 6 | 1907 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1908 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1909 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1910 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1911 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1912 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1913 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1914 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1915 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1916 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1917 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1918 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1919 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1920 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1921 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1922 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1923 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1924 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1925 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1926 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1927 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1928 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1929 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1930 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1931 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1932 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1933 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1934 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1935 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1936 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1937 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1938 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1939 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1940 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1941 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1942 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1943 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1944 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1945 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1946 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1947 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1948 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 84 | OHX | 6 | 1949 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1950 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1951 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1952 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1953 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1954 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1955 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1956 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1957 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1958 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1959 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1960 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1961 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1962 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1963 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1964 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1965 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1966 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1967 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1968 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1969 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1970 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1971 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1972 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1973 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1974 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1975 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1976 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1977 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1978 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1979 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1980 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1981 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1982 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1983 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1984 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1985 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1986 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1987 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1988 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1989 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1990 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 84 | OHX | 6 | 1991 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1992 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1993 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1994 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1995 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1996 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1997 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1998 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 1999 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2000 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2002 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2003 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2004 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2005 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2006 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2007 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2008 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2009 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2010 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2011 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2012 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2013 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2014 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2015 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2016 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2017 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2018 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2019 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2020 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2021 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2022 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2023 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2024 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2025 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2026 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2027 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2028 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2029 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2030 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2031 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2032 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 84 | OHX | 6 | 2033 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2034 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2035 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2036 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2037 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2038 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2039 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2040 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2041 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2042 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2043 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2044 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2045 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2046 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2047 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2048 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2049 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2050 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2051 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2052 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2053 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2054 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2055 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2056 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | 6 | 2057 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1901 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1902 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1903 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1904 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1905 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1906 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1907 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1908 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1909 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1910 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1911 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1912 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1913 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1914 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1915 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1916 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1917 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 84 | OHX | A | 1918 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1919 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1920 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1921 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1922 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1923 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1924 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1925 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1926 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1927 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1928 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1929 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1930 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1931 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1932 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1933 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1934 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1935 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1936 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1937 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1938 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1939 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1940 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1941 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1942 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1943 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1944 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1945 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1946 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1947 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1948 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1949 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1950 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1951 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1952 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1953 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1954 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1955 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1956 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1957 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1958 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1959 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 84 | OHX | A | 1960 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1961 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1962 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1963 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1964 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1965 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1966 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1967 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1968 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1969 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1970 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1971 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1972 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1973 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1974 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1975 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1976 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1977 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1978 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1979 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1980 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1981 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1982 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1983 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1984 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1985 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1986 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1987 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1988 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1989 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1990 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1991 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1992 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1993 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1994 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1995 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1996 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1997 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1998 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 1999 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2000 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2001 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 84 | OHX | A | 2002 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2003 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2004 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2005 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2006 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2007 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2008 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2009 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2010 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2011 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2012 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2013 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2014 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2015 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2016 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2017 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2018 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2019 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2020 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2021 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2022 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2023 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2024 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2025 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2026 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2027 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2028 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2029 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2030 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2031 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2032 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2033 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2034 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2035 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2036 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2037 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2038 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2039 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2040 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2041 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | A | 2042 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AC | 101 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 84 | OHX | AE | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AG | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AK | 102 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AK | 103 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AP | 502 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3401 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3402 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3403 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3404 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3405 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3406 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3407 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3408 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3409 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3410 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3411 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3412 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3413 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3414 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3415 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3416 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3417 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3418 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3419 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3420 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3421 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3422 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3423 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3424 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3425 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3426 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3427 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3428 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3429 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3430 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3431 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3432 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3433 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3434 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3435 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3436 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3437 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 84 | OHX | AR | 3438 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3439 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3440 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3441 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3442 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3443 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3444 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3445 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3446 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3447 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3448 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3449 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3450 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3451 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3452 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3453 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3454 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3455 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3456 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3457 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3458 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3459 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3460 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3461 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3462 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3463 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3464 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3465 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3466 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3467 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3468 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3469 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3470 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3471 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3472 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3473 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3474 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3475 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3476 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3477 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3478 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3479 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 84 | OHX | AR | 3480 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3481 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3482 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3483 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3484 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3485 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3486 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3487 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3488 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3489 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3490 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3491 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3492 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3493 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3494 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3495 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3496 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3497 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3498 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3499 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3500 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3501 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3502 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3503 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3504 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3505 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3506 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3507 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3508 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3509 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3510 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3511 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3512 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3513 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3514 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3515 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3516 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3517 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3518 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3519 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3520 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3521 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 84 | OHX | AR | 3522 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3523 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3524 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3525 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3526 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3527 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3528 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3529 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3530 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3531 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3532 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3533 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3534 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3535 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3536 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3537 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3538 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3539 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3540 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3541 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3542 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3543 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3544 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3545 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3546 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3547 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3548 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3549 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3550 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3551 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3552 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3553 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3554 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3555 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3556 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3557 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3558 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3559 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3560 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3561 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3562 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3563 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 84 | OHX | AR | 3564 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3565 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3566 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3567 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3568 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3569 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3570 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3571 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3572 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3573 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3574 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3575 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3576 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3577 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3578 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3579 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3580 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3581 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3582 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3583 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3584 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3585 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3586 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3587 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3588 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3589 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3590 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3591 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3592 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3593 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3594 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3595 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3596 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3597 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3598 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3599 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3600 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3601 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3602 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3603 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3604 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3605 | - | - | 0/0/0/0 | 0/0/0/0 |

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Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 84 | OHX | AR | 3606 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3607 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3608 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3609 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3610 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3611 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3612 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3613 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3614 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3615 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3616 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3617 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3618 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3619 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3620 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3621 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3622 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3623 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3624 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3625 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3626 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3627 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3628 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3629 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3630 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3631 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3632 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3633 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3634 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3635 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3636 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3637 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3638 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3639 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3640 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3641 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3642 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3643 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3644 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3645 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3646 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3647 | - | - | 0/0/0/0 | 0/0/0/0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 84 | OHX | AR | 3648 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3649 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3650 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3651 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3652 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3653 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3654 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3655 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3656 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3657 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3658 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3659 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3660 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3661 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3662 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3663 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3664 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3665 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3666 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3667 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3668 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3669 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3670 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3671 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3672 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3673 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3674 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3675 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3676 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3677 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3678 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3679 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3680 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3681 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3682 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3683 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3684 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3685 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3686 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3687 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3688 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3689 | - | - | 0/0/0/0 | 0/0/0/0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 84 | OHX | AR | 3690 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3691 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3692 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3693 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3694 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3695 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3696 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3697 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3698 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3699 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3700 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3701 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3702 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3703 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3704 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3705 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3706 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3707 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3708 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3709 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3710 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3711 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3712 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3713 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3714 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3715 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3716 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3717 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3718 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3719 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3720 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3721 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3722 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3723 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3724 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3725 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3726 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3727 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3728 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3729 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3730 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3731 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 84 | OHX | AR | 3732 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3733 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3734 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3735 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3736 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3737 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3738 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AR | 3739 | - | - | 0/0/0/0 | 0/0/0/0 |
| 86 | 7MB | AR | 4239 | - | - | 0/0/45/45 | 0/3/4/4 |
| 84 | OHX | AS | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AS | 202 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AS | 203 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AS | 204 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AS | 205 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AS | 206 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AS | 207 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AS | 208 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AS | 209 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AS | 210 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AT | 202 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AT | 203 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AT | 204 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AT | 205 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AT | 206 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AT | 207 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AT | 208 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AT | 209 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AT | 210 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AT | 211 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AT | 212 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AT | 213 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AT | 214 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AT | 215 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AT | 216 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AT | 217 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AT | 218 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AT | 219 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | AT | 220 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | CE | 402 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | CE | 403 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | CF | 401 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | CF | 402 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|---------|
| 84 | OHX | CG | 301 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | CG | 302 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | CG | 303 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | CK | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | CL | 301 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | CL | 302 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | CM | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | CO | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | CP | 501 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | CV | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | CX | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | CZ | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | DD | 102 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | DG | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | DH | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | DI | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | DL | 101 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | DL | 102 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | H | 301 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | J | 301 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | M | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | O | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | Q | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | T | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | c3 | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | c5 | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | c8 | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | d9 | 101 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | e | 101 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | h | 401 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | k | 401 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | k | 402 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | l | 401 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | r | 301 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | s8 | 301 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | sR | 401 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | v | 301 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | x | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | x | 202 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | y | 201 | - | - | 0/0/0/0 | 0/0/0/0 |
| 84 | OHX | z | 201 | - | - | 0/0/0/0 | 0/0/0/0 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 86 | 1 | 4216 | 7MB | C9-C8 | -2.75 | 1.35 | 1.40 |
| 86 | 1 | 4216 | 7MB | O-C1 | -2.14 | 1.19 | 1.23 |
| 86 | 1 | 4216 | 7MB | C10-C11 | -2.07 | 1.36 | 1.39 |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 86 | 1 | 4216 | 7MB | C6-C2-N1 | -2.82 | 108.36 | 113.23 |
| 86 | 1 | 4216 | 7MB | C3-C2-N1 | 3.39 | 106.22 | 101.21 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

538 monomers are involved in 770 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 84 | 1 | 3401 | OHX | 1 | 0 |
| 84 | 1 | 3402 | OHX | 1 | 0 |
| 84 | 1 | 3403 | OHX | 1 | 0 |
| 84 | 1 | 3404 | OHX | 1 | 0 |
| 84 | 1 | 3405 | OHX | 2 | 0 |
| 84 | 1 | 3406 | OHX | 5 | 0 |
| 84 | 1 | 3408 | OHX | 2 | 0 |
| 84 | 1 | 3409 | OHX | 1 | 0 |
| 84 | 1 | 3410 | OHX | 2 | 0 |
| 84 | 1 | 3413 | OHX | 2 | 0 |
| 84 | 1 | 3414 | OHX | 1 | 0 |
| 84 | 1 | 3415 | OHX | 1 | 0 |
| 84 | 1 | 3416 | OHX | 2 | 0 |
| 84 | 1 | 3419 | OHX | 2 | 0 |
| 84 | 1 | 3420 | OHX | 2 | 0 |
| 84 | 1 | 3422 | OHX | 2 | 0 |
| 84 | 1 | 3427 | OHX | 1 | 0 |
| 84 | 1 | 3428 | OHX | 2 | 0 |
| 84 | 1 | 3430 | OHX | 2 | 0 |
| 84 | 1 | 3433 | OHX | 2 | 0 |
| 84 | 1 | 3437 | OHX | 2 | 0 |
| 84 | 1 | 3438 | OHX | 2 | 0 |
| 84 | 1 | 3440 | OHX | 1 | 0 |
| 84 | 1 | 3441 | OHX | 1 | 0 |
| 84 | 1 | 3442 | OHX | 1 | 0 |
| 84 | 1 | 3444 | OHX | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 84 | 1 | 3446 | OHX | 1 | 0 |
| 84 | 1 | 3447 | OHX | 2 | 0 |
| 84 | 1 | 3448 | OHX | 2 | 0 |
| 84 | 1 | 3450 | OHX | 2 | 0 |
| 84 | 1 | 3453 | OHX | 1 | 0 |
| 84 | 1 | 3454 | OHX | 1 | 0 |
| 84 | 1 | 3459 | OHX | 1 | 0 |
| 84 | 1 | 3461 | OHX | 1 | 0 |
| 84 | 1 | 3463 | OHX | 1 | 0 |
| 84 | 1 | 3465 | OHX | 1 | 0 |
| 84 | 1 | 3466 | OHX | 1 | 0 |
| 84 | 1 | 3471 | OHX | 4 | 0 |
| 84 | 1 | 3472 | OHX | 1 | 0 |
| 84 | 1 | 3474 | OHX | 1 | 0 |
| 84 | 1 | 3478 | OHX | 2 | 0 |
| 84 | 1 | 3482 | OHX | 2 | 0 |
| 84 | 1 | 3485 | OHX | 1 | 0 |
| 84 | 1 | 3491 | OHX | 1 | 0 |
| 84 | 1 | 3493 | OHX | 1 | 0 |
| 84 | 1 | 3494 | OHX | 1 | 0 |
| 84 | 1 | 3495 | OHX | 1 | 0 |
| 84 | 1 | 3496 | OHX | 4 | 0 |
| 84 | 1 | 3497 | OHX | 1 | 0 |
| 84 | 1 | 3500 | OHX | 1 | 0 |
| 84 | 1 | 3502 | OHX | 3 | 0 |
| 84 | 1 | 3503 | OHX | 1 | 0 |
| 84 | 1 | 3504 | OHX | 2 | 0 |
| 84 | 1 | 3505 | OHX | 1 | 0 |
| 84 | 1 | 3506 | OHX | 1 | 0 |
| 84 | 1 | 3507 | OHX | 1 | 0 |
| 84 | 1 | 3511 | OHX | 1 | 0 |
| 84 | 1 | 3513 | OHX | 1 | 0 |
| 84 | 1 | 3514 | OHX | 2 | 0 |
| 84 | 1 | 3515 | OHX | 1 | 0 |
| 84 | 1 | 3516 | OHX | 1 | 0 |
| 84 | 1 | 3521 | OHX | 1 | 0 |
| 84 | 1 | 3522 | OHX | 1 | 0 |
| 84 | 1 | 3523 | OHX | 1 | 0 |
| 84 | 1 | 3524 | OHX | 1 | 0 |
| 84 | 1 | 3527 | OHX | 1 | 0 |
| 84 | 1 | 3529 | OHX | 1 | 0 |
| 84 | 1 | 3530 | OHX | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 84 | 1 | 3534 | OHX | 2 | 0 |
| 84 | 1 | 3535 | OHX | 2 | 0 |
| 84 | 1 | 3536 | OHX | 1 | 0 |
| 84 | 1 | 3537 | OHX | 1 | 0 |
| 84 | 1 | 3538 | OHX | 2 | 0 |
| 84 | 1 | 3539 | OHX | 1 | 0 |
| 84 | 1 | 3540 | OHX | 2 | 0 |
| 84 | 1 | 3541 | OHX | 1 | 0 |
| 84 | 1 | 3542 | OHX | 2 | 0 |
| 84 | 1 | 3544 | OHX | 1 | 0 |
| 84 | 1 | 3546 | OHX | 1 | 0 |
| 84 | 1 | 3547 | OHX | 1 | 0 |
| 84 | 1 | 3548 | OHX | 1 | 0 |
| 84 | 1 | 3552 | OHX | 1 | 0 |
| 84 | 1 | 3553 | OHX | 1 | 0 |
| 84 | 1 | 3554 | OHX | 1 | 0 |
| 84 | 1 | 3556 | OHX | 1 | 0 |
| 84 | 1 | 3558 | OHX | 2 | 0 |
| 84 | 1 | 3563 | OHX | 1 | 0 |
| 84 | 1 | 3565 | OHX | 1 | 0 |
| 84 | 1 | 3567 | OHX | 1 | 0 |
| 84 | 1 | 3568 | OHX | 1 | 0 |
| 84 | 1 | 3572 | OHX | 3 | 0 |
| 84 | 1 | 3577 | OHX | 2 | 0 |
| 84 | 1 | 3578 | OHX | 1 | 0 |
| 84 | 1 | 3579 | OHX | 1 | 0 |
| 84 | 1 | 3582 | OHX | 3 | 0 |
| 84 | 1 | 3585 | OHX | 1 | 0 |
| 84 | 1 | 3586 | OHX | 2 | 0 |
| 84 | 1 | 3587 | OHX | 1 | 0 |
| 84 | 1 | 3588 | OHX | 1 | 0 |
| 84 | 1 | 3594 | OHX | 4 | 0 |
| 84 | 1 | 3595 | OHX | 1 | 0 |
| 84 | 1 | 3596 | OHX | 1 | 0 |
| 84 | 1 | 3597 | OHX | 1 | 0 |
| 84 | 1 | 3598 | OHX | 1 | 0 |
| 84 | 1 | 3603 | OHX | 2 | 0 |
| 84 | 1 | 3604 | OHX | 1 | 0 |
| 84 | 1 | 3605 | OHX | 1 | 0 |
| 84 | 1 | 3610 | OHX | 1 | 0 |
| 84 | 1 | 3612 | OHX | 1 | 0 |
| 84 | 1 | 3613 | OHX | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 84 | 1 | 3614 | OHX | 1 | 0 |
| 84 | 1 | 3616 | OHX | 1 | 0 |
| 84 | 1 | 3617 | OHX | 1 | 0 |
| 84 | 1 | 3618 | OHX | 3 | 0 |
| 84 | 1 | 3619 | OHX | 1 | 0 |
| 84 | 1 | 3624 | OHX | 1 | 0 |
| 84 | 1 | 3628 | OHX | 1 | 0 |
| 84 | 1 | 3629 | OHX | 1 | 0 |
| 84 | 1 | 3631 | OHX | 1 | 0 |
| 84 | 1 | 3632 | OHX | 1 | 0 |
| 84 | 1 | 3634 | OHX | 1 | 0 |
| 84 | 1 | 3637 | OHX | 1 | 0 |
| 84 | 1 | 3639 | OHX | 1 | 0 |
| 84 | 1 | 3641 | OHX | 1 | 0 |
| 84 | 1 | 3644 | OHX | 1 | 0 |
| 84 | 1 | 3646 | OHX | 1 | 0 |
| 84 | 1 | 3650 | OHX | 1 | 0 |
| 84 | 1 | 3654 | OHX | 2 | 0 |
| 84 | 1 | 3656 | OHX | 1 | 0 |
| 84 | 1 | 3657 | OHX | 1 | 0 |
| 84 | 1 | 3661 | OHX | 1 | 0 |
| 84 | 1 | 3662 | OHX | 1 | 0 |
| 84 | 1 | 3663 | OHX | 1 | 0 |
| 84 | 1 | 3665 | OHX | 2 | 0 |
| 84 | 1 | 3666 | OHX | 2 | 0 |
| 84 | 1 | 3667 | OHX | 1 | 0 |
| 84 | 1 | 3668 | OHX | 2 | 0 |
| 84 | 1 | 3669 | OHX | 1 | 0 |
| 84 | 1 | 3672 | OHX | 2 | 0 |
| 84 | 1 | 3674 | OHX | 1 | 0 |
| 84 | 1 | 3676 | OHX | 2 | 0 |
| 84 | 1 | 3677 | OHX | 1 | 0 |
| 84 | 1 | 3681 | OHX | 1 | 0 |
| 84 | 1 | 3682 | OHX | 2 | 0 |
| 84 | 1 | 3684 | OHX | 1 | 0 |
| 84 | 1 | 3687 | OHX | 1 | 0 |
| 84 | 1 | 3688 | OHX | 1 | 0 |
| 84 | 1 | 3689 | OHX | 2 | 0 |
| 84 | 1 | 3690 | OHX | 1 | 0 |
| 84 | 1 | 3691 | OHX | 1 | 0 |
| 84 | 1 | 3696 | OHX | 1 | 0 |
| 84 | 1 | 3698 | OHX | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 84 | 1 | 3702 | OHX | 4 | 0 |
| 84 | 1 | 3709 | OHX | 1 | 0 |
| 84 | 1 | 3712 | OHX | 2 | 0 |
| 84 | 1 | 3713 | OHX | 1 | 0 |
| 84 | 1 | 3714 | OHX | 1 | 0 |
| 84 | 1 | 3717 | OHX | 1 | 0 |
| 84 | 1 | 3720 | OHX | 1 | 0 |
| 84 | 1 | 3722 | OHX | 1 | 0 |
| 84 | 1 | 3724 | OHX | 1 | 0 |
| 84 | 1 | 3725 | OHX | 3 | 0 |
| 84 | 1 | 3730 | OHX | 3 | 0 |
| 86 | 1 | 4216 | 7MB | 4 | 0 |
| 84 | 3 | 201 | OHX | 1 | 0 |
| 84 | 3 | 202 | OHX | 1 | 0 |
| 84 | 3 | 203 | OHX | 1 | 0 |
| 84 | 3 | 206 | OHX | 2 | 0 |
| 84 | 4 | 202 | OHX | 1 | 0 |
| 84 | 4 | 203 | OHX | 1 | 0 |
| 84 | 4 | 204 | OHX | 1 | 0 |
| 84 | 4 | 206 | OHX | 1 | 0 |
| 84 | 4 | 209 | OHX | 1 | 0 |
| 84 | 4 | 211 | OHX | 1 | 0 |
| 84 | 4 | 212 | OHX | 1 | 0 |
| 84 | 6 | 1901 | OHX | 1 | 0 |
| 84 | 6 | 1902 | OHX | 1 | 0 |
| 84 | 6 | 1904 | OHX | 1 | 0 |
| 84 | 6 | 1906 | OHX | 1 | 0 |
| 84 | 6 | 1908 | OHX | 1 | 0 |
| 84 | 6 | 1910 | OHX | 2 | 0 |
| 84 | 6 | 1911 | OHX | 1 | 0 |
| 84 | 6 | 1912 | OHX | 1 | 0 |
| 84 | 6 | 1913 | OHX | 1 | 0 |
| 84 | 6 | 1914 | OHX | 1 | 0 |
| 84 | 6 | 1915 | OHX | 3 | 0 |
| 84 | 6 | 1918 | OHX | 1 | 0 |
| 84 | 6 | 1921 | OHX | 1 | 0 |
| 84 | 6 | 1922 | OHX | 1 | 0 |
| 84 | 6 | 1924 | OHX | 1 | 0 |
| 84 | 6 | 1926 | OHX | 1 | 0 |
| 84 | 6 | 1927 | OHX | 3 | 0 |
| 84 | 6 | 1930 | OHX | 1 | 0 |
| 84 | 6 | 1932 | OHX | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 84 | 6 | 1934 | OHX | 1 | 0 |
| 84 | 6 | 1939 | OHX | 1 | 0 |
| 84 | 6 | 1942 | OHX | 2 | 0 |
| 84 | 6 | 1945 | OHX | 3 | 0 |
| 84 | 6 | 1952 | OHX | 2 | 0 |
| 84 | 6 | 1953 | OHX | 2 | 0 |
| 84 | 6 | 1955 | OHX | 1 | 0 |
| 84 | 6 | 1956 | OHX | 3 | 0 |
| 84 | 6 | 1957 | OHX | 1 | 0 |
| 84 | 6 | 1958 | OHX | 1 | 0 |
| 84 | 6 | 1961 | OHX | 1 | 0 |
| 84 | 6 | 1963 | OHX | 1 | 0 |
| 84 | 6 | 1965 | OHX | 1 | 0 |
| 84 | 6 | 1968 | OHX | 1 | 0 |
| 84 | 6 | 1969 | OHX | 1 | 0 |
| 84 | 6 | 1970 | OHX | 1 | 0 |
| 84 | 6 | 1973 | OHX | 3 | 0 |
| 84 | 6 | 1976 | OHX | 2 | 0 |
| 84 | 6 | 1977 | OHX | 1 | 0 |
| 84 | 6 | 1978 | OHX | 1 | 0 |
| 84 | 6 | 1979 | OHX | 1 | 0 |
| 84 | 6 | 1980 | OHX | 1 | 0 |
| 84 | 6 | 1982 | OHX | 3 | 0 |
| 84 | 6 | 1985 | OHX | 1 | 0 |
| 84 | 6 | 1986 | OHX | 3 | 0 |
| 84 | 6 | 1991 | OHX | 1 | 0 |
| 84 | 6 | 1992 | OHX | 1 | 0 |
| 84 | 6 | 1993 | OHX | 2 | 0 |
| 84 | 6 | 1994 | OHX | 2 | 0 |
| 84 | 6 | 1995 | OHX | 1 | 0 |
| 84 | 6 | 1997 | OHX | 1 | 0 |
| 84 | 6 | 1999 | OHX | 2 | 0 |
| 84 | 6 | 2000 | OHX | 2 | 0 |
| 84 | 6 | 2005 | OHX | 2 | 0 |
| 84 | 6 | 2006 | OHX | 1 | 0 |
| 84 | 6 | 2007 | OHX | 1 | 0 |
| 84 | 6 | 2008 | OHX | 2 | 0 |
| 84 | 6 | 2009 | OHX | 1 | 0 |
| 84 | 6 | 2011 | OHX | 1 | 0 |
| 84 | 6 | 2012 | OHX | 1 | 0 |
| 84 | 6 | 2013 | OHX | 1 | 0 |
| 84 | 6 | 2018 | OHX | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 84 | 6 | 2021 | OHX | 1 | 0 |
| 84 | 6 | 2028 | OHX | 1 | 0 |
| 84 | 6 | 2030 | OHX | 1 | 0 |
| 84 | 6 | 2033 | OHX | 1 | 0 |
| 84 | 6 | 2035 | OHX | 1 | 0 |
| 84 | 6 | 2037 | OHX | 1 | 0 |
| 84 | 6 | 2038 | OHX | 1 | 0 |
| 84 | 6 | 2039 | OHX | 1 | 0 |
| 84 | 6 | 2040 | OHX | 1 | 0 |
| 84 | 6 | 2043 | OHX | 3 | 0 |
| 84 | 6 | 2044 | OHX | 1 | 0 |
| 84 | 6 | 2045 | OHX | 2 | 0 |
| 84 | 6 | 2047 | OHX | 1 | 0 |
| 84 | 6 | 2050 | OHX | 3 | 0 |
| 84 | 6 | 2055 | OHX | 1 | 0 |
| 84 | A | 1901 | OHX | 1 | 0 |
| 84 | A | 1902 | OHX | 1 | 0 |
| 84 | A | 1904 | OHX | 1 | 0 |
| 84 | A | 1905 | OHX | 1 | 0 |
| 84 | A | 1907 | OHX | 1 | 0 |
| 84 | A | 1909 | OHX | 3 | 0 |
| 84 | A | 1910 | OHX | 2 | 0 |
| 84 | A | 1911 | OHX | 1 | 0 |
| 84 | A | 1912 | OHX | 2 | 0 |
| 84 | A | 1913 | OHX | 1 | 0 |
| 84 | A | 1914 | OHX | 2 | 0 |
| 84 | A | 1915 | OHX | 2 | 0 |
| 84 | A | 1916 | OHX | 1 | 0 |
| 84 | A | 1917 | OHX | 1 | 0 |
| 84 | A | 1918 | OHX | 1 | 0 |
| 84 | A | 1919 | OHX | 1 | 0 |
| 84 | A | 1920 | OHX | 1 | 0 |
| 84 | A | 1922 | OHX | 1 | 0 |
| 84 | A | 1923 | OHX | 1 | 0 |
| 84 | A | 1925 | OHX | 3 | 0 |
| 84 | A | 1928 | OHX | 2 | 0 |
| 84 | A | 1931 | OHX | 1 | 0 |
| 84 | A | 1932 | OHX | 2 | 0 |
| 84 | A | 1933 | OHX | 1 | 0 |
| 84 | A | 1937 | OHX | 1 | 0 |
| 84 | A | 1938 | OHX | 2 | 0 |
| 84 | A | 1939 | OHX | 3 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 84 | A | 1943 | OHX | 2 | 0 |
| 84 | A | 1944 | OHX | 3 | 0 |
| 84 | A | 1947 | OHX | 1 | 0 |
| 84 | A | 1948 | OHX | 1 | 0 |
| 84 | A | 1951 | OHX | 1 | 0 |
| 84 | A | 1954 | OHX | 4 | 0 |
| 84 | A | 1955 | OHX | 2 | 0 |
| 84 | A | 1956 | OHX | 1 | 0 |
| 84 | A | 1959 | OHX | 1 | 0 |
| 84 | A | 1961 | OHX | 1 | 0 |
| 84 | A | 1962 | OHX | 1 | 0 |
| 84 | A | 1963 | OHX | 1 | 0 |
| 84 | A | 1964 | OHX | 3 | 0 |
| 84 | A | 1965 | OHX | 1 | 0 |
| 84 | A | 1968 | OHX | 1 | 0 |
| 84 | A | 1970 | OHX | 3 | 0 |
| 84 | A | 1971 | OHX | 1 | 0 |
| 84 | A | 1973 | OHX | 2 | 0 |
| 84 | A | 1974 | OHX | 2 | 0 |
| 84 | A | 1981 | OHX | 1 | 0 |
| 84 | A | 1983 | OHX | 1 | 0 |
| 84 | A | 1984 | OHX | 1 | 0 |
| 84 | A | 1985 | OHX | 1 | 0 |
| 84 | A | 1986 | OHX | 1 | 0 |
| 84 | A | 1987 | OHX | 1 | 0 |
| 84 | A | 1988 | OHX | 3 | 0 |
| 84 | A | 1990 | OHX | 1 | 0 |
| 84 | A | 1992 | OHX | 3 | 0 |
| 84 | A | 1993 | OHX | 1 | 0 |
| 84 | A | 1997 | OHX | 1 | 0 |
| 84 | A | 1998 | OHX | 2 | 0 |
| 84 | A | 1999 | OHX | 1 | 0 |
| 84 | A | 2000 | OHX | 1 | 0 |
| 84 | A | 2003 | OHX | 1 | 0 |
| 84 | A | 2004 | OHX | 1 | 0 |
| 84 | A | 2005 | OHX | 1 | 0 |
| 84 | A | 2008 | OHX | 2 | 0 |
| 84 | A | 2009 | OHX | 2 | 0 |
| 84 | A | 2010 | OHX | 1 | 0 |
| 84 | A | 2012 | OHX | 1 | 0 |
| 84 | A | 2019 | OHX | 1 | 0 |
| 84 | A | 2021 | OHX | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 84 | A | 2022 | OHX | 1 | 0 |
| 84 | A | 2023 | OHX | 1 | 0 |
| 84 | A | 2024 | OHX | 2 | 0 |
| 84 | A | 2025 | OHX | 1 | 0 |
| 84 | A | 2026 | OHX | 2 | 0 |
| 84 | A | 2027 | OHX | 1 | 0 |
| 84 | A | 2029 | OHX | 1 | 0 |
| 84 | A | 2030 | OHX | 3 | 0 |
| 84 | A | 2034 | OHX | 1 | 0 |
| 84 | A | 2035 | OHX | 2 | 0 |
| 84 | A | 2037 | OHX | 1 | 0 |
| 84 | A | 2038 | OHX | 2 | 0 |
| 84 | A | 2041 | OHX | 1 | 0 |
| 84 | AC | 101 | OHX | 1 | 0 |
| 84 | AE | 201 | OHX | 4 | 0 |
| 84 | AK | 102 | OHX | 2 | 0 |
| 84 | AP | 502 | OHX | 3 | 0 |
| 84 | AR | 3401 | OHX | 1 | 0 |
| 84 | AR | 3403 | OHX | 1 | 0 |
| 84 | AR | 3407 | OHX | 1 | 0 |
| 84 | AR | 3408 | OHX | 2 | 0 |
| 84 | AR | 3409 | OHX | 1 | 0 |
| 84 | AR | 3410 | OHX | 2 | 0 |
| 84 | AR | 3413 | OHX | 1 | 0 |
| 84 | AR | 3416 | OHX | 2 | 0 |
| 84 | AR | 3417 | OHX | 2 | 0 |
| 84 | AR | 3418 | OHX | 2 | 0 |
| 84 | AR | 3420 | OHX | 1 | 0 |
| 84 | AR | 3421 | OHX | 1 | 0 |
| 84 | AR | 3423 | OHX | 1 | 0 |
| 84 | AR | 3425 | OHX | 2 | 0 |
| 84 | AR | 3427 | OHX | 1 | 0 |
| 84 | AR | 3429 | OHX | 1 | 0 |
| 84 | AR | 3432 | OHX | 2 | 0 |
| 84 | AR | 3435 | OHX | 1 | 0 |
| 84 | AR | 3437 | OHX | 2 | 0 |
| 84 | AR | 3439 | OHX | 1 | 0 |
| 84 | AR | 3440 | OHX | 2 | 0 |
| 84 | AR | 3441 | OHX | 1 | 0 |
| 84 | AR | 3442 | OHX | 2 | 0 |
| 84 | AR | 3443 | OHX | 7 | 0 |
| 84 | AR | 3444 | OHX | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 84 | AR | 3448 | OHX | 1 | 0 |
| 84 | AR | 3449 | OHX | 1 | 0 |
| 84 | AR | 3453 | OHX | 1 | 0 |
| 84 | AR | 3454 | OHX | 2 | 0 |
| 84 | AR | 3455 | OHX | 1 | 0 |
| 84 | AR | 3456 | OHX | 3 | 0 |
| 84 | AR | 3457 | OHX | 2 | 0 |
| 84 | AR | 3459 | OHX | 1 | 0 |
| 84 | AR | 3460 | OHX | 1 | 0 |
| 84 | AR | 3461 | OHX | 1 | 0 |
| 84 | AR | 3462 | OHX | 1 | 0 |
| 84 | AR | 3466 | OHX | 1 | 0 |
| 84 | AR | 3468 | OHX | 1 | 0 |
| 84 | AR | 3469 | OHX | 3 | 0 |
| 84 | AR | 3470 | OHX | 1 | 0 |
| 84 | AR | 3472 | OHX | 1 | 0 |
| 84 | AR | 3473 | OHX | 1 | 0 |
| 84 | AR | 3474 | OHX | 1 | 0 |
| 84 | AR | 3476 | OHX | 1 | 0 |
| 84 | AR | 3478 | OHX | 2 | 0 |
| 84 | AR | 3480 | OHX | 1 | 0 |
| 84 | AR | 3481 | OHX | 1 | 0 |
| 84 | AR | 3483 | OHX | 1 | 0 |
| 84 | AR | 3484 | OHX | 2 | 0 |
| 84 | AR | 3485 | OHX | 1 | 0 |
| 84 | AR | 3490 | OHX | 2 | 0 |
| 84 | AR | 3492 | OHX | 1 | 0 |
| 84 | AR | 3493 | OHX | 1 | 0 |
| 84 | AR | 3499 | OHX | 1 | 0 |
| 84 | AR | 3500 | OHX | 2 | 0 |
| 84 | AR | 3504 | OHX | 3 | 0 |
| 84 | AR | 3505 | OHX | 1 | 0 |
| 84 | AR | 3507 | OHX | 2 | 0 |
| 84 | AR | 3508 | OHX | 1 | 0 |
| 84 | AR | 3509 | OHX | 2 | 0 |
| 84 | AR | 3511 | OHX | 2 | 0 |
| 84 | AR | 3512 | OHX | 2 | 0 |
| 84 | AR | 3514 | OHX | 1 | 0 |
| 84 | AR | 3515 | OHX | 2 | 0 |
| 84 | AR | 3516 | OHX | 1 | 0 |
| 84 | AR | 3517 | OHX | 1 | 0 |
| 84 | AR | 3518 | OHX | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 84 | AR | 3519 | OHX | 1 | 0 |
| 84 | AR | 3521 | OHX | 1 | 0 |
| 84 | AR | 3522 | OHX | 1 | 0 |
| 84 | AR | 3524 | OHX | 3 | 0 |
| 84 | AR | 3526 | OHX | 2 | 0 |
| 84 | AR | 3527 | OHX | 2 | 0 |
| 84 | AR | 3530 | OHX | 1 | 0 |
| 84 | AR | 3531 | OHX | 1 | 0 |
| 84 | AR | 3532 | OHX | 1 | 0 |
| 84 | AR | 3534 | OHX | 1 | 0 |
| 84 | AR | 3536 | OHX | 2 | 0 |
| 84 | AR | 3538 | OHX | 1 | 0 |
| 84 | AR | 3542 | OHX | 2 | 0 |
| 84 | AR | 3545 | OHX | 1 | 0 |
| 84 | AR | 3548 | OHX | 2 | 0 |
| 84 | AR | 3549 | OHX | 1 | 0 |
| 84 | AR | 3550 | OHX | 2 | 0 |
| 84 | AR | 3552 | OHX | 1 | 0 |
| 84 | AR | 3556 | OHX | 1 | 0 |
| 84 | AR | 3560 | OHX | 1 | 0 |
| 84 | AR | 3563 | OHX | 1 | 0 |
| 84 | AR | 3567 | OHX | 2 | 0 |
| 84 | AR | 3568 | OHX | 3 | 0 |
| 84 | AR | 3570 | OHX | 1 | 0 |
| 84 | AR | 3571 | OHX | 1 | 0 |
| 84 | AR | 3573 | OHX | 1 | 0 |
| 84 | AR | 3574 | OHX | 1 | 0 |
| 84 | AR | 3575 | OHX | 1 | 0 |
| 84 | AR | 3578 | OHX | 1 | 0 |
| 84 | AR | 3580 | OHX | 2 | 0 |
| 84 | AR | 3582 | OHX | 2 | 0 |
| 84 | AR | 3586 | OHX | 1 | 0 |
| 84 | AR | 3589 | OHX | 1 | 0 |
| 84 | AR | 3591 | OHX | 1 | 0 |
| 84 | AR | 3592 | OHX | 1 | 0 |
| 84 | AR | 3594 | OHX | 1 | 0 |
| 84 | AR | 3595 | OHX | 2 | 0 |
| 84 | AR | 3596 | OHX | 1 | 0 |
| 84 | AR | 3598 | OHX | 1 | 0 |
| 84 | AR | 3601 | OHX | 2 | 0 |
| 84 | AR | 3603 | OHX | 2 | 0 |
| 84 | AR | 3604 | OHX | 4 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 84 | AR | 3606 | OHX | 3 | 0 |
| 84 | AR | 3607 | OHX | 1 | 0 |
| 84 | AR | 3608 | OHX | 1 | 0 |
| 84 | AR | 3611 | OHX | 1 | 0 |
| 84 | AR | 3613 | OHX | 1 | 0 |
| 84 | AR | 3614 | OHX | 1 | 0 |
| 84 | AR | 3615 | OHX | 1 | 0 |
| 84 | AR | 3619 | OHX | 2 | 0 |
| 84 | AR | 3620 | OHX | 1 | 0 |
| 84 | AR | 3623 | OHX | 1 | 0 |
| 84 | AR | 3624 | OHX | 1 | 0 |
| 84 | AR | 3628 | OHX | 1 | 0 |
| 84 | AR | 3630 | OHX | 2 | 0 |
| 84 | AR | 3631 | OHX | 1 | 0 |
| 84 | AR | 3635 | OHX | 1 | 0 |
| 84 | AR | 3640 | OHX | 1 | 0 |
| 84 | AR | 3641 | OHX | 1 | 0 |
| 84 | AR | 3643 | OHX | 3 | 0 |
| 84 | AR | 3645 | OHX | 1 | 0 |
| 84 | AR | 3646 | OHX | 1 | 0 |
| 84 | AR | 3647 | OHX | 1 | 0 |
| 84 | AR | 3649 | OHX | 1 | 0 |
| 84 | AR | 3650 | OHX | 2 | 0 |
| 84 | AR | 3652 | OHX | 1 | 0 |
| 84 | AR | 3656 | OHX | 1 | 0 |
| 84 | AR | 3657 | OHX | 1 | 0 |
| 84 | AR | 3658 | OHX | 1 | 0 |
| 84 | AR | 3661 | OHX | 2 | 0 |
| 84 | AR | 3671 | OHX | 2 | 0 |
| 84 | AR | 3674 | OHX | 1 | 0 |
| 84 | AR | 3678 | OHX | 1 | 0 |
| 84 | AR | 3682 | OHX | 1 | 0 |
| 84 | AR | 3683 | OHX | 3 | 0 |
| 84 | AR | 3684 | OHX | 1 | 0 |
| 84 | AR | 3685 | OHX | 1 | 0 |
| 84 | AR | 3689 | OHX | 2 | 0 |
| 84 | AR | 3690 | OHX | 2 | 0 |
| 84 | AR | 3691 | OHX | 1 | 0 |
| 84 | AR | 3696 | OHX | 3 | 0 |
| 84 | AR | 3697 | OHX | 3 | 0 |
| 84 | AR | 3700 | OHX | 2 | 0 |
| 84 | AR | 3701 | OHX | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 84 | AR | 3706 | OHX | 1 | 0 |
| 84 | AR | 3707 | OHX | 1 | 0 |
| 84 | AR | 3708 | OHX | 1 | 0 |
| 84 | AR | 3709 | OHX | 1 | 0 |
| 84 | AR | 3712 | OHX | 1 | 0 |
| 84 | AR | 3713 | OHX | 1 | 0 |
| 84 | AR | 3715 | OHX | 2 | 0 |
| 84 | AR | 3720 | OHX | 1 | 0 |
| 84 | AR | 3721 | OHX | 2 | 0 |
| 84 | AR | 3723 | OHX | 1 | 0 |
| 84 | AR | 3727 | OHX | 1 | 0 |
| 84 | AR | 3728 | OHX | 1 | 0 |
| 84 | AR | 3731 | OHX | 6 | 0 |
| 84 | AR | 3735 | OHX | 1 | 0 |
| 84 | AR | 3736 | OHX | 1 | 0 |
| 84 | AR | 3737 | OHX | 1 | 0 |
| 84 | AR | 3739 | OHX | 2 | 0 |
| 86 | AR | 4239 | 7MB | 3 | 0 |
| 84 | AS | 201 | OHX | 1 | 0 |
| 84 | AS | 202 | OHX | 2 | 0 |
| 84 | AS | 203 | OHX | 1 | 0 |
| 84 | AS | 204 | OHX | 1 | 0 |
| 84 | AS | 209 | OHX | 2 | 0 |
| 84 | AT | 202 | OHX | 1 | 0 |
| 84 | AT | 203 | OHX | 3 | 0 |
| 84 | AT | 205 | OHX | 2 | 0 |
| 84 | AT | 206 | OHX | 1 | 0 |
| 84 | AT | 208 | OHX | 1 | 0 |
| 84 | AT | 210 | OHX | 1 | 0 |
| 84 | AT | 211 | OHX | 2 | 0 |
| 84 | AT | 212 | OHX | 1 | 0 |
| 84 | AT | 213 | OHX | 1 | 0 |
| 84 | AT | 214 | OHX | 2 | 0 |
| 84 | AT | 218 | OHX | 1 | 0 |
| 84 | AT | 219 | OHX | 1 | 0 |
| 84 | AT | 220 | OHX | 1 | 0 |
| 84 | CE | 402 | OHX | 2 | 0 |
| 84 | CF | 401 | OHX | 1 | 0 |
| 84 | CG | 302 | OHX | 4 | 0 |
| 84 | CK | 201 | OHX | 1 | 0 |
| 84 | CL | 301 | OHX | 2 | 0 |
| 84 | CM | 201 | OHX | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 84 | CV | 201 | OHX | 1 | 0 |
| 84 | DI | 201 | OHX | 1 | 0 |
| 84 | DL | 101 | OHX | 1 | 0 |
| 84 | DL | 102 | OHX | 1 | 0 |
| 84 | M | 201 | OHX | 2 | 0 |
| 84 | O | 201 | OHX | 1 | 0 |
| 84 | Q | 201 | OHX | 2 | 0 |
| 84 | T | 201 | OHX | 1 | 0 |

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 |
|-----|-------|------------------|
| 48 | sM | 2 |
| 25 | A | 1 |

All 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 | 44.36 |
| 1 | sM | 139:UNK | C | 155:UNK | N | 36.85 |
| 1 | A | 1716:C | O3' | 1717:G | P | 4.45 |

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 | 3149/3396 (92%) | -0.19 | 56 (1%) 69 60 | 22, 53, 169, 269 | 0 |
| 1 | AR | 3149/3396 (92%) | -0.17 | 58 (1%) 69 60 | 22, 51, 152, 280 | 0 |
| 2 | 3 | 121/121 (100%) | -0.45 | 0 100 100 | 33, 69, 92, 108 | 0 |
| 2 | AS | 121/121 (100%) | -0.50 | 1 (0%) 86 79 | 28, 56, 73, 112 | 0 |
| 3 | 4 | 158/158 (100%) | -0.17 | 1 (0%) 89 84 | 34, 58, 115, 203 | 0 |
| 3 | AT | 158/158 (100%) | -0.22 | 1 (0%) 89 84 | 35, 62, 125, 189 | 0 |
| 4 | CD | 252/252 (100%) | -0.39 | 0 100 100 | 30, 51, 83, 119 | 0 |
| 4 | j | 252/252 (100%) | -0.39 | 0 100 100 | 29, 54, 76, 118 | 0 |
| 5 | CE | 386/386 (100%) | -0.49 | 2 (0%) 90 86 | 21, 40, 65, 139 | 0 |
| 5 | k | 386/386 (100%) | -0.32 | 1 (0%) 93 90 | 28, 54, 77, 122 | 0 |
| 6 | CF | 361/361 (100%) | -0.37 | 0 100 100 | 30, 50, 79, 110 | 0 |
| 6 | l | 361/361 (100%) | -0.42 | 0 100 100 | 28, 49, 82, 101 | 0 |
| 7 | CG | 296/296 (100%) | -0.22 | 4 (1%) 75 67 | 36, 59, 99, 128 | 0 |
| 7 | m | 296/296 (100%) | 0.03 | 2 (0%) 87 82 | 46, 78, 115, 168 | 0 |
| 8 | CH | 156/175 (89%) | -0.30 | 0 100 100 | 35, 49, 88, 129 | 0 |
| 8 | n | 156/175 (89%) | -0.36 | 0 100 100 | 35, 46, 79, 132 | 0 |
| 9 | CI | 222/222 (100%) | -0.49 | 2 (0%) 84 77 | 25, 37, 91, 176 | 0 |
| 9 | o | 222/222 (100%) | -0.42 | 0 100 100 | 28, 40, 80, 161 | 0 |
| 10 | CJ | 233/233 (100%) | 0.64 | 17 (7%) 16 14 | 64, 87, 146, 191 | 0 |
| 10 | p | 233/233 (100%) | 0.15 | 3 (1%) 77 69 | 54, 82, 138, 161 | 0 |
| 11 | CK | 191/191 (100%) | -0.36 | 3 (1%) 72 64 | 33, 46, 77, 143 | 0 |
| 11 | q | 191/191 (100%) | -0.29 | 0 100 100 | 46, 62, 84, 149 | 0 |
| 12 | CL | 211/220 (95%) | -0.06 | 4 (1%) 67 59 | 32, 57, 100, 169 | 0 |
| 12 | r | 211/220 (95%) | -0.36 | 0 100 100 | 35, 53, 108, 127 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 13 | CM | 169/169 (100%) | -0.32 | 0 100 100 | 45, 61, 83, 105 | 0 |
| 13 | s | 169/169 (100%) | -0.00 | 0 100 100 | 61, 80, 102, 115 | 0 |
| 14 | CN | 193/193 (100%) | -0.07 | 1 (0%) 90 86 | 33, 67, 131, 148 | 0 |
| 14 | t | 193/193 (100%) | -0.34 | 1 (0%) 90 86 | 30, 60, 113, 144 | 0 |
| 15 | CO | 136/136 (100%) | -0.57 | 0 100 100 | 30, 44, 72, 97 | 0 |
| 15 | u | 136/136 (100%) | -0.42 | 0 100 100 | 42, 52, 77, 105 | 0 |
| 16 | CP | 203/203 (100%) | -0.32 | 0 100 100 | 37, 55, 71, 75 | 0 |
| 16 | v | 203/203 (100%) | -0.45 | 0 100 100 | 30, 51, 64, 74 | 0 |
| 17 | CQ | 197/197 (100%) | -0.53 | 1 (0%) 90 86 | 22, 33, 79, 88 | 0 |
| 17 | w | 197/197 (100%) | -0.52 | 0 100 100 | 27, 41, 75, 85 | 0 |
| 18 | CR | 183/183 (100%) | 0.61 | 25 (13%) 3 4 | 25, 41, 181, 234 | 0 |
| 18 | x | 183/183 (100%) | -0.19 | 8 (4%) 35 28 | 33, 42, 124, 165 | 0 |
| 19 | CS | 185/185 (100%) | -0.40 | 0 100 100 | 36, 50, 65, 85 | 0 |
| 19 | y | 185/185 (100%) | -0.43 | 0 100 100 | 36, 49, 84, 123 | 0 |
| 20 | CT | 188/188 (100%) | -0.14 | 3 (1%) 72 64 | 42, 61, 148, 170 | 0 |
| 20 | z | 188/188 (100%) | 0.03 | 3 (1%) 72 64 | 53, 73, 158, 171 | 0 |
| 21 | 0 | 172/172 (100%) | -0.24 | 1 (0%) 89 84 | 37, 46, 72, 91 | 0 |
| 21 | CU | 172/172 (100%) | -0.54 | 0 100 100 | 28, 38, 66, 86 | 0 |
| 22 | 2 | 159/159 (100%) | -0.25 | 0 100 100 | 31, 48, 111, 126 | 0 |
| 22 | CV | 159/159 (100%) | -0.38 | 0 100 100 | 25, 42, 94, 108 | 0 |
| 23 | 5 | 100/100 (100%) | 0.54 | 7 (7%) 17 15 | 86, 108, 135, 159 | 0 |
| 23 | CW | 100/100 (100%) | 0.70 | 7 (7%) 17 15 | 70, 94, 120, 162 | 0 |
| 24 | CX | 136/136 (100%) | -0.12 | 0 100 100 | 21, 37, 66, 96 | 0 |
| 24 | l2 | 136/136 (100%) | -0.06 | 0 100 100 | 37, 51, 78, 114 | 0 |
| 25 | 6 | 1783/1800 (99%) | -0.04 | 73 (4%) 38 31 | 34, 76, 201, 266 | 0 |
| 25 | A | 1781/1800 (98%) | 0.10 | 79 (4%) 35 28 | 49, 93, 235, 311 | 0 |
| 26 | 7 | 98/98 (100%) | 1.62 | 32 (32%) 0 0 | 52, 69, 199, 216 | 0 |
| 26 | CY | 98/98 (100%) | 0.56 | 12 (12%) 5 6 | 35, 52, 188, 226 | 0 |
| 27 | 8 | 121/121 (100%) | -0.04 | 0 100 100 | 48, 67, 91, 130 | 0 |
| 27 | CZ | 121/121 (100%) | -0.08 | 2 (1%) 70 62 | 48, 67, 91, 132 | 0 |
| 28 | 9 | 126/126 (100%) | -0.05 | 1 (0%) 86 79 | 42, 58, 80, 111 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 28 | DA | 126/126 (100%) | -0.06 | 1 (0%) 86 79 | 43, 61, 87, 103 | 0 |
| 29 | AA | 135/135 (100%) | 0.70 | 4 (2%) 51 42 | 76, 100, 124, 133 | 0 |
| 29 | DB | 135/135 (100%) | 0.51 | 4 (2%) 51 42 | 77, 99, 124, 136 | 0 |
| 30 | AB | 148/148 (100%) | -0.30 | 0 100 100 | 25, 48, 89, 106 | 0 |
| 30 | DC | 148/148 (100%) | -0.32 | 0 100 100 | 26, 52, 87, 95 | 0 |
| 31 | AC | 58/58 (100%) | -0.41 | 0 100 100 | 31, 55, 111, 132 | 0 |
| 31 | DD | 58/58 (100%) | -0.54 | 0 100 100 | 30, 56, 92, 112 | 0 |
| 32 | AD | 97/97 (100%) | 0.42 | 4 (4%) 38 31 | 77, 92, 122, 140 | 0 |
| 32 | DE | 97/97 (100%) | 0.17 | 1 (1%) 82 75 | 67, 82, 112, 135 | 0 |
| 33 | AE | 109/109 (100%) | -0.03 | 2 (1%) 69 60 | 46, 67, 123, 146 | 0 |
| 33 | DF | 109/109 (100%) | -0.17 | 0 100 100 | 35, 52, 119, 142 | 0 |
| 34 | AF | 127/127 (100%) | -0.32 | 2 (1%) 72 64 | 24, 40, 59, 133 | 0 |
| 34 | DG | 127/127 (100%) | -0.18 | 1 (0%) 86 79 | 24, 46, 66, 132 | 0 |
| 35 | AG | 106/106 (100%) | -0.58 | 0 100 100 | 28, 37, 62, 89 | 0 |
| 35 | DH | 106/106 (100%) | -0.43 | 0 100 100 | 27, 36, 82, 124 | 0 |
| 36 | AH | 112/112 (100%) | -0.09 | 0 100 100 | 53, 73, 130, 149 | 0 |
| 36 | DI | 112/112 (100%) | -0.20 | 0 100 100 | 48, 70, 134, 155 | 0 |
| 37 | AI | 119/119 (100%) | -0.15 | 1 (0%) 86 79 | 45, 68, 85, 92 | 0 |
| 37 | DJ | 119/119 (100%) | -0.10 | 2 (1%) 70 62 | 51, 75, 94, 113 | 0 |
| 38 | AJ | 99/99 (100%) | 0.02 | 2 (2%) 65 57 | 50, 69, 116, 148 | 0 |
| 38 | DK | 99/99 (100%) | 0.20 | 2 (2%) 65 57 | 59, 74, 118, 154 | 0 |
| 39 | AK | 87/87 (100%) | -0.46 | 0 100 100 | 34, 44, 77, 128 | 0 |
| 39 | DL | 87/87 (100%) | -0.41 | 2 (2%) 61 51 | 33, 47, 88, 167 | 0 |
| 40 | AL | 77/77 (100%) | 0.42 | 1 (1%) 77 69 | 78, 94, 120, 130 | 0 |
| 40 | DM | 77/77 (100%) | 1.03 | 9 (11%) 5 6 | 75, 94, 120, 129 | 0 |
| 41 | AM | 50/50 (100%) | -0.43 | 0 100 100 | 44, 53, 64, 76 | 0 |
| 41 | DN | 50/50 (100%) | -0.41 | 0 100 100 | 48, 56, 69, 89 | 0 |
| 42 | AN | 52/52 (100%) | -0.14 | 0 100 100 | 43, 53, 81, 108 | 0 |
| 42 | DO | 52/52 (100%) | -0.49 | 0 100 100 | 32, 39, 54, 81 | 0 |
| 43 | AO | 25/25 (100%) | -0.19 | 0 100 100 | 54, 61, 69, 75 | 0 |
| 43 | DP | 25/25 (100%) | -0.36 | 0 100 100 | 42, 50, 62, 68 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 44 | AP | 105/105 (100%) | 0.21 | 2 (1%) 67 59 | 36, 59, 96, 156 | 0 |
| 44 | DQ | 105/105 (100%) | 0.07 | 0 100 100 | 42, 59, 96, 138 | 0 |
| 45 | AQ | 91/91 (100%) | -0.38 | 0 100 100 | 38, 62, 91, 121 | 0 |
| 45 | DR | 91/91 (100%) | -0.45 | 0 100 100 | 32, 55, 78, 88 | 0 |
| 46 | i | 159/168 (94%) | 0.58 | 17 (10%) 7 7 | 56, 101, 165, 178 | 0 |
| 47 | p0 | 143/220 (65%) | 1.19 | 24 (16%) 2 2 | 100, 113, 177, 185 | 0 |
| 48 | sM | 63/104 (60%) | 0.38 | 4 (6%) 21 17 | 54, 106, 129, 136 | 0 |
| 49 | B | 206/206 (100%) | 0.37 | 10 (4%) 30 24 | 92, 115, 139, 176 | 0 |
| 49 | s0 | 206/206 (100%) | 0.02 | 1 (0%) 90 86 | 72, 95, 124, 136 | 0 |
| 50 | C | 214/216 (99%) | 0.87 | 30 (14%) 3 4 | 101, 141, 172, 181 | 0 |
| 50 | s1 | 216/216 (100%) | 0.35 | 3 (1%) 75 67 | 68, 87, 117, 144 | 0 |
| 51 | D | 217/217 (100%) | 0.03 | 5 (2%) 61 51 | 69, 91, 118, 142 | 0 |
| 51 | s2 | 217/217 (100%) | 0.03 | 1 (0%) 90 86 | 55, 75, 97, 121 | 0 |
| 52 | E | 223/223 (100%) | 0.21 | 8 (3%) 43 37 | 78, 95, 131, 155 | 0 |
| 52 | s3 | 223/223 (100%) | 0.33 | 10 (4%) 34 27 | 74, 111, 145, 158 | 0 |
| 53 | F | 260/260 (100%) | 0.37 | 4 (1%) 74 66 | 73, 95, 113, 153 | 0 |
| 53 | s4 | 260/260 (100%) | 0.02 | 1 (0%) 92 89 | 51, 79, 100, 150 | 0 |
| 54 | G | 206/206 (100%) | 0.73 | 23 (11%) 6 7 | 98, 121, 152, 179 | 0 |
| 54 | s5 | 206/206 (100%) | 0.33 | 12 (5%) 24 20 | 71, 92, 124, 157 | 0 |
| 55 | H | 226/226 (100%) | 0.37 | 6 (2%) 55 46 | 66, 105, 142, 160 | 0 |
| 55 | s6 | 218/226 (96%) | 0.18 | 6 (2%) 53 45 | 51, 83, 123, 148 | 0 |
| 56 | I | 184/186 (98%) | 0.57 | 9 (4%) 30 24 | 85, 126, 160, 187 | 0 |
| 56 | s7 | 186/186 (100%) | 0.33 | 9 (4%) 31 25 | 69, 105, 156, 173 | 0 |
| 57 | J | 188/199 (94%) | 0.32 | 9 (4%) 31 25 | 58, 77, 128, 150 | 0 |
| 57 | s8 | 188/199 (94%) | 0.17 | 5 (2%) 55 46 | 43, 68, 121, 138 | 0 |
| 58 | K | 185/185 (100%) | 0.66 | 16 (8%) 11 11 | 87, 107, 149, 185 | 0 |
| 58 | s9 | 185/185 (100%) | 0.18 | 3 (1%) 72 64 | 63, 80, 128, 169 | 0 |
| 59 | L | 96/105 (91%) | 0.42 | 2 (2%) 64 55 | 80, 111, 141, 172 | 0 |
| 59 | c0 | 96/105 (91%) | 1.29 | 27 (28%) 1 1 | 104, 137, 155, 185 | 0 |
| 60 | M | 155/155 (100%) | 0.50 | 16 (10%) 7 8 | 60, 76, 162, 194 | 0 |
| 60 | c1 | 146/155 (94%) | 0.06 | 7 (4%) 31 25 | 42, 64, 118, 151 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 61 | N | 124/124 (100%) | 1.25 | 24 (19%) 1 1 | 140, 159, 203, 214 | 0 |
| 61 | c2 | 124/124 (100%) | 1.72 | 47 (37%) 0 0 | 159, 186, 216, 234 | 0 |
| 62 | O | 150/150 (100%) | 0.14 | 3 (2%) 65 57 | 60, 90, 112, 129 | 0 |
| 62 | c3 | 150/150 (100%) | -0.23 | 0 100 100 | 53, 76, 100, 121 | 0 |
| 63 | P | 127/128 (99%) | 0.67 | 17 (13%) 4 5 | 65, 128, 158, 165 | 0 |
| 63 | c4 | 128/128 (100%) | 0.61 | 10 (7%) 14 13 | 55, 84, 100, 130 | 0 |
| 64 | Q | 124/141 (87%) | 0.37 | 5 (4%) 39 32 | 80, 103, 150, 165 | 0 |
| 64 | c5 | 135/141 (95%) | 0.41 | 11 (8%) 13 12 | 75, 102, 144, 168 | 0 |
| 65 | R | 141/142 (99%) | 0.71 | 17 (12%) 5 6 | 83, 110, 129, 132 | 0 |
| 65 | c6 | 142/142 (100%) | 0.16 | 2 (1%) 75 67 | 62, 88, 109, 141 | 0 |
| 66 | S | 120/125 (96%) | 0.03 | 2 (1%) 70 62 | 77, 111, 159, 170 | 0 |
| 67 | T | 145/145 (100%) | 0.43 | 10 (6%) 18 15 | 71, 111, 145, 160 | 0 |
| 67 | c8 | 145/145 (100%) | 0.01 | 1 (0%) 87 82 | 71, 88, 121, 137 | 0 |
| 68 | U | 143/143 (100%) | 0.26 | 7 (4%) 30 24 | 89, 112, 136, 148 | 0 |
| 68 | c9 | 143/143 (100%) | 0.03 | 1 (0%) 87 82 | 66, 85, 109, 139 | 0 |
| 69 | V | 107/110 (97%) | 0.48 | 8 (7%) 15 14 | 75, 110, 157, 169 | 0 |
| 69 | d0 | 110/110 (100%) | 1.03 | 23 (20%) 1 1 | 70, 113, 170, 190 | 0 |
| 70 | W | 87/87 (100%) | 0.41 | 3 (3%) 46 38 | 91, 105, 126, 148 | 0 |
| 70 | d1 | 87/87 (100%) | 0.17 | 0 100 100 | 68, 83, 119, 146 | 0 |
| 71 | X | 129/129 (100%) | 0.00 | 0 100 100 | 68, 84, 96, 102 | 0 |
| 71 | d2 | 129/129 (100%) | -0.31 | 0 100 100 | 50, 64, 77, 88 | 0 |
| 72 | Y | 144/144 (100%) | 0.02 | 1 (0%) 87 82 | 57, 67, 88, 124 | 0 |
| 72 | d3 | 144/144 (100%) | -0.25 | 0 100 100 | 40, 49, 73, 108 | 0 |
| 73 | Z | 134/134 (100%) | 0.49 | 5 (3%) 42 35 | 82, 111, 137, 155 | 0 |
| 73 | d4 | 134/134 (100%) | 0.14 | 3 (2%) 62 53 | 59, 89, 117, 159 | 0 |
| 74 | a | 70/70 (100%) | 1.00 | 10 (14%) 3 4 | 117, 134, 148, 160 | 0 |
| 74 | d5 | 69/70 (98%) | 0.62 | 3 (4%) 36 29 | 84, 111, 136, 147 | 0 |
| 75 | b | 97/97 (100%) | 0.38 | 8 (8%) 12 12 | 69, 95, 165, 171 | 0 |
| 75 | d6 | 97/97 (100%) | -0.10 | 0 100 100 | 54, 68, 110, 126 | 0 |
| 76 | c | 81/81 (100%) | 0.67 | 9 (11%) 6 7 | 84, 107, 161, 171 | 0 |
| 76 | d7 | 81/81 (100%) | 0.21 | 5 (6%) 21 18 | 67, 88, 144, 169 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 77 | d | 63/63 (100%) | 1.17 | 13 (20%) 1 1 | 103, 124, 146, 159 | 0 |
| 77 | d8 | 63/63 (100%) | 0.91 | 7 (11%) 6 7 | 82, 104, 132, 141 | 0 |
| 78 | d9 | 53/53 (100%) | 0.21 | 1 (1%) 67 59 | 73, 84, 133, 153 | 0 |
| 78 | e | 53/53 (100%) | -0.24 | 1 (1%) 67 59 | 72, 82, 116, 137 | 0 |
| 79 | e0 | 62/62 (100%) | 0.26 | 2 (3%) 48 40 | 58, 81, 140, 161 | 0 |
| 79 | f | 60/62 (96%) | 0.83 | 6 (10%) 8 8 | 65, 98, 158, 164 | 0 |
| 80 | g | 71/71 (100%) | 0.83 | 12 (16%) 2 2 | 96, 149, 167, 187 | 0 |
| 81 | h | 318/318 (100%) | 0.86 | 40 (12%) 4 5 | 100, 124, 161, 200 | 0 |
| 81 | sR | 318/318 (100%) | 0.80 | 39 (12%) 5 6 | 92, 119, 148, 191 | 0 |
| 82 | c7 | 117/121 (96%) | -0.14 | 1 (0%) 84 77 | 72, 93, 130, 139 | 0 |
| 83 | e1 | 51/51 (100%) | 0.99 | 10 (19%) 1 1 | 143, 176, 189, 200 | 0 |
| All | All | 33004/33818 (97%) | 0.02 | 1086 (3%) 47 39 | 21, 72, 152, 311 | 0 |

The worst 5 of 1086 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 25 | A | 1709 | C | 16.0 |
| 25 | A | 1711 | C | 15.7 |
| 25 | A | 1694 | A | 14.4 |
| 26 | 7 | 75 | THR | 14.3 |
| 26 | 7 | 76 | VAL | 13.2 |

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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 | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 85 | MG | AR | 4139 | 1/1 | 0.97 | 0.65 | 76.32 | 37,37,37,37 | 0 |
| 85 | MG | 1 | 3791 | 1/1 | 0.97 | 0.43 | 54.88 | 21,21,21,21 | 0 |
| 85 | MG | AT | 223 | 1/1 | 0.71 | 0.91 | 49.97 | 55,55,55,55 | 0 |
| 85 | MG | 1 | 3900 | 1/1 | 0.94 | 0.74 | 47.46 | 34,34,34,34 | 0 |
| 85 | MG | 1 | 3801 | 1/1 | 0.71 | 0.52 | 46.61 | 38,38,38,38 | 0 |
| 85 | MG | 1 | 3764 | 1/1 | 0.91 | 0.54 | 42.59 | 38,38,38,38 | 0 |
| 85 | MG | AR | 3858 | 1/1 | 0.97 | 0.47 | 38.78 | 22,22,22,22 | 0 |
| 85 | MG | AR | 3867 | 1/1 | 0.96 | 0.50 | 37.95 | 13,13,13,13 | 0 |
| 84 | OHX | 1 | 3675 | 7/7 | 0.79 | 0.56 | 36.98 | 229,229,230,230 | 0 |
| 85 | MG | AR | 3887 | 1/1 | 0.92 | 0.72 | 35.52 | 35,35,35,35 | 0 |
| 85 | MG | 1 | 4061 | 1/1 | 0.94 | 0.40 | 35.23 | 23,23,23,23 | 0 |
| 85 | MG | AR | 4111 | 1/1 | 0.96 | 0.60 | 34.74 | 48,48,48,48 | 0 |
| 85 | MG | 4 | 217 | 1/1 | 0.80 | 0.48 | 34.49 | 44,44,44,44 | 0 |
| 85 | MG | 6 | 2082 | 1/1 | 0.97 | 0.54 | 33.42 | 25,25,25,25 | 0 |
| 84 | OHX | AR | 3626 | 7/7 | 0.95 | 0.32 | 32.08 | 204,205,205,205 | 0 |
| 85 | MG | 1 | 3843 | 1/1 | 0.97 | 0.66 | 31.65 | 11,11,11,11 | 0 |
| 85 | MG | 1 | 3915 | 1/1 | 0.95 | 0.55 | 31.44 | 19,19,19,19 | 0 |
| 85 | MG | 1 | 3924 | 1/1 | 0.99 | 0.54 | 29.50 | 8,8,8,8 | 0 |
| 85 | MG | 1 | 4060 | 1/1 | 0.93 | 0.55 | 29.36 | 16,16,16,16 | 0 |
| 85 | MG | AR | 3933 | 1/1 | 0.93 | 0.53 | 29.35 | 13,13,13,13 | 0 |
| 85 | MG | 1 | 4215 | 1/1 | 0.97 | 0.34 | 29.31 | 28,28,28,28 | 0 |
| 85 | MG | 1 | 3858 | 1/1 | 0.97 | 0.64 | 28.87 | 12,12,12,12 | 0 |
| 85 | MG | 1 | 3902 | 1/1 | 0.96 | 0.52 | 28.30 | 4,4,4,4 | 0 |
| 84 | OHX | AR | 3701 | 7/7 | 0.90 | 0.41 | 28.20 | 207,208,208,208 | 0 |
| 84 | OHX | 1 | 3705 | 7/7 | 0.87 | 0.42 | 28.10 | 222,222,223,223 | 0 |
| 85 | MG | A | 2079 | 1/1 | 0.95 | 0.58 | 25.85 | 46,46,46,46 | 0 |
| 85 | MG | AR | 3872 | 1/1 | 0.99 | 0.45 | 25.84 | 0,0,0,0 | 0 |
| 85 | MG | AR | 3927 | 1/1 | 0.99 | 0.65 | 25.67 | 11,11,11,11 | 0 |
| 85 | MG | AR | 3909 | 1/1 | 0.99 | 0.37 | 25.58 | 14,14,14,14 | 0 |
| 85 | MG | 6 | 2137 | 1/1 | 0.96 | 0.40 | 25.14 | 82,82,82,82 | 0 |
| 85 | MG | 1 | 3899 | 1/1 | 0.99 | 0.41 | 24.65 | 12,12,12,12 | 0 |
| 85 | MG | 6 | 2113 | 1/1 | 0.97 | 0.42 | 24.48 | 23,23,23,23 | 0 |
| 85 | MG | 1 | 4192 | 1/1 | 0.76 | 0.43 | 24.33 | 38,38,38,38 | 0 |
| 85 | MG | 1 | 3905 | 1/1 | 0.96 | 0.59 | 23.98 | 14,14,14,14 | 0 |
| 85 | MG | 4 | 219 | 1/1 | 0.96 | 0.39 | 23.82 | 24,24,24,24 | 0 |
| 85 | MG | A | 2066 | 1/1 | 0.98 | 0.44 | 23.81 | 62,62,62,62 | 0 |
| 85 | MG | AR | 3853 | 1/1 | 0.96 | 0.58 | 23.75 | 17,17,17,17 | 0 |
| 85 | MG | AT | 224 | 1/1 | 0.93 | 0.54 | 23.66 | 35,35,35,35 | 0 |
| 84 | OHX | AT | 218 | 7/7 | 0.91 | 0.39 | 23.61 | 223,224,224,224 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 84 | OHX | AR | 3686 | 7/7 | 0.92 | 0.48 | 23.16 | 186,187,187,187 | 0 |
| 85 | MG | 1 | 3922 | 1/1 | 0.97 | 0.50 | 23.12 | 15,15,15,15 | 0 |
| 85 | MG | AR | 3905 | 1/1 | 0.97 | 0.52 | 23.06 | 24,24,24,24 | 0 |
| 85 | MG | 1 | 3804 | 1/1 | 0.94 | 0.61 | 23.04 | 18,18,18,18 | 0 |
| 84 | OHX | 1 | 3721 | 7/7 | 0.92 | 0.39 | 22.88 | 191,192,193,193 | 0 |
| 85 | MG | 6 | 2066 | 1/1 | 0.98 | 0.27 | 22.74 | 87,87,87,87 | 0 |
| 85 | MG | A | 2057 | 1/1 | 0.97 | 0.43 | 22.51 | 50,50,50,50 | 0 |
| 85 | MG | AR | 4185 | 1/1 | 0.92 | 0.36 | 22.35 | 40,40,40,40 | 0 |
| 85 | MG | AR | 3756 | 1/1 | 0.95 | 0.72 | 22.18 | 11,11,11,11 | 0 |
| 85 | MG | 1 | 3739 | 1/1 | 0.96 | 0.46 | 21.89 | 15,15,15,15 | 0 |
| 84 | OHX | AR | 3648 | 7/7 | 0.93 | 0.39 | 21.78 | 196,197,198,198 | 0 |
| 85 | MG | 1 | 3829 | 1/1 | 0.95 | 0.38 | 21.27 | 25,25,25,25 | 0 |
| 85 | MG | AR | 3882 | 1/1 | 0.99 | 0.58 | 21.24 | 11,11,11,11 | 0 |
| 85 | MG | 1 | 3904 | 1/1 | 0.98 | 0.44 | 21.22 | 4,4,4,4 | 0 |
| 85 | MG | 1 | 3847 | 1/1 | 0.92 | 0.39 | 20.96 | 23,23,23,23 | 0 |
| 84 | OHX | AR | 3591 | 7/7 | 0.93 | 0.40 | 20.94 | 168,169,169,169 | 0 |
| 85 | MG | 1 | 3870 | 1/1 | 0.98 | 0.51 | 20.93 | 11,11,11,11 | 0 |
| 85 | MG | A | 2125 | 1/1 | 0.83 | 0.54 | 20.66 | 51,51,51,51 | 0 |
| 85 | MG | AR | 3926 | 1/1 | 0.98 | 0.51 | 20.52 | 10,10,10,10 | 0 |
| 85 | MG | AR | 3850 | 1/1 | 0.94 | 0.52 | 20.41 | 11,11,11,11 | 0 |
| 85 | MG | AR | 3937 | 1/1 | 0.99 | 0.43 | 20.17 | 9,9,9,9 | 0 |
| 84 | OHX | AR | 3554 | 7/7 | 0.95 | 0.29 | 20.13 | 159,160,161,161 | 0 |
| 85 | MG | AB | 201 | 1/1 | 0.99 | 0.50 | 19.89 | 15,15,15,15 | 0 |
| 85 | MG | 6 | 2083 | 1/1 | 0.93 | 0.47 | 19.89 | 35,35,35,35 | 0 |
| 85 | MG | 1 | 3852 | 1/1 | 0.95 | 0.59 | 19.80 | 22,22,22,22 | 0 |
| 85 | MG | AR | 3797 | 1/1 | 0.95 | 0.38 | 19.80 | 18,18,18,18 | 0 |
| 85 | MG | 1 | 4195 | 1/1 | 0.97 | 0.36 | 19.62 | 52,52,52,52 | 0 |
| 85 | MG | AR | 4135 | 1/1 | 0.86 | 0.54 | 19.32 | 66,66,66,66 | 0 |
| 84 | OHX | AR | 3691 | 7/7 | 0.96 | 0.45 | 19.07 | 170,171,172,172 | 0 |
| 85 | MG | AR | 4032 | 1/1 | 0.84 | 0.50 | 18.87 | 47,47,47,47 | 0 |
| 84 | OHX | 1 | 3601 | 7/7 | 0.92 | 0.33 | 18.37 | 200,200,201,202 | 0 |
| 85 | MG | 1 | 3857 | 1/1 | 0.98 | 0.39 | 18.36 | 12,12,12,12 | 0 |
| 85 | MG | AR | 3938 | 1/1 | 0.94 | 0.52 | 18.31 | 20,20,20,20 | 0 |
| 85 | MG | 1 | 3927 | 1/1 | 0.96 | 0.50 | 18.24 | 6,6,6,6 | 0 |
| 85 | MG | 1 | 3917 | 1/1 | 0.98 | 0.36 | 18.18 | 18,18,18,18 | 0 |
| 85 | MG | AR | 4138 | 1/1 | 0.97 | 0.42 | 18.16 | 44,44,44,44 | 0 |
| 85 | MG | 6 | 2106 | 1/1 | 0.94 | 0.58 | 17.61 | 32,32,32,32 | 0 |
| 85 | MG | 1 | 3874 | 1/1 | 0.98 | 0.42 | 17.52 | 19,19,19,19 | 0 |
| 85 | MG | CI | 301 | 1/1 | 0.82 | 0.31 | 17.45 | 48,48,48,48 | 0 |
| 85 | MG | 1 | 3989 | 1/1 | 0.94 | 0.48 | 17.40 | 20,20,20,20 | 0 |
| 84 | OHX | AR | 3739 | 7/7 | 0.96 | 0.37 | 17.36 | 151,152,152,152 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 85 | MG | AR | 3842 | 1/1 | 0.97 | 0.38 | 17.28 | 10,10,10,10 | 0 |
| 85 | MG | 1 | 3944 | 1/1 | 0.97 | 0.33 | 17.28 | 33,33,33,33 | 0 |
| 85 | MG | 6 | 2073 | 1/1 | 0.90 | 0.41 | 17.27 | 57,57,57,57 | 0 |
| 85 | MG | 1 | 4204 | 1/1 | 0.97 | 0.41 | 17.08 | 12,12,12,12 | 0 |
| 85 | MG | 1 | 4161 | 1/1 | 0.84 | 0.28 | 17.01 | 37,37,37,37 | 0 |
| 84 | OHX | 1 | 3722 | 7/7 | 0.75 | 0.44 | 16.86 | 268,268,269,269 | 0 |
| 85 | MG | AR | 3846 | 1/1 | 0.95 | 0.58 | 16.84 | 17,17,17,17 | 0 |
| 85 | MG | 1 | 3785 | 1/1 | 0.97 | 0.33 | 16.76 | 21,21,21,21 | 0 |
| 85 | MG | 1 | 3896 | 1/1 | 0.98 | 0.41 | 16.73 | 10,10,10,10 | 0 |
| 85 | MG | 1 | 3883 | 1/1 | 0.90 | 0.47 | 16.32 | 17,17,17,17 | 0 |
| 84 | OHX | AR | 3714 | 7/7 | 0.93 | 0.43 | 16.16 | 192,193,193,194 | 0 |
| 85 | MG | 1 | 4148 | 1/1 | 0.98 | 0.57 | 16.13 | 35,35,35,35 | 0 |
| 85 | MG | AR | 3802 | 1/1 | 0.96 | 0.58 | 16.12 | 16,16,16,16 | 0 |
| 85 | MG | AR | 3852 | 1/1 | 0.99 | 0.44 | 16.10 | 18,18,18,18 | 0 |
| 85 | MG | 1 | 4044 | 1/1 | 0.82 | 0.32 | 16.10 | 40,40,40,40 | 0 |
| 84 | OHX | AR | 3641 | 7/7 | 0.87 | 0.41 | 16.06 | 218,219,219,220 | 0 |
| 85 | MG | 1 | 3745 | 1/1 | 0.95 | 0.48 | 15.89 | 20,20,20,20 | 0 |
| 85 | MG | 6 | 2096 | 1/1 | 0.96 | 0.38 | 15.85 | 48,48,48,48 | 0 |
| 85 | MG | A | 2078 | 1/1 | 0.97 | 0.51 | 15.78 | 28,28,28,28 | 0 |
| 85 | MG | 1 | 4063 | 1/1 | 0.78 | 0.60 | 15.70 | 55,55,55,55 | 0 |
| 85 | MG | AR | 4000 | 1/1 | 0.97 | 0.38 | 15.69 | 30,30,30,30 | 0 |
| 85 | MG | AR | 3900 | 1/1 | 0.95 | 0.33 | 15.59 | 29,29,29,29 | 0 |
| 85 | MG | AR | 4226 | 1/1 | 0.93 | 0.51 | 15.39 | 16,16,16,16 | 0 |
| 85 | MG | AR | 3741 | 1/1 | 0.96 | 0.24 | 15.28 | 14,14,14,14 | 0 |
| 85 | MG | 1 | 3872 | 1/1 | 0.97 | 0.40 | 15.20 | 23,23,23,23 | 0 |
| 85 | MG | AR | 4173 | 1/1 | 0.64 | 0.48 | 15.19 | 38,38,38,38 | 0 |
| 85 | MG | 1 | 3890 | 1/1 | 0.96 | 0.38 | 15.12 | 23,23,23,23 | 0 |
| 85 | MG | AR | 3946 | 1/1 | 0.94 | 0.20 | 15.06 | 28,28,28,28 | 0 |
| 85 | MG | AR | 4102 | 1/1 | 0.94 | 0.33 | 15.03 | 24,24,24,24 | 0 |
| 85 | MG | 1 | 4103 | 1/1 | 0.87 | 0.35 | 14.83 | 60,60,60,60 | 0 |
| 85 | MG | l2 | 201 | 1/1 | 0.99 | 0.28 | 14.81 | 21,21,21,21 | 0 |
| 85 | MG | 1 | 3818 | 1/1 | 0.95 | 0.39 | 14.74 | 19,19,19,19 | 0 |
| 84 | OHX | AR | 3685 | 7/7 | 0.86 | 0.40 | 14.67 | 187,187,188,188 | 0 |
| 84 | OHX | AR | 3694 | 7/7 | 0.91 | 0.40 | 14.59 | 212,212,213,213 | 0 |
| 85 | MG | AR | 4200 | 1/1 | 0.97 | 0.56 | 14.59 | 30,30,30,30 | 0 |
| 85 | MG | 1 | 3949 | 1/1 | 0.77 | 0.44 | 14.49 | 41,41,41,41 | 0 |
| 85 | MG | AR | 3930 | 1/1 | 0.95 | 0.39 | 14.35 | 14,14,14,14 | 0 |
| 84 | OHX | AR | 3683 | 7/7 | 0.96 | 0.36 | 14.14 | 178,179,179,180 | 0 |
| 85 | MG | A | 2047 | 1/1 | 0.99 | 0.38 | 14.09 | 55,55,55,55 | 0 |
| 85 | MG | 1 | 3873 | 1/1 | 0.99 | 0.40 | 14.05 | 18,18,18,18 | 0 |
| 85 | MG | 1 | 3839 | 1/1 | 0.94 | 0.60 | 14.03 | 7,7,7,7 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 85 | MG | AR | 3939 | 1/1 | 0.95 | 0.43 | 14.03 | 16,16,16,16 | 0 |
| 85 | MG | AR | 3934 | 1/1 | 0.97 | 0.37 | 14.02 | 14,14,14,14 | 0 |
| 84 | OHX | 1 | 3660 | 7/7 | 0.94 | 0.29 | 14.01 | 208,209,210,210 | 0 |
| 85 | MG | AR | 3890 | 1/1 | 0.97 | 0.50 | 13.96 | 33,33,33,33 | 0 |
| 84 | OHX | AR | 3611 | 7/7 | 0.96 | 0.33 | 13.94 | 194,196,197,197 | 0 |
| 84 | OHX | 6 | 2005 | 7/7 | 0.94 | 0.28 | 13.89 | 152,153,155,155 | 0 |
| 85 | MG | 1 | 4209 | 1/1 | 0.98 | 0.40 | 13.86 | 22,22,22,22 | 0 |
| 85 | MG | AR | 3856 | 1/1 | 0.98 | 0.53 | 13.86 | 10,10,10,10 | 0 |
| 85 | MG | 1 | 3882 | 1/1 | 0.99 | 0.39 | 13.73 | 11,11,11,11 | 0 |
| 85 | MG | A | 2081 | 1/1 | 0.96 | 0.40 | 13.71 | 48,48,48,48 | 0 |
| 85 | MG | 1 | 4155 | 1/1 | 0.97 | 0.48 | 13.69 | 66,66,66,66 | 0 |
| 85 | MG | 1 | 4191 | 1/1 | 0.99 | 0.45 | 13.64 | 22,22,22,22 | 0 |
| 85 | MG | AK | 104 | 1/1 | 0.96 | 0.38 | 13.61 | 44,44,44,44 | 0 |
| 85 | MG | AR | 4187 | 1/1 | 0.95 | 0.67 | 13.59 | 27,27,27,27 | 0 |
| 85 | MG | DG | 202 | 1/1 | 0.94 | 0.36 | 13.49 | 21,21,21,21 | 0 |
| 85 | MG | 6 | 2076 | 1/1 | 0.95 | 0.33 | 13.46 | 18,18,18,18 | 0 |
| 85 | MG | 1 | 3833 | 1/1 | 0.87 | 0.30 | 13.33 | 41,41,41,41 | 0 |
| 84 | OHX | AR | 3652 | 7/7 | 0.90 | 0.36 | 13.30 | 196,196,197,197 | 0 |
| 85 | MG | 1 | 3918 | 1/1 | 0.95 | 0.36 | 13.23 | 26,26,26,26 | 0 |
| 85 | MG | 1 | 4064 | 1/1 | 0.84 | 0.35 | 13.19 | 59,59,59,59 | 0 |
| 85 | MG | A | 2101 | 1/1 | 0.92 | 0.24 | 13.14 | 64,64,64,64 | 0 |
| 85 | MG | AR | 3992 | 1/1 | 0.94 | 0.50 | 13.12 | 19,19,19,19 | 0 |
| 85 | MG | AR | 3765 | 1/1 | 0.98 | 0.44 | 13.08 | 23,23,23,23 | 0 |
| 85 | MG | AR | 4242 | 1/1 | 0.93 | 0.73 | 13.06 | 56,56,56,56 | 0 |
| 85 | MG | AR | 4095 | 1/1 | 0.87 | 0.34 | 13.03 | 36,36,36,36 | 0 |
| 85 | MG | 6 | 2093 | 1/1 | 0.88 | 0.33 | 12.98 | 47,47,47,47 | 0 |
| 85 | MG | 1 | 3838 | 1/1 | 0.98 | 0.36 | 12.96 | 20,20,20,20 | 0 |
| 84 | OHX | 1 | 3595 | 7/7 | 0.93 | 0.44 | 12.90 | 190,191,192,192 | 0 |
| 84 | OHX | 6 | 2027 | 7/7 | 0.86 | 0.32 | 12.78 | 187,188,189,190 | 0 |
| 84 | OHX | AR | 3650 | 7/7 | 0.95 | 0.39 | 12.77 | 177,177,178,178 | 0 |
| 85 | MG | A | 2052 | 1/1 | 0.91 | 0.46 | 12.77 | 27,27,27,27 | 0 |
| 85 | MG | 1 | 3903 | 1/1 | 0.93 | 0.32 | 12.75 | 32,32,32,32 | 0 |
| 85 | MG | A | 2056 | 1/1 | 0.97 | 0.38 | 12.66 | 39,39,39,39 | 0 |
| 85 | MG | 1 | 4099 | 1/1 | 0.99 | 0.31 | 12.62 | 16,16,16,16 | 0 |
| 85 | MG | 1 | 4086 | 1/1 | 0.99 | 0.31 | 12.54 | 16,16,16,16 | 0 |
| 84 | OHX | AR | 3660 | 7/7 | 0.93 | 0.35 | 12.45 | 167,168,169,170 | 0 |
| 84 | OHX | AR | 3734 | 7/7 | 0.88 | 0.30 | 12.26 | 223,224,224,225 | 0 |
| 84 | OHX | AR | 3696 | 7/7 | 0.90 | 0.34 | 12.25 | 176,176,177,178 | 0 |
| 85 | MG | AR | 3985 | 1/1 | 0.94 | 0.23 | 12.21 | 19,19,19,19 | 0 |
| 85 | MG | 1 | 3929 | 1/1 | 0.97 | 0.43 | 12.14 | 20,20,20,20 | 0 |
| 85 | MG | AR | 3925 | 1/1 | 0.97 | 0.38 | 12.06 | 14,14,14,14 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 85 | MG | 1 | 3832 | 1/1 | 0.99 | 0.34 | 11.98 | 13,13,13,13 | 0 |
| 85 | MG | CE | 406 | 1/1 | 0.83 | 0.58 | 11.97 | 48,48,48,48 | 0 |
| 85 | MG | A | 2087 | 1/1 | 0.88 | 0.28 | 11.92 | 57,57,57,57 | 0 |
| 85 | MG | 1 | 4048 | 1/1 | 0.97 | 0.32 | 11.81 | 27,27,27,27 | 0 |
| 85 | MG | 1 | 3914 | 1/1 | 0.93 | 0.54 | 11.77 | 31,31,31,31 | 0 |
| 84 | OHX | 1 | 3728 | 7/7 | 0.88 | 0.36 | 11.74 | 233,233,233,234 | 0 |
| 84 | OHX | A | 2013 | 7/7 | 0.92 | 0.32 | 11.62 | 203,205,206,206 | 0 |
| 84 | OHX | 1 | 3667 | 7/7 | 0.91 | 0.35 | 11.62 | 189,189,190,191 | 0 |
| 84 | OHX | 6 | 1982 | 7/7 | 0.88 | 0.42 | 11.61 | 171,172,173,174 | 0 |
| 85 | MG | AR | 3971 | 1/1 | 0.71 | 0.35 | 11.59 | 38,38,38,38 | 0 |
| 84 | OHX | AR | 3655 | 7/7 | 0.91 | 0.36 | 11.51 | 216,218,218,219 | 0 |
| 84 | OHX | AR | 3729 | 7/7 | 0.87 | 0.32 | 11.46 | 214,215,216,216 | 0 |
| 85 | MG | 1 | 4142 | 1/1 | 0.89 | 0.57 | 11.43 | 47,47,47,47 | 0 |
| 85 | MG | 1 | 3768 | 1/1 | 0.98 | 0.30 | 11.16 | 24,24,24,24 | 0 |
| 84 | OHX | AR | 3584 | 7/7 | 0.95 | 0.37 | 11.09 | 169,169,170,171 | 0 |
| 84 | OHX | 1 | 3731 | 7/7 | 0.84 | 0.28 | 11.08 | 201,202,205,205 | 0 |
| 84 | OHX | AR | 3577 | 7/7 | 0.93 | 0.30 | 10.97 | 201,201,202,202 | 0 |
| 84 | OHX | 6 | 1965 | 7/7 | 0.97 | 0.28 | 10.96 | 161,162,163,163 | 0 |
| 85 | MG | 6 | 2058 | 1/1 | 0.93 | 0.39 | 10.96 | 33,33,33,33 | 0 |
| 84 | OHX | 1 | 3701 | 7/7 | 0.92 | 0.24 | 10.95 | 181,182,182,182 | 0 |
| 84 | OHX | 1 | 3650 | 7/7 | 0.90 | 0.32 | 10.94 | 179,181,181,182 | 0 |
| 84 | OHX | AR | 3674 | 7/7 | 0.94 | 0.41 | 10.86 | 215,215,216,216 | 0 |
| 85 | MG | 1 | 3866 | 1/1 | 0.86 | 0.34 | 10.86 | 46,46,46,46 | 0 |
| 85 | MG | AR | 3896 | 1/1 | 0.94 | 0.43 | 10.82 | 37,37,37,37 | 0 |
| 84 | OHX | 6 | 1980 | 7/7 | 0.90 | 0.39 | 10.80 | 206,206,208,208 | 0 |
| 85 | MG | 1 | 3976 | 1/1 | 0.79 | 0.35 | 10.77 | 61,61,61,61 | 0 |
| 84 | OHX | A | 2003 | 7/7 | 0.94 | 0.41 | 10.71 | 196,198,199,199 | 0 |
| 84 | OHX | 6 | 2038 | 7/7 | 0.87 | 0.37 | 10.64 | 213,215,217,217 | 0 |
| 85 | MG | AR | 4201 | 1/1 | 0.90 | 0.37 | 10.53 | 31,31,31,31 | 0 |
| 85 | MG | AR | 3783 | 1/1 | 0.98 | 0.39 | 10.50 | 15,15,15,15 | 0 |
| 85 | MG | 6 | 2091 | 1/1 | 0.94 | 0.33 | 10.49 | 54,54,54,54 | 0 |
| 85 | MG | 1 | 3962 | 1/1 | 0.94 | 0.25 | 10.48 | 33,33,33,33 | 0 |
| 85 | MG | AR | 3851 | 1/1 | 0.99 | 0.34 | 10.44 | 29,29,29,29 | 0 |
| 84 | OHX | 4 | 209 | 7/7 | 0.86 | 0.36 | 10.39 | 194,194,195,195 | 0 |
| 85 | MG | AR | 4081 | 1/1 | 0.91 | 0.30 | 10.29 | 52,52,52,52 | 0 |
| 84 | OHX | 4 | 210 | 7/7 | 0.83 | 0.31 | 10.19 | 236,236,236,236 | 0 |
| 85 | MG | CX | 202 | 1/1 | 0.97 | 0.32 | 10.09 | 6,6,6,6 | 0 |
| 85 | MG | AR | 3922 | 1/1 | 0.97 | 0.36 | 10.07 | 20,20,20,20 | 0 |
| 84 | OHX | 1 | 3718 | 7/7 | 0.91 | 0.39 | 10.00 | 220,221,221,222 | 0 |
| 84 | OHX | AR | 3653 | 7/7 | 0.95 | 0.31 | 9.99 | 178,178,179,179 | 0 |
| 85 | MG | AR | 4083 | 1/1 | 0.96 | 0.35 | 9.96 | 23,23,23,23 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 85 | MG | 6 | 2087 | 1/1 | 0.92 | 0.39 | 9.94 | 28,28,28,28 | 0 |
| 84 | OHX | AR | 3677 | 7/7 | 0.92 | 0.36 | 9.92 | 180,180,181,181 | 0 |
| 84 | OHX | 6 | 1983 | 7/7 | 0.95 | 0.35 | 9.92 | 169,169,170,170 | 0 |
| 85 | MG | AR | 4001 | 1/1 | 0.84 | 0.43 | 9.85 | 41,41,41,41 | 0 |
| 84 | OHX | AT | 219 | 7/7 | 0.92 | 0.37 | 9.85 | 190,190,190,191 | 0 |
| 85 | MG | 6 | 2068 | 1/1 | 0.98 | 0.35 | 9.83 | 76,76,76,76 | 0 |
| 85 | MG | AT | 221 | 1/1 | 0.93 | 0.40 | 9.83 | 26,26,26,26 | 0 |
| 85 | MG | 1 | 3817 | 1/1 | 0.97 | 0.30 | 9.80 | 32,32,32,32 | 0 |
| 84 | OHX | 6 | 2045 | 7/7 | 0.85 | 0.39 | 9.80 | 196,197,198,199 | 0 |
| 84 | OHX | AR | 3645 | 7/7 | 0.94 | 0.25 | 9.77 | 174,175,176,176 | 0 |
| 85 | MG | AR | 3817 | 1/1 | 0.98 | 0.31 | 9.77 | 20,20,20,20 | 0 |
| 85 | MG | AR | 4050 | 1/1 | 0.82 | 0.28 | 9.67 | 46,46,46,46 | 0 |
| 84 | OHX | 1 | 3702 | 7/7 | 0.94 | 0.33 | 9.67 | 179,180,181,182 | 0 |
| 84 | OHX | 1 | 3679 | 7/7 | 0.92 | 0.24 | 9.63 | 230,231,232,232 | 0 |
| 84 | OHX | AR | 3545 | 7/7 | 0.96 | 0.23 | 9.59 | 181,182,182,183 | 0 |
| 84 | OHX | 1 | 3651 | 7/7 | 0.91 | 0.31 | 9.57 | 207,208,209,209 | 0 |
| 85 | MG | AR | 3963 | 1/1 | 0.94 | 0.38 | 9.54 | 23,23,23,23 | 0 |
| 84 | OHX | 1 | 3717 | 7/7 | 0.82 | 0.48 | 9.48 | 217,218,219,219 | 0 |
| 85 | MG | A | 2130 | 1/1 | 0.90 | 0.30 | 9.44 | 49,49,49,49 | 0 |
| 84 | OHX | A | 2035 | 7/7 | 0.95 | 0.30 | 9.43 | 177,178,180,181 | 0 |
| 85 | MG | AR | 3895 | 1/1 | 0.98 | 0.39 | 9.37 | 21,21,21,21 | 0 |
| 84 | OHX | x | 201 | 7/7 | 0.89 | 0.45 | 9.34 | 169,169,170,170 | 0 |
| 84 | OHX | 6 | 2035 | 7/7 | 0.92 | 0.32 | 9.31 | 157,158,159,159 | 0 |
| 84 | OHX | 1 | 3647 | 7/7 | 0.94 | 0.30 | 9.27 | 203,204,205,206 | 0 |
| 84 | OHX | 6 | 2036 | 7/7 | 0.91 | 0.38 | 9.20 | 172,174,175,176 | 0 |
| 85 | MG | CP | 502 | 1/1 | 0.82 | 0.38 | 9.14 | 25,25,25,25 | 0 |
| 85 | MG | A | 2053 | 1/1 | 0.95 | 0.33 | 9.14 | 39,39,39,39 | 0 |
| 84 | OHX | 1 | 3686 | 7/7 | 0.93 | 0.34 | 9.13 | 207,208,209,209 | 0 |
| 85 | MG | AR | 3862 | 1/1 | 0.95 | 0.26 | 9.12 | 20,20,20,20 | 0 |
| 85 | MG | AR | 3898 | 1/1 | 0.96 | 0.42 | 9.08 | 16,16,16,16 | 0 |
| 85 | MG | AR | 3847 | 1/1 | 0.95 | 0.29 | 9.08 | 35,35,35,35 | 0 |
| 85 | MG | 1 | 3979 | 1/1 | 0.92 | 0.29 | 9.02 | 47,47,47,47 | 0 |
| 85 | MG | 1 | 4007 | 1/1 | 0.97 | 0.30 | 9.00 | 16,16,16,16 | 0 |
| 85 | MG | 1 | 3753 | 1/1 | 0.92 | 0.32 | 8.98 | 28,28,28,28 | 0 |
| 84 | OHX | A | 1903 | 7/7 | 0.99 | 0.26 | 8.97 | 117,118,118,119 | 0 |
| 85 | MG | AR | 4228 | 1/1 | 0.97 | 0.31 | 8.92 | 12,12,12,12 | 0 |
| 85 | MG | AR | 3911 | 1/1 | 0.98 | 0.43 | 8.85 | 16,16,16,16 | 0 |
| 84 | OHX | AR | 3684 | 7/7 | 0.94 | 0.47 | 8.81 | 181,182,183,183 | 0 |
| 84 | OHX | AR | 3601 | 7/7 | 0.94 | 0.29 | 8.76 | 171,172,173,173 | 0 |
| 84 | OHX | A | 1996 | 7/7 | 0.90 | 0.27 | 8.62 | 208,209,211,212 | 0 |
| 85 | MG | A | 2119 | 1/1 | 0.97 | 0.38 | 8.58 | 55,55,55,55 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | OHX | 6 | 2015 | 7/7 | 0.89 | 0.41 | 8.57 | 230,231,232,233 | 0 |
| 84 | OHX | A | 1985 | 7/7 | 0.79 | 0.36 | 8.51 | 221,222,223,224 | 0 |
| 85 | MG | AR | 3891 | 1/1 | 0.94 | 0.36 | 8.49 | 36,36,36,36 | 0 |
| 84 | OHX | 1 | 3664 | 7/7 | 0.89 | 0.35 | 8.46 | 232,233,234,235 | 0 |
| 84 | OHX | 4 | 206 | 7/7 | 0.93 | 0.27 | 8.42 | 179,179,180,180 | 0 |
| 85 | MG | 1 | 3945 | 1/1 | 0.90 | 0.29 | 8.40 | 17,17,17,17 | 0 |
| 85 | MG | AR | 3864 | 1/1 | 0.91 | 0.26 | 8.34 | 21,21,21,21 | 0 |
| 84 | OHX | 1 | 3687 | 7/7 | 0.93 | 0.31 | 8.33 | 196,196,197,197 | 0 |
| 85 | MG | 1 | 3822 | 1/1 | 0.97 | 0.31 | 8.33 | 22,22,22,22 | 0 |
| 85 | MG | 1 | 3925 | 1/1 | 0.98 | 0.38 | 8.27 | 15,15,15,15 | 0 |
| 85 | MG | 1 | 4117 | 1/1 | 0.98 | 0.34 | 8.27 | 26,26,26,26 | 0 |
| 85 | MG | AR | 3840 | 1/1 | 0.99 | 0.33 | 8.26 | 22,22,22,22 | 0 |
| 84 | OHX | 1 | 3662 | 7/7 | 0.94 | 0.22 | 8.25 | 178,179,180,180 | 0 |
| 85 | MG | x | 205 | 1/1 | 0.97 | 0.48 | 8.24 | 20,20,20,20 | 0 |
| 85 | MG | 1 | 3772 | 1/1 | 0.93 | 0.34 | 8.18 | 32,32,32,32 | 0 |
| 84 | OHX | 1 | 3668 | 7/7 | 0.95 | 0.28 | 8.14 | 179,179,180,181 | 0 |
| 85 | MG | A | 2100 | 1/1 | 0.88 | 0.32 | 8.12 | 60,60,60,60 | 0 |
| 85 | MG | 1 | 3987 | 1/1 | 0.99 | 0.24 | 8.10 | 32,32,32,32 | 0 |
| 85 | MG | 1 | 4135 | 1/1 | 0.72 | 0.32 | 8.09 | 64,64,64,64 | 0 |
| 84 | OHX | AR | 3633 | 7/7 | 0.94 | 0.32 | 8.09 | 173,173,174,174 | 0 |
| 85 | MG | 1 | 3806 | 1/1 | 0.99 | 0.28 | 8.06 | 31,31,31,31 | 0 |
| 84 | OHX | A | 2026 | 7/7 | 0.92 | 0.32 | 8.06 | 191,192,194,194 | 0 |
| 84 | OHX | AS | 209 | 7/7 | 0.92 | 0.26 | 8.06 | 175,176,177,177 | 0 |
| 85 | MG | AR | 3983 | 1/1 | 0.97 | 0.28 | 8.06 | 24,24,24,24 | 0 |
| 84 | OHX | AR | 3635 | 7/7 | 0.96 | 0.34 | 8.03 | 173,175,175,175 | 0 |
| 85 | MG | 1 | 3884 | 1/1 | 0.98 | 0.38 | 7.99 | 27,27,27,27 | 0 |
| 84 | OHX | AR | 3587 | 7/7 | 0.96 | 0.19 | 7.96 | 175,176,177,177 | 0 |
| 84 | OHX | AS | 210 | 7/7 | 0.79 | 0.33 | 7.96 | 235,237,238,238 | 0 |
| 85 | MG | AR | 3866 | 1/1 | 0.97 | 0.26 | 7.88 | 20,20,20,20 | 0 |
| 84 | OHX | 1 | 3693 | 7/7 | 0.81 | 0.45 | 7.81 | 264,265,266,266 | 0 |
| 85 | MG | 1 | 3912 | 1/1 | 0.92 | 0.34 | 7.80 | 30,30,30,30 | 0 |
| 85 | MG | 6 | 2147 | 1/1 | 0.86 | 0.31 | 7.80 | 75,75,75,75 | 0 |
| 85 | MG | 6 | 2162 | 1/1 | 0.96 | 0.30 | 7.79 | 69,69,69,69 | 0 |
| 85 | MG | 6 | 2103 | 1/1 | 0.98 | 0.41 | 7.73 | 40,40,40,40 | 0 |
| 84 | OHX | 1 | 3602 | 7/7 | 0.94 | 0.29 | 7.68 | 228,229,229,230 | 0 |
| 84 | OHX | AR | 3581 | 7/7 | 0.93 | 0.32 | 7.57 | 205,205,205,205 | 0 |
| 85 | MG | 6 | 2108 | 1/1 | 0.95 | 0.29 | 7.57 | 44,44,44,44 | 0 |
| 85 | MG | 1 | 3738 | 1/1 | 0.92 | 0.27 | 7.54 | 57,57,57,57 | 0 |
| 85 | MG | 1 | 3953 | 1/1 | 0.94 | 0.29 | 7.50 | 32,32,32,32 | 0 |
| 84 | OHX | 1 | 3584 | 7/7 | 0.95 | 0.29 | 7.45 | 154,155,156,156 | 0 |
| 84 | OHX | AR | 3663 | 7/7 | 0.85 | 0.26 | 7.39 | 208,209,210,210 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 85 | MG | 6 | 2184 | 1/1 | 0.94 | 0.27 | 7.37 | 43,43,43,43 | 0 |
| 84 | OHX | A | 1990 | 7/7 | 0.96 | 0.42 | 7.36 | 212,215,216,216 | 0 |
| 84 | OHX | AR | 3407 | 7/7 | 0.99 | 0.24 | 7.34 | 88,88,88,88 | 0 |
| 85 | MG | 1 | 4071 | 1/1 | 0.99 | 0.37 | 7.33 | 16,16,16,16 | 0 |
| 85 | MG | AR | 3957 | 1/1 | 0.95 | 0.55 | 7.31 | 37,37,37,37 | 0 |
| 85 | MG | AR | 3936 | 1/1 | 0.94 | 0.32 | 7.30 | 20,20,20,20 | 0 |
| 84 | OHX | 1 | 3729 | 7/7 | 0.90 | 0.37 | 7.29 | 206,207,207,208 | 0 |
| 84 | OHX | AR | 3661 | 7/7 | 0.94 | 0.53 | 7.25 | 176,177,178,178 | 0 |
| 85 | MG | AR | 4011 | 1/1 | 0.96 | 0.47 | 7.24 | 31,31,31,31 | 0 |
| 85 | MG | 1 | 4065 | 1/1 | 0.99 | 0.26 | 7.21 | 35,35,35,35 | 0 |
| 85 | MG | 6 | 2165 | 1/1 | 0.96 | 0.29 | 7.20 | 45,45,45,45 | 0 |
| 85 | MG | 1 | 3889 | 1/1 | 0.98 | 0.28 | 7.09 | 19,19,19,19 | 0 |
| 84 | OHX | AR | 3712 | 7/7 | 0.88 | 0.31 | 7.09 | 183,183,184,184 | 0 |
| 85 | MG | AR | 3915 | 1/1 | 0.98 | 0.29 | 7.08 | 20,20,20,20 | 0 |
| 84 | OHX | AR | 3728 | 7/7 | 0.82 | 0.35 | 7.04 | 238,238,239,239 | 0 |
| 85 | MG | A | 2055 | 1/1 | 0.88 | 0.26 | 7.02 | 48,48,48,48 | 0 |
| 85 | MG | AR | 3991 | 1/1 | 0.97 | 0.26 | 6.99 | 15,15,15,15 | 0 |
| 84 | OHX | 1 | 3700 | 7/7 | 0.92 | 0.26 | 6.98 | 161,162,163,163 | 0 |
| 85 | MG | AR | 3964 | 1/1 | 0.88 | 0.30 | 6.96 | 28,28,28,28 | 0 |
| 84 | OHX | 1 | 3409 | 7/7 | 0.99 | 0.21 | 6.89 | 85,85,85,85 | 0 |
| 85 | MG | 1 | 3913 | 1/1 | 0.98 | 0.26 | 6.89 | 38,38,38,38 | 0 |
| 84 | OHX | AR | 3415 | 7/7 | 0.99 | 0.23 | 6.87 | 86,86,86,87 | 0 |
| 85 | MG | 6 | 2064 | 1/1 | 0.88 | 0.31 | 6.84 | 62,62,62,62 | 0 |
| 85 | MG | 1 | 3732 | 1/1 | 0.96 | 0.31 | 6.84 | 27,27,27,27 | 0 |
| 85 | MG | AR | 3901 | 1/1 | 0.97 | 0.26 | 6.77 | 17,17,17,17 | 0 |
| 84 | OHX | 1 | 3542 | 7/7 | 0.94 | 0.28 | 6.70 | 156,157,158,158 | 0 |
| 85 | MG | AR | 3952 | 1/1 | 0.88 | 0.24 | 6.67 | 28,28,28,28 | 0 |
| 84 | OHX | AR | 3575 | 7/7 | 0.96 | 0.22 | 6.66 | 156,158,159,159 | 0 |
| 84 | OHX | 1 | 3403 | 7/7 | 0.99 | 0.23 | 6.59 | 90,90,90,90 | 0 |
| 85 | MG | 6 | 2149 | 1/1 | 0.96 | 0.31 | 6.56 | 75,75,75,75 | 0 |
| 84 | OHX | 1 | 3727 | 7/7 | 0.84 | 0.33 | 6.54 | 253,254,255,256 | 0 |
| 84 | OHX | 1 | 3587 | 7/7 | 0.94 | 0.25 | 6.53 | 188,189,189,190 | 0 |
| 84 | OHX | 1 | 3401 | 7/7 | 1.00 | 0.26 | 6.52 | 89,89,90,90 | 0 |
| 84 | OHX | AR | 3692 | 7/7 | 0.96 | 0.34 | 6.51 | 184,186,186,187 | 0 |
| 84 | OHX | 1 | 3405 | 7/7 | 0.99 | 0.26 | 6.48 | 97,98,98,98 | 0 |
| 84 | OHX | 1 | 3632 | 7/7 | 0.89 | 0.31 | 6.46 | 202,202,204,204 | 0 |
| 84 | OHX | AR | 3643 | 7/7 | 0.96 | 0.28 | 6.44 | 157,158,159,160 | 0 |
| 85 | MG | v | 302 | 1/1 | 0.93 | 0.39 | 6.42 | 43,43,43,43 | 0 |
| 84 | OHX | 6 | 2019 | 7/7 | 0.95 | 0.31 | 6.40 | 191,192,193,194 | 0 |
| 85 | MG | AR | 4030 | 1/1 | 0.93 | 0.26 | 6.35 | 37,37,37,37 | 0 |
| 85 | MG | d3 | 202 | 1/1 | 0.93 | 0.54 | 6.30 | 56,56,56,56 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 85 | MG | AR | 4037 | 1/1 | 0.90 | 0.30 | 6.29 | 33,33,33,33 | 0 |
| 84 | OHX | 6 | 1958 | 7/7 | 0.95 | 0.21 | 6.27 | 153,153,155,156 | 0 |
| 84 | OHX | AR | 3526 | 7/7 | 0.95 | 0.21 | 6.25 | 164,166,167,167 | 0 |
| 85 | MG | AR | 3779 | 1/1 | 0.98 | 0.28 | 6.18 | 20,20,20,20 | 0 |
| 85 | MG | AR | 3801 | 1/1 | 0.86 | 0.35 | 6.16 | 30,30,30,30 | 0 |
| 84 | OHX | A | 2038 | 7/7 | 0.89 | 0.56 | 6.13 | 217,217,220,220 | 0 |
| 85 | MG | AF | 202 | 1/1 | 0.87 | 0.27 | 6.10 | 32,32,32,32 | 0 |
| 85 | MG | 1 | 4039 | 1/1 | 0.92 | 0.23 | 6.09 | 40,40,40,40 | 0 |
| 84 | OHX | 1 | 3672 | 7/7 | 0.92 | 0.40 | 6.06 | 161,162,164,164 | 0 |
| 85 | MG | CU | 202 | 1/1 | 0.97 | 0.20 | 6.04 | 31,31,31,31 | 0 |
| 85 | MG | AR | 3914 | 1/1 | 0.98 | 0.35 | 6.02 | 13,13,13,13 | 0 |
| 85 | MG | 1 | 3934 | 1/1 | 0.89 | 0.17 | 6.02 | 61,61,61,61 | 0 |
| 84 | OHX | DL | 102 | 7/7 | 0.88 | 0.39 | 6.00 | 212,212,213,213 | 0 |
| 85 | MG | 1 | 4147 | 1/1 | 0.97 | 0.25 | 5.98 | 28,28,28,28 | 0 |
| 84 | OHX | 1 | 3594 | 7/7 | 0.95 | 0.26 | 5.96 | 150,150,151,151 | 0 |
| 84 | OHX | AR | 3613 | 7/7 | 0.95 | 0.29 | 5.95 | 165,166,167,167 | 0 |
| 84 | OHX | 1 | 3666 | 7/7 | 0.88 | 0.39 | 5.93 | 186,187,188,188 | 0 |
| 84 | OHX | AR | 3578 | 7/7 | 0.97 | 0.38 | 5.92 | 188,188,189,189 | 0 |
| 84 | OHX | AT | 215 | 7/7 | 0.95 | 0.23 | 5.91 | 212,213,213,213 | 0 |
| 84 | OHX | AR | 3672 | 7/7 | 0.97 | 0.32 | 5.90 | 137,138,138,138 | 0 |
| 85 | MG | 1 | 4149 | 1/1 | 0.94 | 0.21 | 5.89 | 45,45,45,45 | 0 |
| 84 | OHX | 1 | 3708 | 7/7 | 0.92 | 0.30 | 5.87 | 210,211,211,211 | 0 |
| 85 | MG | AR | 3889 | 1/1 | 0.91 | 0.25 | 5.86 | 42,42,42,42 | 0 |
| 84 | OHX | AR | 3606 | 7/7 | 0.94 | 0.30 | 5.85 | 155,156,157,157 | 0 |
| 85 | MG | A | 2072 | 1/1 | 0.92 | 0.28 | 5.83 | 44,44,44,44 | 0 |
| 85 | MG | 1 | 3996 | 1/1 | 0.98 | 0.25 | 5.79 | 51,51,51,51 | 0 |
| 85 | MG | AR | 4033 | 1/1 | 0.95 | 0.30 | 5.79 | 63,63,63,63 | 0 |
| 84 | OHX | A | 2014 | 7/7 | 0.94 | 0.34 | 5.77 | 198,199,200,200 | 0 |
| 84 | OHX | 1 | 3654 | 7/7 | 0.92 | 0.29 | 5.75 | 192,194,194,194 | 0 |
| 84 | OHX | AR | 3602 | 7/7 | 0.92 | 0.33 | 5.71 | 192,193,194,194 | 0 |
| 84 | OHX | A | 1970 | 7/7 | 0.95 | 0.31 | 5.68 | 178,180,182,182 | 0 |
| 84 | OHX | AR | 3402 | 7/7 | 0.99 | 0.27 | 5.68 | 89,89,89,89 | 0 |
| 84 | OHX | AR | 3659 | 7/7 | 0.91 | 0.26 | 5.68 | 195,196,196,197 | 0 |
| 85 | MG | 1 | 3747 | 1/1 | 0.93 | 0.31 | 5.64 | 28,28,28,28 | 0 |
| 85 | MG | AR | 4136 | 1/1 | 0.94 | 0.22 | 5.59 | 41,41,41,41 | 0 |
| 85 | MG | 1 | 4170 | 1/1 | 0.95 | 0.22 | 5.50 | 33,33,33,33 | 0 |
| 84 | OHX | 1 | 3620 | 7/7 | 0.95 | 0.27 | 5.50 | 208,208,209,209 | 0 |
| 84 | OHX | AR | 3608 | 7/7 | 0.96 | 0.33 | 5.50 | 186,187,188,188 | 0 |
| 84 | OHX | AR | 3524 | 7/7 | 0.95 | 0.23 | 5.49 | 152,153,154,155 | 0 |
| 84 | OHX | A | 2024 | 7/7 | 0.90 | 0.36 | 5.47 | 219,222,223,223 | 0 |
| 84 | OHX | 1 | 3636 | 7/7 | 0.95 | 0.36 | 5.46 | 170,171,172,172 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 85 | MG | AR | 3749 | 1/1 | 0.95 | 0.25 | 5.44 | 19,19,19,19 | 0 |
| 84 | OHX | AR | 3700 | 7/7 | 0.94 | 0.37 | 5.42 | 174,175,175,176 | 0 |
| 84 | OHX | 1 | 3406 | 7/7 | 0.99 | 0.22 | 5.40 | 85,85,85,85 | 0 |
| 85 | MG | AR | 3910 | 1/1 | 0.99 | 0.32 | 5.38 | 17,17,17,17 | 0 |
| 85 | MG | AR | 4090 | 1/1 | 0.93 | 0.27 | 5.35 | 62,62,62,62 | 0 |
| 84 | OHX | A | 2006 | 7/7 | 0.92 | 0.25 | 5.31 | 215,218,219,219 | 0 |
| 85 | MG | A | 2108 | 1/1 | 0.96 | 0.38 | 5.29 | 39,39,39,39 | 0 |
| 84 | OHX | 1 | 3566 | 7/7 | 0.93 | 0.25 | 5.27 | 182,182,183,183 | 0 |
| 85 | MG | 1 | 4208 | 1/1 | 0.96 | 0.30 | 5.21 | 30,30,30,30 | 0 |
| 85 | MG | AR | 4177 | 1/1 | 0.95 | 0.23 | 5.21 | 18,18,18,18 | 0 |
| 84 | OHX | 1 | 3583 | 7/7 | 0.97 | 0.29 | 5.20 | 144,144,145,145 | 0 |
| 85 | MG | AR | 3763 | 1/1 | 0.97 | 0.26 | 5.16 | 18,18,18,18 | 0 |
| 85 | MG | CR | 201 | 1/1 | 0.94 | 0.44 | 5.15 | 14,14,14,14 | 0 |
| 84 | OHX | 6 | 2023 | 7/7 | 0.86 | 0.27 | 5.14 | 201,203,204,205 | 0 |
| 84 | OHX | AR | 3671 | 7/7 | 0.86 | 0.27 | 5.11 | 166,166,167,167 | 0 |
| 84 | OHX | 1 | 3592 | 7/7 | 0.94 | 0.26 | 5.11 | 166,166,167,167 | 0 |
| 84 | OHX | 6 | 1997 | 7/7 | 0.94 | 0.20 | 5.11 | 198,199,201,201 | 0 |
| 84 | OHX | 1 | 3646 | 7/7 | 0.94 | 0.23 | 5.10 | 182,183,184,185 | 0 |
| 84 | OHX | AR | 3617 | 7/7 | 0.97 | 0.27 | 4.97 | 158,158,159,159 | 0 |
| 85 | MG | A | 2115 | 1/1 | 0.95 | 0.27 | 4.95 | 85,85,85,85 | 0 |
| 84 | OHX | 1 | 3608 | 7/7 | 0.92 | 0.29 | 4.92 | 177,177,179,179 | 0 |
| 85 | MG | CE | 404 | 1/1 | 0.98 | 0.27 | 4.91 | 24,24,24,24 | 0 |
| 84 | OHX | 6 | 1907 | 7/7 | 0.98 | 0.19 | 4.87 | 100,101,101,101 | 0 |
| 84 | OHX | A | 1964 | 7/7 | 0.96 | 0.30 | 4.86 | 168,169,170,170 | 0 |
| 84 | OHX | 1 | 3715 | 7/7 | 0.89 | 0.43 | 4.85 | 219,220,222,222 | 0 |
| 84 | OHX | AR | 3715 | 7/7 | 0.96 | 0.21 | 4.85 | 144,146,147,147 | 0 |
| 84 | OHX | AR | 3695 | 7/7 | 0.88 | 0.24 | 4.84 | 225,226,227,227 | 0 |
| 84 | OHX | 1 | 3546 | 7/7 | 0.96 | 0.20 | 4.83 | 147,148,149,150 | 0 |
| 84 | OHX | 1 | 3596 | 7/7 | 0.95 | 0.29 | 4.81 | 183,184,185,185 | 0 |
| 85 | MG | AR | 3757 | 1/1 | 0.94 | 0.28 | 4.76 | 32,32,32,32 | 0 |
| 84 | OHX | 1 | 3448 | 7/7 | 0.98 | 0.24 | 4.75 | 104,105,106,106 | 0 |
| 84 | OHX | 1 | 3692 | 7/7 | 0.90 | 0.31 | 4.75 | 189,190,191,191 | 0 |
| 85 | MG | 1 | 4221 | 1/1 | 0.97 | 0.36 | 4.74 | 22,22,22,22 | 0 |
| 85 | MG | CE | 405 | 1/1 | 0.93 | 0.41 | 4.72 | 34,34,34,34 | 0 |
| 84 | OHX | 6 | 1979 | 7/7 | 0.95 | 0.29 | 4.71 | 165,165,166,167 | 0 |
| 85 | MG | A | 2092 | 1/1 | 0.95 | 0.37 | 4.66 | 87,87,87,87 | 0 |
| 84 | OHX | 1 | 3607 | 7/7 | 0.95 | 0.24 | 4.64 | 190,192,193,193 | 0 |
| 85 | MG | CR | 205 | 1/1 | 0.84 | 0.44 | 4.63 | 29,29,29,29 | 0 |
| 84 | OHX | 1 | 3698 | 7/7 | 0.89 | 0.47 | 4.63 | 177,178,178,179 | 0 |
| 84 | OHX | A | 2021 | 7/7 | 0.95 | 0.34 | 4.63 | 176,177,179,179 | 0 |
| 85 | MG | 6 | 2145 | 1/1 | 0.86 | 0.19 | 4.60 | 51,51,51,51 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 85 | MG | 6 | 2062 | 1/1 | 0.94 | 0.36 | 4.58 | 32,32,32,32 | 0 |
| 85 | MG | CQ | 203 | 1/1 | 0.89 | 0.40 | 4.54 | 28,28,28,28 | 0 |
| 84 | OHX | AR | 3638 | 7/7 | 0.89 | 0.41 | 4.49 | 208,208,209,209 | 0 |
| 84 | OHX | AR | 3620 | 7/7 | 0.94 | 0.27 | 4.48 | 180,182,183,184 | 0 |
| 84 | OHX | 1 | 3684 | 7/7 | 0.97 | 0.22 | 4.46 | 170,171,172,173 | 0 |
| 84 | OHX | AR | 3705 | 7/7 | 0.88 | 0.28 | 4.45 | 212,213,213,214 | 0 |
| 84 | OHX | 1 | 3658 | 7/7 | 0.86 | 0.22 | 4.41 | 211,212,212,213 | 0 |
| 85 | MG | AR | 3906 | 1/1 | 0.99 | 0.23 | 4.35 | 15,15,15,15 | 0 |
| 84 | OHX | AR | 3609 | 7/7 | 0.87 | 0.31 | 4.32 | 201,201,202,202 | 0 |
| 84 | OHX | A | 1982 | 7/7 | 0.95 | 0.29 | 4.30 | 164,166,167,167 | 0 |
| 84 | OHX | 6 | 2033 | 7/7 | 0.92 | 0.29 | 4.27 | 199,200,201,202 | 0 |
| 85 | MG | 1 | 3819 | 1/1 | 0.98 | 0.25 | 4.24 | 25,25,25,25 | 0 |
| 84 | OHX | 1 | 3572 | 7/7 | 0.97 | 0.27 | 4.18 | 168,168,169,170 | 0 |
| 85 | MG | AR | 3810 | 1/1 | 0.95 | 0.29 | 4.17 | 28,28,28,28 | 0 |
| 85 | MG | 1 | 3960 | 1/1 | 0.86 | 0.30 | 4.16 | 27,27,27,27 | 0 |
| 85 | MG | AR | 4224 | 1/1 | 0.96 | 0.25 | 4.15 | 26,26,26,26 | 0 |
| 84 | OHX | AR | 3646 | 7/7 | 0.89 | 0.30 | 4.13 | 167,168,169,169 | 0 |
| 85 | MG | 1 | 4188 | 1/1 | 0.94 | 0.21 | 4.13 | 34,34,34,34 | 0 |
| 84 | OHX | AR | 3640 | 7/7 | 0.88 | 0.29 | 4.11 | 197,198,199,199 | 0 |
| 85 | MG | A | 2109 | 1/1 | 0.79 | 0.31 | 4.10 | 50,50,50,50 | 0 |
| 84 | OHX | 4 | 205 | 7/7 | 0.95 | 0.23 | 4.09 | 172,173,174,174 | 0 |
| 84 | OHX | 1 | 3537 | 7/7 | 0.95 | 0.25 | 4.08 | 160,161,162,162 | 0 |
| 85 | MG | 1 | 3898 | 1/1 | 0.92 | 0.33 | 4.04 | 22,22,22,22 | 0 |
| 84 | OHX | A | 1994 | 7/7 | 0.96 | 0.23 | 4.01 | 200,203,204,205 | 0 |
| 84 | OHX | 1 | 3680 | 7/7 | 0.90 | 0.39 | 4.01 | 212,212,213,213 | 0 |
| 85 | MG | 1 | 3748 | 1/1 | 0.96 | 0.25 | 3.95 | 23,23,23,23 | 0 |
| 84 | OHX | 1 | 3407 | 7/7 | 0.99 | 0.20 | 3.95 | 83,83,83,83 | 0 |
| 84 | OHX | AR | 3689 | 7/7 | 0.91 | 0.23 | 3.91 | 195,197,198,198 | 0 |
| 84 | OHX | 1 | 3412 | 7/7 | 0.99 | 0.22 | 3.90 | 88,88,88,88 | 0 |
| 85 | MG | 1 | 3737 | 1/1 | 0.93 | 0.26 | 3.86 | 36,36,36,36 | 0 |
| 85 | MG | 1 | 3835 | 1/1 | 0.96 | 0.28 | 3.85 | 19,19,19,19 | 0 |
| 85 | MG | AR | 3935 | 1/1 | 0.97 | 0.28 | 3.82 | 22,22,22,22 | 0 |
| 84 | OHX | 6 | 1971 | 7/7 | 0.94 | 0.18 | 3.79 | 177,178,179,180 | 0 |
| 85 | MG | AR | 4084 | 1/1 | 0.91 | 0.20 | 3.74 | 31,31,31,31 | 0 |
| 84 | OHX | AR | 3497 | 7/7 | 0.97 | 0.23 | 3.70 | 140,140,141,141 | 0 |
| 85 | MG | AR | 4040 | 1/1 | 0.91 | 0.24 | 3.64 | 27,27,27,27 | 0 |
| 84 | OHX | AR | 3494 | 7/7 | 0.96 | 0.23 | 3.62 | 144,145,146,146 | 0 |
| 85 | MG | AR | 4174 | 1/1 | 0.97 | 0.21 | 3.62 | 23,23,23,23 | 0 |
| 84 | OHX | 1 | 3578 | 7/7 | 0.94 | 0.24 | 3.61 | 168,170,170,171 | 0 |
| 84 | OHX | 6 | 1991 | 7/7 | 0.95 | 0.20 | 3.59 | 184,185,187,187 | 0 |
| 84 | OHX | 6 | 1972 | 7/7 | 0.94 | 0.34 | 3.55 | 196,197,198,199 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 85 | MG | AR | 3885 | 1/1 | 0.94 | 0.37 | 3.55 | 38,38,38,38 | 0 |
| 84 | OHX | AT | 203 | 7/7 | 0.99 | 0.21 | 3.55 | 83,83,83,83 | 0 |
| 85 | MG | 6 | 2159 | 1/1 | 0.92 | 0.32 | 3.54 | 39,39,39,39 | 0 |
| 85 | MG | 1 | 3803 | 1/1 | 0.96 | 0.23 | 3.52 | 22,22,22,22 | 0 |
| 85 | MG | F | 301 | 1/1 | 0.78 | 0.34 | 3.51 | 71,71,71,71 | 0 |
| 85 | MG | 6 | 2150 | 1/1 | 0.93 | 0.21 | 3.49 | 51,51,51,51 | 0 |
| 84 | OHX | A | 1993 | 7/7 | 0.88 | 0.40 | 3.49 | 236,237,239,240 | 0 |
| 84 | OHX | DI | 201 | 7/7 | 0.90 | 0.58 | 3.49 | 194,195,195,196 | 0 |
| 85 | MG | CQ | 201 | 1/1 | 0.95 | 0.30 | 3.42 | 23,23,23,23 | 0 |
| 84 | OHX | AR | 3403 | 7/7 | 0.99 | 0.19 | 3.42 | 86,86,86,86 | 0 |
| 84 | OHX | 6 | 1981 | 7/7 | 0.95 | 0.34 | 3.41 | 195,197,199,199 | 0 |
| 84 | OHX | AT | 211 | 7/7 | 0.93 | 0.26 | 3.41 | 179,179,180,180 | 0 |
| 85 | MG | 1 | 4219 | 1/1 | 0.98 | 0.34 | 3.41 | 47,47,47,47 | 0 |
| 85 | MG | 6 | 2132 | 1/1 | 0.94 | 0.22 | 3.40 | 38,38,38,38 | 0 |
| 85 | MG | A | 2061 | 1/1 | 0.94 | 0.22 | 3.40 | 27,27,27,27 | 0 |
| 85 | MG | 1 | 3859 | 1/1 | 0.97 | 0.21 | 3.39 | 33,33,33,33 | 0 |
| 84 | OHX | AR | 3644 | 7/7 | 0.88 | 0.26 | 3.38 | 197,197,198,199 | 0 |
| 84 | OHX | 6 | 2050 | 7/7 | 0.95 | 0.27 | 3.35 | 190,191,192,193 | 0 |
| 84 | OHX | 1 | 3420 | 7/7 | 0.99 | 0.20 | 3.35 | 91,91,92,92 | 0 |
| 84 | OHX | AR | 3731 | 7/7 | 0.90 | 0.37 | 3.33 | 175,176,177,178 | 0 |
| 85 | MG | AR | 4205 | 1/1 | 0.86 | 0.24 | 3.32 | 30,30,30,30 | 0 |
| 84 | OHX | AR | 3703 | 7/7 | 0.94 | 0.42 | 3.32 | 214,214,214,214 | 0 |
| 84 | OHX | AR | 3730 | 7/7 | 0.87 | 0.34 | 3.31 | 271,272,273,273 | 0 |
| 84 | OHX | 6 | 2040 | 7/7 | 0.92 | 0.29 | 3.28 | 199,200,201,202 | 0 |
| 84 | OHX | AR | 3406 | 7/7 | 0.99 | 0.23 | 3.27 | 86,86,86,86 | 0 |
| 84 | OHX | 6 | 1996 | 7/7 | 0.94 | 0.17 | 3.26 | 190,191,192,193 | 0 |
| 85 | MG | 6 | 2129 | 1/1 | 0.94 | 0.22 | 3.26 | 53,53,53,53 | 0 |
| 84 | OHX | 1 | 3681 | 7/7 | 0.93 | 0.29 | 3.25 | 210,211,212,212 | 0 |
| 84 | OHX | A | 2031 | 7/7 | 0.88 | 0.24 | 3.23 | 244,246,248,248 | 0 |
| 85 | MG | A | 2086 | 1/1 | 0.73 | 0.29 | 3.23 | 50,50,50,50 | 0 |
| 84 | OHX | 1 | 3605 | 7/7 | 0.94 | 0.31 | 3.22 | 171,171,172,172 | 0 |
| 84 | OHX | 1 | 3644 | 7/7 | 0.94 | 0.27 | 3.22 | 170,171,173,173 | 0 |
| 84 | OHX | 1 | 3612 | 7/7 | 0.95 | 0.24 | 3.22 | 173,174,175,175 | 0 |
| 84 | OHX | 6 | 2037 | 7/7 | 0.92 | 0.40 | 3.21 | 203,204,206,206 | 0 |
| 84 | OHX | AR | 3690 | 7/7 | 0.94 | 0.23 | 3.19 | 179,179,180,181 | 0 |
| 84 | OHX | A | 2009 | 7/7 | 0.95 | 0.32 | 3.18 | 191,192,194,195 | 0 |
| 84 | OHX | 6 | 1903 | 7/7 | 0.99 | 0.20 | 3.18 | 89,89,90,90 | 0 |
| 84 | OHX | 1 | 3411 | 7/7 | 0.99 | 0.19 | 3.18 | 93,93,93,93 | 0 |
| 85 | MG | AR | 4092 | 1/1 | 0.92 | 0.20 | 3.17 | 25,25,25,25 | 0 |
| 84 | OHX | A | 1997 | 7/7 | 0.92 | 0.25 | 3.15 | 211,214,214,215 | 0 |
| 84 | OHX | 1 | 3554 | 7/7 | 0.96 | 0.22 | 3.12 | 167,168,169,169 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | OHX | AR | 3717 | 7/7 | 0.86 | 0.32 | 3.09 | 281,282,283,283 | 0 |
| 85 | MG | AR | 3943 | 1/1 | 0.92 | 0.27 | 3.09 | 73,73,73,73 | 0 |
| 84 | OHX | 1 | 3402 | 7/7 | 0.99 | 0.24 | 3.07 | 90,90,91,91 | 0 |
| 84 | OHX | 1 | 3575 | 7/7 | 0.94 | 0.21 | 3.05 | 187,188,189,189 | 0 |
| 85 | MG | AR | 4225 | 1/1 | 0.97 | 0.25 | 3.00 | 23,23,23,23 | 0 |
| 84 | OHX | 6 | 1998 | 7/7 | 0.93 | 0.19 | 2.94 | 239,240,243,244 | 0 |
| 84 | OHX | AR | 3409 | 7/7 | 0.99 | 0.20 | 2.93 | 92,92,92,92 | 0 |
| 85 | MG | 1 | 4190 | 1/1 | 0.94 | 0.25 | 2.91 | 26,26,26,26 | 0 |
| 84 | OHX | 1 | 3617 | 7/7 | 0.88 | 0.38 | 2.91 | 201,202,203,204 | 0 |
| 84 | OHX | 6 | 2016 | 7/7 | 0.93 | 0.21 | 2.90 | 194,194,196,196 | 0 |
| 84 | OHX | 6 | 2030 | 7/7 | 0.95 | 0.38 | 2.89 | 160,161,162,162 | 0 |
| 84 | OHX | A | 2017 | 7/7 | 0.92 | 0.24 | 2.88 | 220,223,224,224 | 0 |
| 84 | OHX | y | 201 | 7/7 | 0.93 | 0.26 | 2.87 | 204,205,207,208 | 0 |
| 85 | MG | AR | 3836 | 1/1 | 0.97 | 0.31 | 2.86 | 15,15,15,15 | 0 |
| 85 | MG | 1 | 3777 | 1/1 | 0.96 | 0.26 | 2.85 | 40,40,40,40 | 0 |
| 84 | OHX | A | 1954 | 7/7 | 0.96 | 0.20 | 2.84 | 172,174,175,175 | 0 |
| 85 | MG | AR | 4191 | 1/1 | 0.93 | 0.20 | 2.83 | 38,38,38,38 | 0 |
| 85 | MG | 1 | 3956 | 1/1 | 0.96 | 0.22 | 2.82 | 15,15,15,15 | 0 |
| 85 | MG | 6 | 2154 | 1/1 | 0.93 | 0.20 | 2.82 | 38,38,38,38 | 0 |
| 84 | OHX | 1 | 3635 | 7/7 | 0.90 | 0.27 | 2.80 | 219,220,221,222 | 0 |
| 84 | OHX | 1 | 3710 | 7/7 | 0.85 | 0.34 | 2.77 | 247,248,248,249 | 0 |
| 84 | OHX | 1 | 3516 | 7/7 | 0.97 | 0.23 | 2.76 | 131,132,133,133 | 0 |
| 84 | OHX | AR | 3485 | 7/7 | 0.98 | 0.26 | 2.75 | 135,136,137,137 | 0 |
| 84 | OHX | 1 | 3581 | 7/7 | 0.95 | 0.24 | 2.71 | 153,153,154,154 | 0 |
| 84 | OHX | AR | 3597 | 7/7 | 0.92 | 0.20 | 2.70 | 176,177,178,178 | 0 |
| 85 | MG | 1 | 4217 | 1/1 | 0.88 | 0.29 | 2.69 | 18,18,18,18 | 0 |
| 84 | OHX | A | 1980 | 7/7 | 0.94 | 0.26 | 2.69 | 194,196,197,197 | 0 |
| 85 | MG | 1 | 3881 | 1/1 | 0.96 | 0.31 | 2.63 | 35,35,35,35 | 0 |
| 85 | MG | 6 | 2061 | 1/1 | 0.96 | 0.21 | 2.63 | 64,64,64,64 | 0 |
| 84 | OHX | 1 | 3529 | 7/7 | 0.96 | 0.23 | 2.63 | 143,144,145,146 | 0 |
| 85 | MG | AR | 3975 | 1/1 | 0.96 | 0.27 | 2.60 | 31,31,31,31 | 0 |
| 84 | OHX | 6 | 2042 | 7/7 | 0.82 | 0.55 | 2.58 | 246,246,248,248 | 0 |
| 84 | OHX | A | 1947 | 7/7 | 0.95 | 0.30 | 2.52 | 162,164,165,165 | 0 |
| 84 | OHX | A | 1986 | 7/7 | 0.96 | 0.25 | 2.51 | 215,218,220,222 | 0 |
| 84 | OHX | 6 | 1902 | 7/7 | 0.99 | 0.24 | 2.50 | 102,102,102,102 | 0 |
| 84 | OHX | 4 | 208 | 7/7 | 0.96 | 0.27 | 2.48 | 187,187,188,188 | 0 |
| 85 | MG | AR | 3973 | 1/1 | 0.92 | 0.19 | 2.48 | 27,27,27,27 | 0 |
| 84 | OHX | 1 | 3544 | 7/7 | 0.94 | 0.17 | 2.47 | 187,188,190,190 | 0 |
| 84 | OHX | AR | 3572 | 7/7 | 0.96 | 0.21 | 2.47 | 174,175,176,176 | 0 |
| 85 | MG | AR | 4026 | 1/1 | 0.79 | 0.21 | 2.46 | 62,62,62,62 | 0 |
| 84 | OHX | 1 | 3657 | 7/7 | 0.92 | 0.40 | 2.42 | 170,171,171,171 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | OHX | AR | 3721 | 7/7 | 0.92 | 0.30 | 2.42 | 212,213,213,214 | 0 |
| 84 | OHX | AR | 3668 | 7/7 | 0.89 | 0.32 | 2.41 | 216,216,217,218 | 0 |
| 84 | OHX | 6 | 2006 | 7/7 | 0.91 | 0.21 | 2.39 | 199,199,201,201 | 0 |
| 84 | OHX | AR | 3699 | 7/7 | 0.96 | 0.38 | 2.36 | 194,195,196,196 | 0 |
| 85 | MG | 1 | 3741 | 1/1 | 0.97 | 0.21 | 2.34 | 40,40,40,40 | 0 |
| 85 | MG | A | 2128 | 1/1 | 0.94 | 0.26 | 2.31 | 53,53,53,53 | 0 |
| 84 | OHX | AR | 3589 | 7/7 | 0.94 | 0.19 | 2.31 | 186,187,188,189 | 0 |
| 84 | OHX | 1 | 3585 | 7/7 | 0.96 | 0.24 | 2.30 | 173,174,174,175 | 0 |
| 85 | MG | 1 | 3813 | 1/1 | 0.96 | 0.18 | 2.30 | 24,24,24,24 | 0 |
| 84 | OHX | AT | 202 | 7/7 | 1.00 | 0.20 | 2.28 | 86,86,87,87 | 0 |
| 84 | OHX | 1 | 3491 | 7/7 | 0.93 | 0.18 | 2.24 | 138,138,139,139 | 0 |
| 84 | OHX | 1 | 3417 | 7/7 | 0.99 | 0.19 | 2.23 | 97,97,97,97 | 0 |
| 85 | MG | A | 2085 | 1/1 | 0.92 | 0.20 | 2.19 | 47,47,47,47 | 0 |
| 85 | MG | A | 2054 | 1/1 | 0.87 | 0.21 | 2.18 | 59,59,59,59 | 0 |
| 84 | OHX | 1 | 3682 | 7/7 | 0.92 | 0.27 | 2.18 | 204,206,207,207 | 0 |
| 85 | MG | AR | 3768 | 1/1 | 0.96 | 0.24 | 2.18 | 23,23,23,23 | 0 |
| 84 | OHX | AR | 3594 | 7/7 | 0.95 | 0.17 | 2.17 | 169,170,171,171 | 0 |
| 84 | OHX | 1 | 3603 | 7/7 | 0.97 | 0.34 | 2.17 | 162,162,164,164 | 0 |
| 85 | MG | A | 2105 | 1/1 | 0.92 | 0.25 | 2.16 | 71,71,71,71 | 0 |
| 84 | OHX | 1 | 3441 | 7/7 | 0.96 | 0.17 | 2.14 | 168,169,169,170 | 0 |
| 84 | OHX | 1 | 3712 | 7/7 | 0.91 | 0.41 | 2.13 | 215,215,216,217 | 0 |
| 84 | OHX | 6 | 2032 | 7/7 | 0.90 | 0.36 | 2.11 | 236,237,238,239 | 0 |
| 84 | OHX | 6 | 1901 | 7/7 | 0.99 | 0.23 | 2.11 | 92,92,92,92 | 0 |
| 84 | OHX | 1 | 3613 | 7/7 | 0.94 | 0.23 | 2.08 | 166,166,167,168 | 0 |
| 85 | MG | AR | 3845 | 1/1 | 0.98 | 0.23 | 2.06 | 32,32,32,32 | 0 |
| 85 | MG | AB | 204 | 1/1 | 0.97 | 0.27 | 2.03 | 42,42,42,42 | 0 |
| 85 | MG | 6 | 2135 | 1/1 | 0.99 | 0.22 | 2.02 | 38,38,38,38 | 0 |
| 84 | OHX | 1 | 3569 | 7/7 | 0.97 | 0.27 | 2.00 | 166,166,167,168 | 0 |
| 84 | OHX | 6 | 2008 | 7/7 | 0.93 | 0.29 | 2.00 | 211,213,214,216 | 0 |
| 84 | OHX | 6 | 1989 | 7/7 | 0.93 | 0.29 | 2.00 | 169,170,172,172 | 0 |
| 85 | MG | 1 | 3840 | 1/1 | 0.83 | 0.18 | 1.98 | 39,39,39,39 | 0 |
| 85 | MG | AR | 3816 | 1/1 | 0.97 | 0.21 | 1.96 | 27,27,27,27 | 0 |
| 85 | MG | AR | 3787 | 1/1 | 0.89 | 0.18 | 1.95 | 31,31,31,31 | 0 |
| 85 | MG | DH | 203 | 1/1 | 0.99 | 0.23 | 1.92 | 41,41,41,41 | 0 |
| 85 | MG | AT | 230 | 1/1 | 0.98 | 0.23 | 1.92 | 48,48,48,48 | 0 |
| 85 | MG | AR | 4188 | 1/1 | 0.98 | 0.19 | 1.91 | 35,35,35,35 | 0 |
| 85 | MG | A | 2123 | 1/1 | 0.88 | 0.20 | 1.91 | 40,40,40,40 | 0 |
| 84 | OHX | AR | 3427 | 7/7 | 0.98 | 0.22 | 1.90 | 87,87,87,87 | 0 |
| 84 | OHX | AR | 3704 | 7/7 | 0.91 | 0.37 | 1.88 | 223,224,225,225 | 0 |
| 84 | OHX | AT | 217 | 7/7 | 0.96 | 0.25 | 1.88 | 184,185,185,186 | 0 |
| 85 | MG | A | 2153 | 1/1 | 0.88 | 0.31 | 1.88 | 66,66,66,66 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | OHX | A | 2030 | 7/7 | 0.87 | 0.24 | 1.85 | 208,209,211,212 | 0 |
| 84 | OHX | AR | 3401 | 7/7 | 0.99 | 0.26 | 1.83 | 93,93,93,93 | 0 |
| 84 | OHX | AT | 220 | 7/7 | 0.91 | 0.26 | 1.83 | 197,197,198,198 | 0 |
| 84 | OHX | 1 | 3618 | 7/7 | 0.92 | 0.35 | 1.80 | 189,190,191,192 | 0 |
| 84 | OHX | 1 | 3713 | 7/7 | 0.91 | 0.33 | 1.78 | 217,217,218,218 | 0 |
| 84 | OHX | AR | 3722 | 7/7 | 0.90 | 0.30 | 1.77 | 200,201,201,202 | 0 |
| 84 | OHX | 1 | 3637 | 7/7 | 0.97 | 0.21 | 1.76 | 180,181,181,181 | 0 |
| 84 | OHX | 1 | 3433 | 7/7 | 0.98 | 0.21 | 1.76 | 90,90,90,90 | 0 |
| 84 | OHX | AR | 3413 | 7/7 | 0.99 | 0.16 | 1.73 | 84,84,84,84 | 0 |
| 85 | MG | AR | 3875 | 1/1 | 0.92 | 0.19 | 1.72 | 48,48,48,48 | 0 |
| 84 | OHX | AR | 3662 | 7/7 | 0.96 | 0.19 | 1.72 | 168,169,169,170 | 0 |
| 84 | OHX | A | 2012 | 7/7 | 0.89 | 0.20 | 1.71 | 218,220,220,222 | 0 |
| 85 | MG | 1 | 4186 | 1/1 | 0.96 | 0.26 | 1.71 | 51,51,51,51 | 0 |
| 85 | MG | AH | 201 | 1/1 | 0.79 | 0.32 | 1.70 | 60,60,60,60 | 0 |
| 84 | OHX | 1 | 3466 | 7/7 | 0.96 | 0.18 | 1.69 | 120,121,122,123 | 0 |
| 84 | OHX | AR | 3529 | 7/7 | 0.95 | 0.18 | 1.69 | 161,162,163,163 | 0 |
| 84 | OHX | AR | 3675 | 7/7 | 0.88 | 0.27 | 1.69 | 210,211,212,212 | 0 |
| 84 | OHX | AR | 3424 | 7/7 | 0.99 | 0.19 | 1.69 | 86,87,87,87 | 0 |
| 85 | MG | 1 | 3937 | 1/1 | 0.95 | 0.29 | 1.69 | 58,58,58,58 | 0 |
| 84 | OHX | A | 1901 | 7/7 | 0.99 | 0.21 | 1.69 | 101,101,102,102 | 0 |
| 84 | OHX | AG | 201 | 7/7 | 0.95 | 0.27 | 1.69 | 186,187,188,188 | 0 |
| 84 | OHX | AR | 3414 | 7/7 | 0.99 | 0.18 | 1.67 | 90,90,90,90 | 0 |
| 84 | OHX | A | 1908 | 7/7 | 0.98 | 0.16 | 1.67 | 111,111,113,114 | 0 |
| 84 | OHX | 1 | 3523 | 7/7 | 0.95 | 0.21 | 1.66 | 157,158,159,160 | 0 |
| 84 | OHX | AR | 3590 | 7/7 | 0.95 | 0.19 | 1.65 | 172,173,173,173 | 0 |
| 85 | MG | d9 | 102 | 1/1 | 0.93 | 0.45 | 1.65 | 106,106,106,106 | 0 |
| 85 | MG | AR | 4196 | 1/1 | 0.94 | 0.22 | 1.64 | 39,39,39,39 | 0 |
| 84 | OHX | 1 | 3690 | 7/7 | 0.96 | 0.28 | 1.63 | 174,175,176,176 | 0 |
| 84 | OHX | AR | 3404 | 7/7 | 0.99 | 0.19 | 1.61 | 88,89,89,89 | 0 |
| 85 | MG | AR | 3947 | 1/1 | 0.95 | 0.18 | 1.61 | 26,26,26,26 | 0 |
| 85 | MG | AR | 4141 | 1/1 | 0.89 | 0.23 | 1.61 | 53,53,53,53 | 0 |
| 84 | OHX | AR | 3505 | 7/7 | 0.95 | 0.17 | 1.59 | 138,140,141,141 | 0 |
| 85 | MG | 6 | 2122 | 1/1 | 0.96 | 0.18 | 1.56 | 48,48,48,48 | 0 |
| 84 | OHX | AR | 3582 | 7/7 | 0.94 | 0.21 | 1.55 | 166,167,167,168 | 0 |
| 84 | OHX | A | 1968 | 7/7 | 0.96 | 0.20 | 1.55 | 168,170,171,172 | 0 |
| 84 | OHX | AR | 3592 | 7/7 | 0.94 | 0.28 | 1.55 | 151,152,152,153 | 0 |
| 84 | OHX | 1 | 3410 | 7/7 | 0.99 | 0.20 | 1.54 | 88,88,88,88 | 0 |
| 84 | OHX | 1 | 3683 | 7/7 | 0.84 | 0.30 | 1.53 | 197,198,199,199 | 0 |
| 85 | MG | A | 2142 | 1/1 | 0.97 | 0.29 | 1.50 | 90,90,90,90 | 0 |
| 85 | MG | 1 | 4055 | 1/1 | 0.92 | 0.24 | 1.50 | 33,33,33,33 | 0 |
| 84 | OHX | 1 | 3656 | 7/7 | 0.91 | 0.26 | 1.49 | 229,230,231,231 | 0 |
| 84 | OHX | A | 2040 | 7/7 | 0.88 | 0.24 | 1.49 | 246,248,249,250 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 85 | MG | AR | 4157 | 1/1 | 0.99 | 0.22 | 1.49 | 29,29,29,29 | 0 |
| 84 | OHX | CG | 303 | 7/7 | 0.88 | 0.60 | 1.49 | 212,213,214,214 | 0 |
| 85 | MG | o | 301 | 1/1 | 0.94 | 0.25 | 1.45 | 39,39,39,39 | 0 |
| 85 | MG | 1 | 3746 | 1/1 | 0.82 | 0.27 | 1.45 | 59,59,59,59 | 0 |
| 84 | OHX | AR | 3503 | 7/7 | 0.97 | 0.33 | 1.44 | 152,153,154,154 | 0 |
| 84 | OHX | 6 | 2009 | 7/7 | 0.95 | 0.21 | 1.44 | 181,181,183,183 | 0 |
| 84 | OHX | 1 | 3553 | 7/7 | 0.93 | 0.22 | 1.43 | 184,185,186,186 | 0 |
| 84 | OHX | 1 | 3424 | 7/7 | 0.99 | 0.19 | 1.43 | 92,93,93,93 | 0 |
| 84 | OHX | AR | 3619 | 7/7 | 0.96 | 0.28 | 1.42 | 169,169,170,170 | 0 |
| 84 | OHX | 1 | 3638 | 7/7 | 0.88 | 0.22 | 1.42 | 245,246,247,248 | 0 |
| 84 | OHX | 6 | 2034 | 7/7 | 0.90 | 0.26 | 1.41 | 236,238,239,240 | 0 |
| 84 | OHX | 1 | 3655 | 7/7 | 0.93 | 0.20 | 1.41 | 203,204,205,205 | 0 |
| 84 | OHX | AR | 3484 | 7/7 | 0.97 | 0.20 | 1.40 | 133,134,135,135 | 0 |
| 84 | OHX | 6 | 1973 | 7/7 | 0.94 | 0.26 | 1.39 | 161,162,163,163 | 0 |
| 84 | OHX | d9 | 101 | 7/7 | 0.91 | 0.33 | 1.37 | 234,235,236,237 | 0 |
| 84 | OHX | 4 | 212 | 7/7 | 0.92 | 0.24 | 1.37 | 201,202,202,202 | 0 |
| 84 | OHX | 1 | 3571 | 7/7 | 0.98 | 0.27 | 1.37 | 144,145,145,146 | 0 |
| 84 | OHX | AR | 3654 | 7/7 | 0.98 | 0.20 | 1.35 | 161,162,163,164 | 0 |
| 85 | MG | AR | 3931 | 1/1 | 0.98 | 0.18 | 1.35 | 13,13,13,13 | 0 |
| 84 | OHX | 1 | 3694 | 7/7 | 0.75 | 0.29 | 1.34 | 251,252,254,254 | 0 |
| 85 | MG | A | 2062 | 1/1 | 0.92 | 0.29 | 1.34 | 48,48,48,48 | 0 |
| 85 | MG | AR | 3806 | 1/1 | 0.92 | 0.22 | 1.31 | 68,68,68,68 | 0 |
| 85 | MG | AR | 3745 | 1/1 | 0.97 | 0.19 | 1.31 | 32,32,32,32 | 0 |
| 84 | OHX | AR | 3530 | 7/7 | 0.94 | 0.20 | 1.30 | 147,148,148,148 | 0 |
| 84 | OHX | AT | 209 | 7/7 | 0.96 | 0.18 | 1.30 | 163,163,163,163 | 0 |
| 85 | MG | AR | 3755 | 1/1 | 0.94 | 0.18 | 1.30 | 34,34,34,34 | 0 |
| 85 | MG | 6 | 2140 | 1/1 | 0.93 | 0.22 | 1.28 | 46,46,46,46 | 0 |
| 85 | MG | 6 | 2098 | 1/1 | 0.96 | 0.23 | 1.27 | 38,38,38,38 | 0 |
| 85 | MG | 1 | 4165 | 1/1 | 0.98 | 0.19 | 1.27 | 38,38,38,38 | 0 |
| 84 | OHX | A | 1999 | 7/7 | 0.92 | 0.24 | 1.25 | 214,215,217,217 | 0 |
| 84 | OHX | 6 | 1995 | 7/7 | 0.94 | 0.18 | 1.21 | 171,173,174,175 | 0 |
| 85 | MG | 1 | 4084 | 1/1 | 0.92 | 0.21 | 1.19 | 44,44,44,44 | 0 |
| 84 | OHX | AR | 3523 | 7/7 | 0.97 | 0.23 | 1.17 | 175,176,176,177 | 0 |
| 84 | OHX | AR | 3688 | 7/7 | 0.90 | 0.28 | 1.17 | 199,200,201,201 | 0 |
| 84 | OHX | 1 | 3540 | 7/7 | 0.95 | 0.24 | 1.15 | 145,146,146,148 | 0 |
| 85 | MG | AF | 201 | 1/1 | 0.93 | 0.24 | 1.14 | 27,27,27,27 | 0 |
| 84 | OHX | AR | 3466 | 7/7 | 0.96 | 0.17 | 1.13 | 114,115,116,116 | 0 |
| 84 | OHX | x | 202 | 7/7 | 0.89 | 0.27 | 1.12 | 223,224,225,225 | 0 |
| 84 | OHX | A | 1902 | 7/7 | 0.99 | 0.16 | 1.11 | 96,97,97,97 | 0 |
| 85 | MG | 1 | 4189 | 1/1 | 0.98 | 0.22 | 1.08 | 48,48,48,48 | 0 |
| 85 | MG | 6 | 2092 | 1/1 | 0.86 | 0.30 | 1.08 | 45,45,45,45 | 0 |
| 84 | OHX | AC | 101 | 7/7 | 0.99 | 0.18 | 1.08 | 89,90,90,90 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | OHX | M | 201 | 7/7 | 0.93 | 0.33 | 1.07 | 202,204,205,206 | 0 |
| 84 | OHX | 1 | 3580 | 7/7 | 0.94 | 0.17 | 1.05 | 162,164,164,165 | 0 |
| 85 | MG | AB | 202 | 1/1 | 0.99 | 0.22 | 1.05 | 34,34,34,34 | 0 |
| 84 | OHX | 1 | 3611 | 7/7 | 0.94 | 0.23 | 1.04 | 184,185,185,186 | 0 |
| 84 | OHX | CE | 403 | 7/7 | 0.90 | 0.50 | 1.03 | 237,238,239,240 | 0 |
| 84 | OHX | 1 | 3539 | 7/7 | 0.95 | 0.20 | 1.03 | 169,169,170,170 | 0 |
| 84 | OHX | A | 2002 | 7/7 | 0.82 | 0.30 | 1.03 | 242,245,246,247 | 0 |
| 85 | MG | 1 | 3930 | 1/1 | 0.91 | 0.21 | 1.03 | 19,19,19,19 | 0 |
| 84 | OHX | 1 | 3706 | 7/7 | 0.95 | 0.17 | 1.02 | 144,145,146,146 | 0 |
| 84 | OHX | 6 | 1993 | 7/7 | 0.92 | 0.24 | 1.00 | 191,192,193,194 | 0 |
| 84 | OHX | 6 | 2043 | 7/7 | 0.86 | 0.32 | 0.99 | 196,196,198,198 | 0 |
| 84 | OHX | AR | 3673 | 7/7 | 0.94 | 0.20 | 0.96 | 179,180,180,180 | 0 |
| 85 | MG | A | 2095 | 1/1 | 0.91 | 0.18 | 0.95 | 94,94,94,94 | 0 |
| 84 | OHX | 6 | 2049 | 7/7 | 0.90 | 0.27 | 0.93 | 218,219,220,221 | 0 |
| 84 | OHX | AR | 3612 | 7/7 | 0.94 | 0.19 | 0.92 | 182,183,184,184 | 0 |
| 84 | OHX | AR | 3607 | 7/7 | 0.97 | 0.23 | 0.92 | 166,166,167,167 | 0 |
| 84 | OHX | AR | 3504 | 7/7 | 0.98 | 0.21 | 0.92 | 116,117,117,118 | 0 |
| 84 | OHX | 1 | 3640 | 7/7 | 0.93 | 0.19 | 0.91 | 194,195,196,196 | 0 |
| 84 | OHX | 1 | 3422 | 7/7 | 0.99 | 0.17 | 0.91 | 94,94,94,94 | 0 |
| 85 | MG | 6 | 2183 | 1/1 | 0.98 | 0.23 | 0.90 | 44,44,44,44 | 0 |
| 84 | OHX | AR | 3593 | 7/7 | 0.94 | 0.20 | 0.90 | 173,174,174,174 | 0 |
| 84 | OHX | 1 | 3510 | 7/7 | 0.98 | 0.22 | 0.90 | 148,148,149,149 | 0 |
| 84 | OHX | AR | 3547 | 7/7 | 0.95 | 0.20 | 0.89 | 147,147,147,148 | 0 |
| 85 | MG | 6 | 2109 | 1/1 | 0.97 | 0.24 | 0.89 | 39,39,39,39 | 0 |
| 84 | OHX | AR | 3698 | 7/7 | 0.97 | 0.20 | 0.86 | 166,167,167,168 | 0 |
| 86 | 7MB | 1 | 4216 | 20/20 | 0.94 | 0.20 | 0.84 | 48,48,48,48 | 0 |
| 84 | OHX | CV | 201 | 7/7 | 0.99 | 0.21 | 0.84 | 91,91,91,91 | 0 |
| 84 | OHX | 6 | 1909 | 7/7 | 0.99 | 0.16 | 0.84 | 103,104,104,104 | 0 |
| 85 | MG | z | 202 | 1/1 | 0.86 | 0.24 | 0.80 | 62,62,62,62 | 0 |
| 84 | OHX | A | 2042 | 7/7 | 0.83 | 0.17 | 0.80 | 240,242,244,245 | 0 |
| 84 | OHX | 1 | 3688 | 7/7 | 0.92 | 0.24 | 0.79 | 220,221,221,222 | 0 |
| 84 | OHX | A | 1958 | 7/7 | 0.94 | 0.18 | 0.79 | 206,207,210,210 | 0 |
| 84 | OHX | AR | 3514 | 7/7 | 0.96 | 0.26 | 0.78 | 146,147,147,148 | 0 |
| 84 | OHX | 1 | 3622 | 7/7 | 0.92 | 0.19 | 0.78 | 211,212,213,213 | 0 |
| 84 | OHX | AR | 3707 | 7/7 | 0.90 | 0.27 | 0.77 | 207,207,207,207 | 0 |
| 85 | MG | AR | 4068 | 1/1 | 0.96 | 0.18 | 0.77 | 25,25,25,25 | 0 |
| 84 | OHX | 1 | 3625 | 7/7 | 0.93 | 0.24 | 0.76 | 186,186,187,187 | 0 |
| 84 | OHX | 6 | 2039 | 7/7 | 0.92 | 0.18 | 0.76 | 204,204,206,206 | 0 |
| 85 | MG | 1 | 3848 | 1/1 | 0.99 | 0.20 | 0.76 | 26,26,26,26 | 0 |
| 84 | OHX | 1 | 3548 | 7/7 | 0.94 | 0.20 | 0.76 | 179,180,181,181 | 0 |
| 84 | OHX | 6 | 1932 | 7/7 | 0.94 | 0.21 | 0.74 | 129,129,131,131 | 0 |
| 85 | MG | 1 | 3755 | 1/1 | 0.95 | 0.21 | 0.74 | 41,41,41,41 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 85 | MG | AR | 4114 | 1/1 | 0.92 | 0.17 | 0.74 | 30,30,30,30 | 0 |
| 84 | OHX | AR | 3506 | 7/7 | 0.97 | 0.17 | 0.74 | 158,159,159,160 | 0 |
| 84 | OHX | AR | 3631 | 7/7 | 0.95 | 0.16 | 0.74 | 153,155,155,155 | 0 |
| 85 | MG | 4 | 225 | 1/1 | 0.98 | 0.18 | 0.72 | 43,43,43,43 | 0 |
| 84 | OHX | 1 | 3425 | 7/7 | 0.99 | 0.16 | 0.72 | 93,93,93,93 | 0 |
| 84 | OHX | 4 | 203 | 7/7 | 0.95 | 0.25 | 0.71 | 181,182,183,184 | 0 |
| 84 | OHX | AR | 3568 | 7/7 | 0.96 | 0.17 | 0.70 | 162,163,164,165 | 0 |
| 84 | OHX | 6 | 2056 | 7/7 | 0.89 | 0.22 | 0.70 | 214,215,217,218 | 0 |
| 84 | OHX | 6 | 1960 | 7/7 | 0.88 | 0.21 | 0.70 | 155,157,157,158 | 0 |
| 84 | OHX | 3 | 207 | 7/7 | 0.94 | 0.17 | 0.68 | 188,189,190,191 | 0 |
| 84 | OHX | 6 | 2011 | 7/7 | 0.90 | 0.21 | 0.68 | 205,205,207,207 | 0 |
| 84 | OHX | 1 | 3716 | 7/7 | 0.94 | 0.17 | 0.66 | 205,206,208,209 | 0 |
| 84 | OHX | 1 | 3527 | 7/7 | 0.97 | 0.18 | 0.66 | 138,139,140,140 | 0 |
| 84 | OHX | 1 | 3609 | 7/7 | 0.93 | 0.21 | 0.65 | 191,193,194,195 | 0 |
| 84 | OHX | AR | 3518 | 7/7 | 0.97 | 0.16 | 0.65 | 161,162,163,163 | 0 |
| 84 | OHX | 6 | 2052 | 7/7 | 0.90 | 0.25 | 0.65 | 244,244,246,246 | 0 |
| 84 | OHX | l | 401 | 7/7 | 0.93 | 0.38 | 0.64 | 208,209,210,210 | 0 |
| 84 | OHX | AR | 3556 | 7/7 | 0.94 | 0.19 | 0.61 | 138,139,140,140 | 0 |
| 84 | OHX | A | 1991 | 7/7 | 0.92 | 0.21 | 0.60 | 218,220,221,221 | 0 |
| 84 | OHX | AR | 3408 | 7/7 | 0.99 | 0.22 | 0.59 | 83,83,83,83 | 0 |
| 85 | MG | 1 | 3825 | 1/1 | 0.98 | 0.17 | 0.59 | 42,42,42,42 | 0 |
| 84 | OHX | k | 401 | 7/7 | 0.97 | 0.24 | 0.59 | 169,170,170,170 | 0 |
| 84 | OHX | AR | 3736 | 7/7 | 0.90 | 0.17 | 0.58 | 184,185,186,187 | 0 |
| 84 | OHX | 1 | 3695 | 7/7 | 0.90 | 0.23 | 0.57 | 200,201,202,202 | 0 |
| 84 | OHX | 6 | 2026 | 7/7 | 0.93 | 0.21 | 0.56 | 218,219,220,222 | 0 |
| 84 | OHX | 1 | 3621 | 7/7 | 0.92 | 0.24 | 0.55 | 221,223,224,224 | 0 |
| 85 | MG | DI | 202 | 1/1 | 0.90 | 0.26 | 0.55 | 32,32,32,32 | 0 |
| 84 | OHX | A | 2015 | 7/7 | 0.84 | 0.35 | 0.54 | 248,250,254,254 | 0 |
| 85 | MG | 6 | 2177 | 1/1 | 0.94 | 0.24 | 0.53 | 25,25,25,25 | 0 |
| 85 | MG | AB | 203 | 1/1 | 0.83 | 0.31 | 0.50 | 37,37,37,37 | 0 |
| 84 | OHX | H | 301 | 7/7 | 0.73 | 0.32 | 0.48 | 231,233,235,235 | 0 |
| 84 | OHX | 6 | 1906 | 7/7 | 0.99 | 0.19 | 0.47 | 94,94,95,95 | 0 |
| 84 | OHX | AR | 3622 | 7/7 | 0.94 | 0.29 | 0.47 | 203,203,204,205 | 0 |
| 84 | OHX | AR | 3618 | 7/7 | 0.94 | 0.19 | 0.47 | 195,196,196,196 | 0 |
| 84 | OHX | 6 | 1941 | 7/7 | 0.94 | 0.17 | 0.47 | 158,159,160,161 | 0 |
| 84 | OHX | AR | 3667 | 7/7 | 0.94 | 0.23 | 0.46 | 207,209,210,210 | 0 |
| 84 | OHX | 1 | 3577 | 7/7 | 0.97 | 0.25 | 0.46 | 177,178,179,179 | 0 |
| 85 | MG | AR | 4047 | 1/1 | 0.89 | 0.21 | 0.45 | 30,30,30,30 | 0 |
| 84 | OHX | AR | 3697 | 7/7 | 0.98 | 0.22 | 0.45 | 115,116,116,116 | 0 |
| 84 | OHX | 1 | 3503 | 7/7 | 0.97 | 0.18 | 0.44 | 145,146,147,148 | 0 |
| 84 | OHX | AR | 3538 | 7/7 | 0.96 | 0.20 | 0.44 | 184,185,186,186 | 0 |
| 85 | MG | AR | 3959 | 1/1 | 0.94 | 0.22 | 0.43 | 32,32,32,32 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | OHX | AR | 3565 | 7/7 | 0.94 | 0.16 | 0.43 | 161,162,163,164 | 0 |
| 84 | OHX | 6 | 1940 | 7/7 | 0.96 | 0.15 | 0.43 | 149,151,152,153 | 0 |
| 84 | OHX | AR | 3567 | 7/7 | 0.95 | 0.16 | 0.41 | 159,159,160,160 | 0 |
| 84 | OHX | AR | 3564 | 7/7 | 0.94 | 0.18 | 0.40 | 189,190,190,190 | 0 |
| 84 | OHX | A | 1918 | 7/7 | 0.97 | 0.17 | 0.40 | 120,122,123,123 | 0 |
| 85 | MG | AR | 3974 | 1/1 | 0.93 | 0.25 | 0.39 | 28,28,28,28 | 0 |
| 85 | MG | CD | 301 | 1/1 | 0.96 | 0.21 | 0.39 | 28,28,28,28 | 0 |
| 84 | OHX | A | 2016 | 7/7 | 0.91 | 0.19 | 0.39 | 207,209,210,211 | 0 |
| 84 | OHX | A | 2028 | 7/7 | 0.93 | 0.23 | 0.38 | 252,254,254,256 | 0 |
| 85 | MG | A | 2082 | 1/1 | 0.96 | 0.19 | 0.37 | 65,65,65,65 | 0 |
| 84 | OHX | AR | 3555 | 7/7 | 0.95 | 0.18 | 0.36 | 148,149,149,150 | 0 |
| 85 | MG | AR | 4076 | 1/1 | 0.96 | 0.16 | 0.36 | 38,38,38,38 | 0 |
| 84 | OHX | 1 | 3642 | 7/7 | 0.92 | 0.21 | 0.34 | 193,193,195,195 | 0 |
| 84 | OHX | AR | 3549 | 7/7 | 0.96 | 0.19 | 0.33 | 156,157,158,158 | 0 |
| 84 | OHX | AT | 216 | 7/7 | 0.91 | 0.17 | 0.32 | 193,193,193,193 | 0 |
| 84 | OHX | A | 2004 | 7/7 | 0.95 | 0.22 | 0.31 | 192,194,196,196 | 0 |
| 84 | OHX | 1 | 3723 | 7/7 | 0.93 | 0.19 | 0.29 | 201,202,203,204 | 0 |
| 85 | MG | AT | 225 | 1/1 | 0.92 | 0.17 | 0.28 | 60,60,60,60 | 0 |
| 84 | OHX | 6 | 2013 | 7/7 | 0.97 | 0.20 | 0.27 | 149,151,152,153 | 0 |
| 84 | OHX | A | 1976 | 7/7 | 0.96 | 0.16 | 0.27 | 165,166,167,168 | 0 |
| 84 | OHX | AR | 3546 | 7/7 | 0.95 | 0.17 | 0.25 | 140,140,141,141 | 0 |
| 85 | MG | AR | 3743 | 1/1 | 0.85 | 0.18 | 0.24 | 41,41,41,41 | 0 |
| 84 | OHX | 6 | 1945 | 7/7 | 0.97 | 0.16 | 0.23 | 149,150,151,152 | 0 |
| 84 | OHX | A | 1953 | 7/7 | 0.96 | 0.18 | 0.23 | 180,182,184,184 | 0 |
| 84 | OHX | A | 2023 | 7/7 | 0.90 | 0.23 | 0.23 | 202,204,206,206 | 0 |
| 85 | MG | 1 | 3820 | 1/1 | 0.92 | 0.26 | 0.22 | 30,30,30,30 | 0 |
| 84 | OHX | CL | 302 | 7/7 | 0.83 | 0.24 | 0.21 | 200,201,201,202 | 0 |
| 84 | OHX | AR | 3709 | 7/7 | 0.95 | 0.18 | 0.20 | 163,163,164,164 | 0 |
| 84 | OHX | 1 | 3517 | 7/7 | 0.96 | 0.17 | 0.20 | 141,142,143,143 | 0 |
| 84 | OHX | 1 | 3557 | 7/7 | 0.91 | 0.20 | 0.19 | 186,187,188,188 | 0 |
| 85 | MG | AR | 3776 | 1/1 | 0.95 | 0.17 | 0.19 | 32,32,32,32 | 0 |
| 85 | MG | AR | 4008 | 1/1 | 0.96 | 0.16 | 0.17 | 33,33,33,33 | 0 |
| 84 | OHX | AR | 3455 | 7/7 | 0.98 | 0.17 | 0.16 | 106,107,108,108 | 0 |
| 84 | OHX | A | 1921 | 7/7 | 0.97 | 0.17 | 0.14 | 139,141,143,143 | 0 |
| 85 | MG | DC | 202 | 1/1 | 0.93 | 0.21 | 0.14 | 28,28,28,28 | 0 |
| 84 | OHX | AR | 3542 | 7/7 | 0.99 | 0.19 | 0.14 | 133,134,134,134 | 0 |
| 84 | OHX | A | 1940 | 7/7 | 0.97 | 0.16 | 0.13 | 174,175,177,178 | 0 |
| 84 | OHX | 6 | 2024 | 7/7 | 0.93 | 0.18 | 0.12 | 207,208,210,211 | 0 |
| 84 | OHX | 1 | 3475 | 7/7 | 0.96 | 0.17 | 0.12 | 128,129,130,130 | 0 |
| 84 | OHX | CK | 201 | 7/7 | 0.94 | 0.24 | 0.12 | 185,185,186,187 | 0 |
| 84 | OHX | AR | 3621 | 7/7 | 0.92 | 0.22 | 0.12 | 208,209,210,211 | 0 |
| 84 | OHX | AR | 3520 | 7/7 | 0.89 | 0.20 | 0.11 | 175,175,176,176 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 84 | OHX | 6 | 1984 | 7/7 | 0.97 | 0.19 | 0.10 | 198,200,201,201 | 0 |
| 84 | OHX | AR | 3463 | 7/7 | 0.97 | 0.18 | 0.10 | 114,114,115,115 | 0 |
| 84 | OHX | 1 | 3419 | 7/7 | 0.99 | 0.19 | 0.10 | 93,93,93,93 | 0 |
| 84 | OHX | AR | 3405 | 7/7 | 0.99 | 0.23 | 0.09 | 94,94,94,94 | 0 |
| 85 | MG | AR | 3825 | 1/1 | 0.96 | 0.18 | 0.09 | 30,30,30,30 | 0 |
| 84 | OHX | 1 | 3643 | 7/7 | 0.96 | 0.14 | 0.09 | 192,193,194,194 | 0 |
| 84 | OHX | AR | 3411 | 7/7 | 0.99 | 0.20 | 0.08 | 83,83,83,83 | 0 |
| 84 | OHX | A | 2029 | 7/7 | 0.86 | 0.14 | 0.08 | 261,263,265,265 | 0 |
| 84 | OHX | AR | 3439 | 7/7 | 0.99 | 0.15 | 0.06 | 91,91,92,92 | 0 |
| 84 | OHX | A | 1941 | 7/7 | 0.96 | 0.17 | 0.06 | 195,197,198,198 | 0 |
| 84 | OHX | e | 101 | 7/7 | 0.97 | 0.22 | 0.05 | 205,208,210,210 | 0 |
| 84 | OHX | 6 | 1994 | 7/7 | 0.95 | 0.26 | 0.04 | 168,169,171,171 | 0 |
| 84 | OHX | A | 1965 | 7/7 | 0.98 | 0.19 | 0.04 | 167,169,170,171 | 0 |
| 84 | OHX | 6 | 1962 | 7/7 | 0.94 | 0.21 | 0.03 | 187,188,189,190 | 0 |
| 84 | OHX | 1 | 3574 | 7/7 | 0.97 | 0.20 | 0.01 | 138,139,140,140 | 0 |
| 84 | OHX | 1 | 3427 | 7/7 | 0.99 | 0.15 | 0.00 | 87,87,87,87 | 0 |
| 84 | OHX | 6 | 2025 | 7/7 | 0.84 | 0.20 | -0.01 | 248,249,250,252 | 0 |
| 84 | OHX | 1 | 3531 | 7/7 | 0.94 | 0.17 | -0.02 | 179,180,181,181 | 0 |
| 85 | MG | AR | 3753 | 1/1 | 0.90 | 0.16 | -0.03 | 51,51,51,51 | 0 |
| 84 | OHX | 6 | 1904 | 7/7 | 1.00 | 0.15 | -0.04 | 96,96,96,96 | 0 |
| 84 | OHX | 6 | 1968 | 7/7 | 0.97 | 0.17 | -0.05 | 145,146,147,148 | 0 |
| 84 | OHX | 1 | 3404 | 7/7 | 0.99 | 0.20 | -0.05 | 93,93,93,93 | 0 |
| 84 | OHX | AR | 3477 | 7/7 | 0.96 | 0.18 | -0.05 | 119,119,119,120 | 0 |
| 84 | OHX | AR | 3580 | 7/7 | 0.98 | 0.18 | -0.06 | 139,139,140,140 | 0 |
| 84 | OHX | 1 | 3545 | 7/7 | 0.95 | 0.18 | -0.07 | 156,157,158,159 | 0 |
| 84 | OHX | 6 | 1955 | 7/7 | 0.92 | 0.16 | -0.08 | 191,193,195,196 | 0 |
| 85 | MG | AR | 4065 | 1/1 | 0.95 | 0.17 | -0.09 | 54,54,54,54 | 0 |
| 85 | MG | o | 302 | 1/1 | 0.96 | 0.23 | -0.09 | 27,27,27,27 | 0 |
| 84 | OHX | 1 | 3507 | 7/7 | 0.96 | 0.17 | -0.09 | 149,149,150,150 | 0 |
| 84 | OHX | AT | 206 | 7/7 | 0.96 | 0.17 | -0.10 | 155,155,156,156 | 0 |
| 84 | OHX | A | 1998 | 7/7 | 0.95 | 0.19 | -0.11 | 213,217,219,219 | 0 |
| 85 | MG | 1 | 4137 | 1/1 | 0.99 | 0.20 | -0.11 | 38,38,38,38 | 0 |
| 84 | OHX | AT | 214 | 7/7 | 0.94 | 0.25 | -0.11 | 173,173,174,174 | 0 |
| 84 | OHX | A | 1950 | 7/7 | 0.97 | 0.17 | -0.12 | 168,169,170,171 | 0 |
| 84 | OHX | AR | 3693 | 7/7 | 0.90 | 0.28 | -0.12 | 238,239,240,240 | 0 |
| 84 | OHX | AR | 3583 | 7/7 | 0.97 | 0.18 | -0.13 | 148,149,150,150 | 0 |
| 84 | OHX | A | 2018 | 7/7 | 0.95 | 0.16 | -0.14 | 214,215,216,217 | 0 |
| 85 | MG | A | 2150 | 1/1 | 0.94 | 0.17 | -0.14 | 52,52,52,52 | 0 |
| 84 | OHX | 1 | 3582 | 7/7 | 0.97 | 0.20 | -0.15 | 152,153,154,155 | 0 |
| 84 | OHX | AR | 3563 | 7/7 | 0.96 | 0.17 | -0.15 | 173,173,174,174 | 0 |
| 85 | MG | AR | 3762 | 1/1 | 0.88 | 0.19 | -0.15 | 40,40,40,40 | 0 |
| 84 | OHX | 6 | 1977 | 7/7 | 0.93 | 0.15 | -0.16 | 193,194,196,196 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 84 | OHX | 6 | 2000 | 7/7 | 0.92 | 0.16 | -0.16 | 210,211,212,213 | 0 |
| 85 | MG | 1 | 3810 | 1/1 | 0.93 | 0.23 | -0.16 | 86,86,86,86 | 0 |
| 84 | OHX | 6 | 1974 | 7/7 | 0.93 | 0.20 | -0.17 | 176,176,178,178 | 0 |
| 85 | MG | 1 | 3815 | 1/1 | 0.97 | 0.18 | -0.19 | 40,40,40,40 | 0 |
| 84 | OHX | A | 1979 | 7/7 | 0.96 | 0.15 | -0.19 | 200,203,204,205 | 0 |
| 85 | MG | DA | 201 | 1/1 | 0.86 | 0.20 | -0.19 | 29,29,29,29 | 0 |
| 84 | OHX | 1 | 3461 | 7/7 | 0.94 | 0.17 | -0.22 | 136,137,137,138 | 0 |
| 84 | OHX | A | 1971 | 7/7 | 0.85 | 0.17 | -0.22 | 216,218,220,221 | 0 |
| 84 | OHX | A | 1905 | 7/7 | 0.99 | 0.18 | -0.22 | 102,102,103,103 | 0 |
| 85 | MG | 1 | 4034 | 1/1 | 0.77 | 0.16 | -0.23 | 33,33,33,33 | 0 |
| 84 | OHX | 1 | 3511 | 7/7 | 0.94 | 0.16 | -0.23 | 166,167,168,168 | 0 |
| 84 | OHX | AR | 3595 | 7/7 | 0.97 | 0.20 | -0.26 | 160,161,161,162 | 0 |
| 85 | MG | A | 2144 | 1/1 | 0.97 | 0.24 | -0.27 | 49,49,49,49 | 0 |
| 85 | MG | A | 2152 | 1/1 | 0.91 | 0.17 | -0.27 | 78,78,78,78 | 0 |
| 84 | OHX | DD | 102 | 7/7 | 0.99 | 0.17 | -0.29 | 88,89,89,89 | 0 |
| 84 | OHX | A | 2033 | 7/7 | 0.95 | 0.19 | -0.29 | 210,212,214,214 | 0 |
| 85 | MG | 6 | 2198 | 1/1 | 0.95 | 0.19 | -0.30 | 53,53,53,53 | 0 |
| 84 | OHX | 1 | 3551 | 7/7 | 0.92 | 0.16 | -0.32 | 191,192,192,193 | 0 |
| 84 | OHX | A | 1959 | 7/7 | 0.90 | 0.15 | -0.32 | 180,182,183,184 | 0 |
| 84 | OHX | AE | 201 | 7/7 | 0.89 | 0.20 | -0.34 | 194,195,195,196 | 0 |
| 85 | MG | 6 | 2120 | 1/1 | 0.90 | 0.17 | -0.34 | 61,61,61,61 | 0 |
| 84 | OHX | 6 | 1985 | 7/7 | 0.94 | 0.16 | -0.35 | 191,193,194,195 | 0 |
| 84 | OHX | 1 | 3485 | 7/7 | 0.97 | 0.19 | -0.35 | 151,152,153,153 | 0 |
| 84 | OHX | k | 402 | 7/7 | 0.95 | 0.20 | -0.35 | 156,157,158,158 | 0 |
| 84 | OHX | 1 | 3590 | 7/7 | 0.97 | 0.18 | -0.36 | 208,209,210,211 | 0 |
| 84 | OHX | A | 1977 | 7/7 | 0.94 | 0.17 | -0.36 | 202,205,207,207 | 0 |
| 85 | MG | s6 | 301 | 1/1 | 0.95 | 0.27 | -0.36 | 64,64,64,64 | 0 |
| 85 | MG | 6 | 2161 | 1/1 | 0.95 | 0.17 | -0.36 | 51,51,51,51 | 0 |
| 85 | MG | 1 | 3910 | 1/1 | 0.95 | 0.20 | -0.37 | 30,30,30,30 | 0 |
| 84 | OHX | AR | 3417 | 7/7 | 0.99 | 0.15 | -0.37 | 86,86,86,86 | 0 |
| 84 | OHX | 1 | 3526 | 7/7 | 0.95 | 0.13 | -0.38 | 167,168,169,170 | 0 |
| 85 | MG | 1 | 4157 | 1/1 | 0.92 | 0.21 | -0.39 | 37,37,37,37 | 0 |
| 84 | OHX | 1 | 3430 | 7/7 | 0.99 | 0.14 | -0.39 | 97,97,97,98 | 0 |
| 84 | OHX | A | 2001 | 7/7 | 0.94 | 0.18 | -0.40 | 185,188,189,189 | 0 |
| 84 | OHX | 6 | 2002 | 7/7 | 0.92 | 0.19 | -0.40 | 218,220,221,221 | 0 |
| 84 | OHX | 1 | 3496 | 7/7 | 0.97 | 0.18 | -0.41 | 115,116,117,117 | 0 |
| 84 | OHX | AR | 3536 | 7/7 | 0.97 | 0.17 | -0.41 | 141,141,142,142 | 0 |
| 84 | OHX | AR | 3515 | 7/7 | 0.97 | 0.16 | -0.42 | 159,160,161,162 | 0 |
| 84 | OHX | 1 | 3550 | 7/7 | 0.94 | 0.15 | -0.43 | 196,197,198,199 | 0 |
| 84 | OHX | 1 | 3458 | 7/7 | 0.96 | 0.14 | -0.44 | 131,132,133,133 | 0 |
| 85 | MG | CP | 503 | 1/1 | 0.94 | 0.25 | -0.44 | 95,95,95,95 | 0 |
| 84 | OHX | 1 | 3714 | 7/7 | 0.93 | 0.18 | -0.44 | 155,156,157,158 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 84 | OHX | 1 | 3509 | 7/7 | 0.98 | 0.18 | -0.44 | 155,155,157,157 | 0 |
| 84 | OHX | c5 | 201 | 7/7 | 0.85 | 0.32 | -0.45 | 228,229,230,231 | 0 |
| 84 | OHX | 1 | 3534 | 7/7 | 0.95 | 0.18 | -0.46 | 148,149,149,150 | 0 |
| 86 | 7MB | AR | 4239 | 20/20 | 0.97 | 0.19 | -0.47 | 44,44,44,44 | 0 |
| 85 | MG | 1 | 4052 | 1/1 | 0.85 | 0.12 | -0.48 | 48,48,48,48 | 0 |
| 84 | OHX | 6 | 2057 | 7/7 | 0.84 | 0.18 | -0.48 | 247,247,250,250 | 0 |
| 85 | MG | 1 | 4091 | 1/1 | 0.95 | 0.15 | -0.48 | 49,49,49,49 | 0 |
| 87 | ZN | d7 | 101 | 1/1 | 0.95 | 0.28 | -0.49 | 176,176,176,176 | 0 |
| 84 | OHX | 1 | 3588 | 7/7 | 0.97 | 0.16 | -0.50 | 168,169,170,170 | 0 |
| 84 | OHX | AR | 3533 | 7/7 | 0.95 | 0.15 | -0.50 | 166,166,167,167 | 0 |
| 84 | OHX | AR | 3570 | 7/7 | 0.95 | 0.17 | -0.51 | 161,162,163,163 | 0 |
| 84 | OHX | 6 | 1970 | 7/7 | 0.98 | 0.19 | -0.52 | 178,179,180,180 | 0 |
| 84 | OHX | AR | 3433 | 7/7 | 0.98 | 0.17 | -0.52 | 94,94,94,95 | 0 |
| 85 | MG | 1 | 4124 | 1/1 | 0.67 | 0.23 | -0.53 | 52,52,52,52 | 0 |
| 84 | OHX | AR | 3474 | 7/7 | 0.97 | 0.15 | -0.54 | 119,120,121,121 | 0 |
| 85 | MG | AR | 3824 | 1/1 | 0.94 | 0.14 | -0.54 | 62,62,62,62 | 0 |
| 84 | OHX | 1 | 3586 | 7/7 | 0.96 | 0.17 | -0.55 | 182,183,185,186 | 0 |
| 84 | OHX | DG | 201 | 7/7 | 0.98 | 0.16 | -0.55 | 132,133,133,134 | 0 |
| 84 | OHX | AR | 3681 | 7/7 | 0.89 | 0.21 | -0.56 | 198,199,200,201 | 0 |
| 84 | OHX | A | 1909 | 7/7 | 0.98 | 0.13 | -0.57 | 124,125,128,129 | 0 |
| 84 | OHX | s8 | 301 | 7/7 | 0.95 | 0.32 | -0.57 | 214,216,216,218 | 0 |
| 84 | OHX | A | 2027 | 7/7 | 0.93 | 0.18 | -0.58 | 236,239,240,241 | 0 |
| 84 | OHX | AR | 3416 | 7/7 | 0.99 | 0.17 | -0.58 | 88,88,88,89 | 0 |
| 84 | OHX | 1 | 3558 | 7/7 | 0.96 | 0.19 | -0.59 | 166,167,168,168 | 0 |
| 84 | OHX | 1 | 3597 | 7/7 | 0.89 | 0.13 | -0.60 | 237,238,240,240 | 0 |
| 84 | OHX | 1 | 3488 | 7/7 | 0.97 | 0.14 | -0.60 | 140,140,141,141 | 0 |
| 84 | OHX | AR | 3532 | 7/7 | 0.98 | 0.17 | -0.60 | 129,130,130,131 | 0 |
| 84 | OHX | CP | 501 | 7/7 | 0.95 | 0.22 | -0.62 | 177,178,178,178 | 0 |
| 84 | OHX | AR | 3473 | 7/7 | 0.95 | 0.16 | -0.62 | 121,122,122,122 | 0 |
| 84 | OHX | 1 | 3445 | 7/7 | 0.98 | 0.14 | -0.62 | 95,95,95,96 | 0 |
| 84 | OHX | A | 1932 | 7/7 | 0.94 | 0.17 | -0.62 | 178,180,182,182 | 0 |
| 84 | OHX | 1 | 3482 | 7/7 | 0.97 | 0.14 | -0.62 | 116,116,117,117 | 0 |
| 84 | OHX | AR | 3489 | 7/7 | 0.97 | 0.12 | -0.62 | 149,150,151,152 | 0 |
| 84 | OHX | 1 | 3678 | 7/7 | 0.87 | 0.17 | -0.62 | 228,228,229,230 | 0 |
| 84 | OHX | 1 | 3568 | 7/7 | 0.93 | 0.20 | -0.63 | 195,196,196,197 | 0 |
| 84 | OHX | AR | 3422 | 7/7 | 0.99 | 0.15 | -0.64 | 86,86,86,86 | 0 |
| 84 | OHX | 1 | 3473 | 7/7 | 0.98 | 0.12 | -0.65 | 119,120,121,121 | 0 |
| 85 | MG | 6 | 2127 | 1/1 | 0.92 | 0.17 | -0.65 | 52,52,52,52 | 0 |
| 84 | OHX | A | 1945 | 7/7 | 0.95 | 0.16 | -0.65 | 201,203,204,205 | 0 |
| 84 | OHX | AR | 3475 | 7/7 | 0.97 | 0.17 | -0.66 | 114,115,115,116 | 0 |
| 84 | OHX | AR | 3723 | 7/7 | 0.90 | 0.19 | -0.67 | 240,241,242,242 | 0 |
| 84 | OHX | A | 1973 | 7/7 | 0.96 | 0.15 | -0.67 | 201,204,206,208 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 84 | OHX | r | 301 | 7/7 | 0.91 | 0.19 | -0.67 | 167,168,168,169 | 0 |
| 84 | OHX | 1 | 3518 | 7/7 | 0.97 | 0.17 | -0.67 | 134,135,135,136 | 0 |
| 84 | OHX | 6 | 2017 | 7/7 | 0.97 | 0.19 | -0.67 | 158,159,160,161 | 0 |
| 87 | ZN | AP | 501 | 1/1 | 0.97 | 0.26 | -0.68 | 115,115,115,115 | 0 |
| 84 | OHX | 1 | 3521 | 7/7 | 0.95 | 0.16 | -0.68 | 144,145,147,147 | 0 |
| 84 | OHX | AR | 3669 | 7/7 | 0.85 | 0.16 | -0.68 | 245,246,247,248 | 0 |
| 84 | OHX | 1 | 3501 | 7/7 | 0.96 | 0.16 | -0.69 | 123,124,125,125 | 0 |
| 84 | OHX | 6 | 2053 | 7/7 | 0.84 | 0.22 | -0.69 | 250,252,253,254 | 0 |
| 84 | OHX | 1 | 3541 | 7/7 | 0.97 | 0.12 | -0.69 | 154,155,156,156 | 0 |
| 84 | OHX | 6 | 2004 | 7/7 | 0.93 | 0.17 | -0.70 | 193,194,195,196 | 0 |
| 84 | OHX | A | 2010 | 7/7 | 0.95 | 0.14 | -0.70 | 192,195,197,197 | 0 |
| 85 | MG | 1 | 4057 | 1/1 | 0.97 | 0.17 | -0.70 | 30,30,30,30 | 0 |
| 84 | OHX | AR | 3507 | 7/7 | 0.98 | 0.17 | -0.71 | 136,136,137,137 | 0 |
| 84 | OHX | 1 | 3416 | 7/7 | 0.99 | 0.15 | -0.71 | 86,86,86,86 | 0 |
| 84 | OHX | 1 | 3413 | 7/7 | 0.99 | 0.18 | -0.72 | 88,88,89,89 | 0 |
| 84 | OHX | A | 1936 | 7/7 | 0.95 | 0.15 | -0.72 | 160,162,163,163 | 0 |
| 85 | MG | 1 | 4172 | 1/1 | 0.96 | 0.16 | -0.73 | 76,76,76,76 | 0 |
| 84 | OHX | 6 | 2003 | 7/7 | 0.96 | 0.18 | -0.74 | 180,182,183,184 | 0 |
| 84 | OHX | 1 | 3426 | 7/7 | 0.99 | 0.15 | -0.74 | 93,93,93,94 | 0 |
| 84 | OHX | A | 1946 | 7/7 | 0.88 | 0.17 | -0.76 | 212,214,216,217 | 0 |
| 84 | OHX | 1 | 3576 | 7/7 | 0.96 | 0.15 | -0.76 | 189,189,191,191 | 0 |
| 84 | OHX | CG | 302 | 7/7 | 0.85 | 0.24 | -0.77 | 210,211,212,213 | 0 |
| 84 | OHX | AS | 201 | 7/7 | 0.98 | 0.16 | -0.77 | 98,99,100,101 | 0 |
| 84 | OHX | AR | 3441 | 7/7 | 0.98 | 0.14 | -0.77 | 109,110,110,111 | 0 |
| 84 | OHX | AR | 3483 | 7/7 | 0.99 | 0.16 | -0.78 | 124,125,125,126 | 0 |
| 85 | MG | AR | 4145 | 1/1 | 0.93 | 0.14 | -0.79 | 38,38,38,38 | 0 |
| 84 | OHX | AS | 206 | 7/7 | 0.97 | 0.14 | -0.79 | 146,146,148,148 | 0 |
| 84 | OHX | 6 | 1919 | 7/7 | 0.97 | 0.14 | -0.79 | 112,113,114,114 | 0 |
| 84 | OHX | 1 | 3418 | 7/7 | 0.99 | 0.13 | -0.79 | 85,85,85,85 | 0 |
| 84 | OHX | 1 | 3414 | 7/7 | 0.99 | 0.17 | -0.80 | 90,90,90,90 | 0 |
| 84 | OHX | 1 | 3462 | 7/7 | 0.96 | 0.16 | -0.80 | 115,116,117,118 | 0 |
| 84 | OHX | 6 | 1929 | 7/7 | 0.98 | 0.14 | -0.83 | 147,148,151,152 | 0 |
| 84 | OHX | 1 | 3474 | 7/7 | 0.98 | 0.14 | -0.84 | 131,132,133,133 | 0 |
| 84 | OHX | 1 | 3435 | 7/7 | 0.98 | 0.15 | -0.85 | 103,104,105,105 | 0 |
| 84 | OHX | 1 | 3627 | 7/7 | 0.95 | 0.15 | -0.86 | 176,176,178,179 | 0 |
| 85 | MG | 6 | 2111 | 1/1 | 0.93 | 0.16 | -0.86 | 42,42,42,42 | 0 |
| 85 | MG | 1 | 4087 | 1/1 | 0.97 | 0.13 | -0.86 | 37,37,37,37 | 0 |
| 84 | OHX | 6 | 1908 | 7/7 | 0.99 | 0.16 | -0.87 | 91,91,91,91 | 0 |
| 84 | OHX | 6 | 1987 | 7/7 | 0.96 | 0.15 | -0.87 | 179,179,180,181 | 0 |
| 84 | OHX | 1 | 3533 | 7/7 | 0.96 | 0.19 | -0.88 | 196,197,198,199 | 0 |
| 84 | OHX | AR | 3517 | 7/7 | 0.95 | 0.15 | -0.88 | 134,135,135,136 | 0 |
| 84 | OHX | AR | 3540 | 7/7 | 0.96 | 0.16 | -0.89 | 151,152,153,154 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 85 | MG | 1 | 3765 | 1/1 | 0.93 | 0.13 | -0.89 | 41,41,41,41 | 0 |
| 84 | OHX | AR | 3418 | 7/7 | 0.99 | 0.14 | -0.91 | 92,92,93,93 | 0 |
| 84 | OHX | 6 | 1911 | 7/7 | 0.99 | 0.15 | -0.92 | 99,100,100,100 | 0 |
| 84 | OHX | AT | 207 | 7/7 | 0.97 | 0.10 | -0.92 | 162,163,164,164 | 0 |
| 84 | OHX | AR | 3458 | 7/7 | 0.99 | 0.12 | -0.94 | 100,101,101,102 | 0 |
| 84 | OHX | A | 1987 | 7/7 | 0.97 | 0.14 | -0.94 | 172,173,174,175 | 0 |
| 85 | MG | AR | 4058 | 1/1 | 0.82 | 0.18 | -0.95 | 57,57,57,57 | 0 |
| 84 | OHX | CX | 201 | 7/7 | 0.98 | 0.17 | -0.95 | 121,122,123,124 | 0 |
| 87 | ZN | d9 | 103 | 1/1 | 0.98 | 0.10 | -0.95 | 86,86,86,86 | 0 |
| 84 | OHX | 1 | 3470 | 7/7 | 0.96 | 0.13 | -0.96 | 141,142,143,143 | 0 |
| 84 | OHX | 1 | 3444 | 7/7 | 0.98 | 0.16 | -0.96 | 103,104,104,105 | 0 |
| 84 | OHX | 1 | 3593 | 7/7 | 0.95 | 0.15 | -0.96 | 206,207,208,209 | 0 |
| 84 | OHX | AT | 212 | 7/7 | 0.96 | 0.16 | -0.97 | 160,160,161,161 | 0 |
| 84 | OHX | 1 | 3493 | 7/7 | 0.98 | 0.16 | -0.99 | 147,148,148,149 | 0 |
| 84 | OHX | A | 2020 | 7/7 | 0.95 | 0.17 | -0.99 | 188,191,192,192 | 0 |
| 84 | OHX | A | 1972 | 7/7 | 0.97 | 0.13 | -0.99 | 195,196,198,199 | 0 |
| 85 | MG | AR | 3951 | 1/1 | 0.90 | 0.16 | -1.00 | 26,26,26,26 | 0 |
| 84 | OHX | AR | 3614 | 7/7 | 0.97 | 0.15 | -1.00 | 164,165,165,166 | 0 |
| 84 | OHX | A | 1926 | 7/7 | 0.98 | 0.11 | -1.00 | 149,150,151,152 | 0 |
| 84 | OHX | AR | 3440 | 7/7 | 0.99 | 0.12 | -1.00 | 98,98,98,99 | 0 |
| 85 | MG | A | 2064 | 1/1 | 0.97 | 0.15 | -1.00 | 49,49,49,49 | 0 |
| 84 | OHX | 6 | 1924 | 7/7 | 0.98 | 0.12 | -1.01 | 123,124,126,127 | 0 |
| 84 | OHX | 6 | 1913 | 7/7 | 0.99 | 0.13 | -1.02 | 105,105,106,107 | 0 |
| 84 | OHX | AR | 3442 | 7/7 | 0.98 | 0.15 | -1.02 | 110,111,111,111 | 0 |
| 84 | OHX | AR | 3559 | 7/7 | 0.95 | 0.14 | -1.02 | 177,178,179,179 | 0 |
| 84 | OHX | AR | 3459 | 7/7 | 0.98 | 0.14 | -1.04 | 97,97,98,99 | 0 |
| 84 | OHX | 1 | 3428 | 7/7 | 0.99 | 0.14 | -1.04 | 96,96,96,96 | 0 |
| 84 | OHX | AR | 3543 | 7/7 | 0.97 | 0.17 | -1.05 | 181,181,182,182 | 0 |
| 84 | OHX | 1 | 3494 | 7/7 | 0.98 | 0.11 | -1.05 | 141,142,144,144 | 0 |
| 84 | OHX | AR | 3579 | 7/7 | 0.96 | 0.13 | -1.05 | 183,184,185,185 | 0 |
| 84 | OHX | A | 2019 | 7/7 | 0.90 | 0.14 | -1.05 | 252,253,255,256 | 0 |
| 84 | OHX | CF | 401 | 7/7 | 0.81 | 0.27 | -1.06 | 245,246,247,247 | 0 |
| 84 | OHX | AT | 204 | 7/7 | 0.98 | 0.10 | -1.06 | 143,143,143,143 | 0 |
| 84 | OHX | 1 | 3438 | 7/7 | 0.99 | 0.13 | -1.06 | 91,91,92,92 | 0 |
| 84 | OHX | 6 | 1944 | 7/7 | 0.98 | 0.12 | -1.06 | 154,155,157,158 | 0 |
| 84 | OHX | 2 | 201 | 7/7 | 0.99 | 0.17 | -1.07 | 94,94,94,94 | 0 |
| 85 | MG | t | 202 | 1/1 | 0.90 | 0.21 | -1.07 | 64,64,64,64 | 0 |
| 84 | OHX | 1 | 3528 | 7/7 | 0.96 | 0.14 | -1.08 | 169,170,171,171 | 0 |
| 84 | OHX | AR | 3500 | 7/7 | 0.95 | 0.12 | -1.08 | 136,138,139,140 | 0 |
| 84 | OHX | AR | 3576 | 7/7 | 0.96 | 0.14 | -1.08 | 168,169,169,170 | 0 |
| 84 | OHX | 6 | 1933 | 7/7 | 0.97 | 0.14 | -1.09 | 121,122,123,123 | 0 |
| 84 | OHX | T | 201 | 7/7 | 0.97 | 0.13 | -1.11 | 133,135,137,138 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 84 | OHX | 1 | 3481 | 7/7 | 0.98 | 0.11 | -1.11 | 130,131,132,133 | 0 |
| 84 | OHX | 6 | 1925 | 7/7 | 0.99 | 0.12 | -1.11 | 116,116,118,118 | 0 |
| 84 | OHX | 6 | 1961 | 7/7 | 0.96 | 0.15 | -1.12 | 152,153,154,155 | 0 |
| 84 | OHX | 1 | 3530 | 7/7 | 0.97 | 0.13 | -1.13 | 151,151,151,152 | 0 |
| 84 | OHX | AR | 3521 | 7/7 | 0.98 | 0.12 | -1.13 | 160,161,161,162 | 0 |
| 84 | OHX | Q | 201 | 7/7 | 0.90 | 0.25 | -1.14 | 245,246,248,249 | 0 |
| 84 | OHX | 6 | 1978 | 7/7 | 0.94 | 0.13 | -1.15 | 176,178,180,181 | 0 |
| 84 | OHX | 1 | 3589 | 7/7 | 0.96 | 0.15 | -1.15 | 179,180,181,181 | 0 |
| 87 | ZN | d6 | 102 | 1/1 | 0.99 | 0.10 | -1.15 | 59,59,59,59 | 0 |
| 84 | OHX | 1 | 3476 | 7/7 | 0.97 | 0.16 | -1.16 | 121,121,122,123 | 0 |
| 84 | OHX | 1 | 3665 | 7/7 | 0.92 | 0.16 | -1.16 | 209,210,211,211 | 0 |
| 84 | OHX | A | 1967 | 7/7 | 0.96 | 0.14 | -1.16 | 167,168,169,170 | 0 |
| 84 | OHX | A | 1911 | 7/7 | 0.98 | 0.13 | -1.16 | 115,117,118,120 | 0 |
| 87 | ZN | DO | 201 | 1/1 | 1.00 | 0.13 | -1.17 | 31,31,31,31 | 0 |
| 84 | OHX | AR | 3492 | 7/7 | 0.96 | 0.16 | -1.17 | 134,135,135,135 | 0 |
| 84 | OHX | 1 | 3434 | 7/7 | 0.99 | 0.14 | -1.17 | 94,95,95,95 | 0 |
| 84 | OHX | AR | 3465 | 7/7 | 0.99 | 0.12 | -1.18 | 100,101,102,102 | 0 |
| 84 | OHX | 6 | 1923 | 7/7 | 0.99 | 0.14 | -1.19 | 136,138,139,139 | 0 |
| 84 | OHX | AR | 3499 | 7/7 | 0.96 | 0.14 | -1.19 | 130,131,133,133 | 0 |
| 84 | OHX | 3 | 206 | 7/7 | 0.96 | 0.09 | -1.19 | 176,177,179,179 | 0 |
| 84 | OHX | sR | 401 | 7/7 | 0.93 | 0.15 | -1.20 | 215,216,219,219 | 0 |
| 84 | OHX | AK | 102 | 7/7 | 0.98 | 0.10 | -1.21 | 121,122,122,122 | 0 |
| 85 | MG | 1 | 4069 | 1/1 | 0.96 | 0.18 | -1.22 | 39,39,39,39 | 0 |
| 84 | OHX | AR | 3539 | 7/7 | 0.94 | 0.12 | -1.22 | 169,170,172,172 | 0 |
| 84 | OHX | 4 | 201 | 7/7 | 0.96 | 0.16 | -1.22 | 143,143,144,144 | 0 |
| 85 | MG | AR | 4091 | 1/1 | 0.97 | 0.16 | -1.22 | 53,53,53,53 | 0 |
| 84 | OHX | A | 1935 | 7/7 | 0.97 | 0.13 | -1.23 | 191,193,195,195 | 0 |
| 85 | MG | c6 | 201 | 1/1 | 0.96 | 0.16 | -1.24 | 67,67,67,67 | 0 |
| 84 | OHX | A | 1957 | 7/7 | 0.96 | 0.18 | -1.24 | 169,171,172,173 | 0 |
| 84 | OHX | 6 | 1953 | 7/7 | 0.97 | 0.13 | -1.25 | 154,155,157,158 | 0 |
| 84 | OHX | 1 | 3522 | 7/7 | 0.96 | 0.14 | -1.25 | 133,134,134,135 | 0 |
| 84 | OHX | 1 | 3520 | 7/7 | 0.98 | 0.08 | -1.25 | 149,150,152,152 | 0 |
| 84 | OHX | AR | 3426 | 7/7 | 0.99 | 0.13 | -1.26 | 88,88,88,89 | 0 |
| 84 | OHX | 1 | 3484 | 7/7 | 0.95 | 0.14 | -1.27 | 131,131,133,133 | 0 |
| 84 | OHX | A | 1910 | 7/7 | 0.98 | 0.11 | -1.27 | 123,125,127,128 | 0 |
| 85 | MG | c9 | 201 | 1/1 | 0.76 | 0.11 | -1.28 | 73,73,73,73 | 0 |
| 84 | OHX | AR | 3412 | 7/7 | 0.99 | 0.16 | -1.28 | 85,85,85,85 | 0 |
| 85 | MG | AR | 3773 | 1/1 | 0.81 | 0.12 | -1.28 | 113,113,113,113 | 0 |
| 84 | OHX | A | 1931 | 7/7 | 0.96 | 0.11 | -1.28 | 166,168,169,169 | 0 |
| 84 | OHX | AR | 3509 | 7/7 | 0.98 | 0.14 | -1.29 | 135,136,136,137 | 0 |
| 84 | OHX | AS | 202 | 7/7 | 0.98 | 0.11 | -1.30 | 122,123,124,124 | 0 |
| 85 | MG | 6 | 2156 | 1/1 | 0.91 | 0.14 | -1.30 | 50,50,50,50 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 84 | OHX | 6 | 1950 | 7/7 | 0.96 | 0.12 | -1.30 | 171,171,173,174 | 0 |
| 84 | OHX | 6 | 1963 | 7/7 | 0.97 | 0.15 | -1.31 | 159,159,161,161 | 0 |
| 85 | MG | 4 | 221 | 1/1 | 0.98 | 0.15 | -1.32 | 52,52,52,52 | 0 |
| 85 | MG | 1 | 3797 | 1/1 | 0.98 | 0.13 | -1.34 | 41,41,41,41 | 0 |
| 84 | OHX | 6 | 1966 | 7/7 | 0.95 | 0.14 | -1.34 | 164,165,166,167 | 0 |
| 84 | OHX | AR | 3604 | 7/7 | 0.96 | 0.15 | -1.35 | 150,151,151,151 | 0 |
| 85 | MG | CR | 206 | 1/1 | 0.94 | 0.15 | -1.35 | 30,30,30,30 | 0 |
| 84 | OHX | 1 | 3505 | 7/7 | 0.98 | 0.13 | -1.35 | 139,139,140,140 | 0 |
| 84 | OHX | 1 | 3504 | 7/7 | 0.94 | 0.12 | -1.38 | 154,156,157,158 | 0 |
| 85 | MG | 1 | 4156 | 1/1 | 1.00 | 0.13 | -1.38 | 65,65,65,65 | 0 |
| 84 | OHX | 1 | 3456 | 7/7 | 0.98 | 0.13 | -1.38 | 114,115,116,117 | 0 |
| 84 | OHX | AR | 3541 | 7/7 | 0.96 | 0.12 | -1.38 | 170,171,172,174 | 0 |
| 85 | MG | AR | 3857 | 1/1 | 0.95 | 0.14 | -1.38 | 46,46,46,46 | 0 |
| 84 | OHX | A | 1988 | 7/7 | 0.96 | 0.12 | -1.39 | 158,160,162,162 | 0 |
| 84 | OHX | 1 | 3440 | 7/7 | 0.99 | 0.14 | -1.39 | 94,95,95,95 | 0 |
| 85 | MG | sM | 201 | 1/1 | 0.94 | 0.10 | -1.39 | 41,41,41,41 | 0 |
| 84 | OHX | 1 | 3495 | 7/7 | 0.97 | 0.12 | -1.39 | 133,134,135,135 | 0 |
| 84 | OHX | DL | 101 | 7/7 | 0.97 | 0.14 | -1.41 | 144,144,144,144 | 0 |
| 87 | ZN | b | 102 | 1/1 | 0.99 | 0.10 | -1.42 | 68,68,68,68 | 0 |
| 84 | OHX | 1 | 3555 | 7/7 | 0.95 | 0.11 | -1.42 | 190,191,192,192 | 0 |
| 85 | MG | 1 | 3992 | 1/1 | 0.98 | 0.14 | -1.42 | 53,53,53,53 | 0 |
| 84 | OHX | AS | 205 | 7/7 | 0.98 | 0.11 | -1.42 | 144,146,147,147 | 0 |
| 84 | OHX | AR | 3436 | 7/7 | 0.99 | 0.16 | -1.42 | 87,87,87,87 | 0 |
| 84 | OHX | AR | 3420 | 7/7 | 0.99 | 0.16 | -1.43 | 87,87,87,87 | 0 |
| 84 | OHX | 6 | 1921 | 7/7 | 0.98 | 0.14 | -1.43 | 121,124,124,126 | 0 |
| 85 | MG | AR | 4018 | 1/1 | 0.93 | 0.12 | -1.44 | 40,40,40,40 | 0 |
| 84 | OHX | 6 | 1957 | 7/7 | 0.98 | 0.14 | -1.44 | 144,145,146,147 | 0 |
| 84 | OHX | AR | 3560 | 7/7 | 0.96 | 0.12 | -1.44 | 173,174,175,175 | 0 |
| 84 | OHX | J | 301 | 7/7 | 0.91 | 0.25 | -1.45 | 244,245,247,247 | 0 |
| 87 | ZN | AK | 101 | 1/1 | 0.99 | 0.13 | -1.45 | 38,38,38,38 | 0 |
| 84 | OHX | A | 1962 | 7/7 | 0.96 | 0.14 | -1.45 | 175,176,177,178 | 0 |
| 84 | OHX | AR | 3553 | 7/7 | 0.98 | 0.12 | -1.46 | 160,160,161,162 | 0 |
| 84 | OHX | AR | 3479 | 7/7 | 0.98 | 0.15 | -1.46 | 119,119,120,120 | 0 |
| 84 | OHX | 6 | 1914 | 7/7 | 0.96 | 0.14 | -1.47 | 119,120,121,123 | 0 |
| 84 | OHX | 1 | 3471 | 7/7 | 0.98 | 0.13 | -1.47 | 118,118,121,121 | 0 |
| 84 | OHX | A | 1925 | 7/7 | 0.97 | 0.09 | -1.48 | 171,172,174,175 | 0 |
| 84 | OHX | A | 1907 | 7/7 | 0.99 | 0.09 | -1.48 | 117,118,120,121 | 0 |
| 84 | OHX | A | 1913 | 7/7 | 0.98 | 0.14 | -1.48 | 121,122,123,124 | 0 |
| 84 | OHX | v | 301 | 7/7 | 0.97 | 0.14 | -1.49 | 155,155,156,156 | 0 |
| 84 | OHX | AR | 3423 | 7/7 | 0.99 | 0.14 | -1.50 | 85,85,85,85 | 0 |
| 85 | MG | CX | 203 | 1/1 | 0.94 | 0.15 | -1.50 | 45,45,45,45 | 0 |
| 84 | OHX | 3 | 204 | 7/7 | 0.98 | 0.08 | -1.50 | 163,164,165,166 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 84 | OHX | 6 | 1937 | 7/7 | 0.98 | 0.11 | -1.51 | 140,141,141,141 | 0 |
| 84 | OHX | AR | 3496 | 7/7 | 0.95 | 0.15 | -1.52 | 147,147,148,149 | 0 |
| 84 | OHX | A | 1963 | 7/7 | 0.98 | 0.10 | -1.52 | 185,187,189,190 | 0 |
| 84 | OHX | A | 1984 | 7/7 | 0.99 | 0.12 | -1.52 | 151,152,153,154 | 0 |
| 84 | OHX | AP | 502 | 7/7 | 0.97 | 0.14 | -1.53 | 124,124,126,127 | 0 |
| 85 | MG | AR | 4240 | 1/1 | 0.94 | 0.14 | -1.54 | 33,33,33,33 | 0 |
| 84 | OHX | A | 1942 | 7/7 | 0.98 | 0.14 | -1.55 | 163,165,166,167 | 0 |
| 87 | ZN | e | 102 | 1/1 | 0.99 | 0.06 | -1.55 | 74,74,74,74 | 0 |
| 84 | OHX | 6 | 1954 | 7/7 | 0.95 | 0.11 | -1.57 | 181,182,184,185 | 0 |
| 84 | OHX | 1 | 3579 | 7/7 | 0.97 | 0.12 | -1.58 | 175,175,177,177 | 0 |
| 85 | MG | A | 2136 | 1/1 | 0.97 | 0.08 | -1.59 | 110,110,110,110 | 0 |
| 84 | OHX | AR | 3534 | 7/7 | 0.97 | 0.12 | -1.62 | 162,163,164,165 | 0 |
| 87 | ZN | DQ | 501 | 1/1 | 0.97 | 0.15 | -1.62 | 105,105,105,105 | 0 |
| 84 | OHX | 1 | 3487 | 7/7 | 0.98 | 0.10 | -1.63 | 139,140,142,142 | 0 |
| 84 | OHX | A | 1975 | 7/7 | 0.97 | 0.08 | -1.65 | 190,193,195,195 | 0 |
| 84 | OHX | 1 | 3452 | 7/7 | 0.98 | 0.14 | -1.66 | 111,111,112,113 | 0 |
| 84 | OHX | 1 | 3626 | 7/7 | 0.98 | 0.16 | -1.66 | 137,137,138,138 | 0 |
| 84 | OHX | A | 1927 | 7/7 | 0.96 | 0.12 | -1.67 | 158,160,162,162 | 0 |
| 84 | OHX | 6 | 2007 | 7/7 | 0.97 | 0.15 | -1.68 | 148,150,151,151 | 0 |
| 84 | OHX | 1 | 3515 | 7/7 | 0.97 | 0.13 | -1.72 | 128,128,129,129 | 0 |
| 85 | MG | DC | 204 | 1/1 | 0.99 | 0.17 | -1.72 | 45,45,45,45 | 0 |
| 84 | OHX | 6 | 1999 | 7/7 | 0.98 | 0.18 | -1.75 | 177,179,179,181 | 0 |
| 84 | OHX | 1 | 3432 | 7/7 | 0.96 | 0.15 | -1.76 | 131,131,132,132 | 0 |
| 84 | OHX | AR | 3437 | 7/7 | 0.99 | 0.11 | -1.76 | 89,89,89,89 | 0 |
| 85 | MG | AR | 4175 | 1/1 | 0.95 | 0.14 | -1.77 | 27,27,27,27 | 0 |
| 84 | OHX | 6 | 1988 | 7/7 | 0.96 | 0.12 | -1.79 | 191,193,195,195 | 0 |
| 85 | MG | 6 | 2155 | 1/1 | 0.92 | 0.14 | -1.81 | 61,61,61,61 | 0 |
| 84 | OHX | 1 | 3443 | 7/7 | 0.99 | 0.12 | -1.81 | 95,95,95,95 | 0 |
| 84 | OHX | 1 | 3561 | 7/7 | 0.96 | 0.14 | -1.83 | 184,184,185,186 | 0 |
| 85 | MG | j | 302 | 1/1 | 0.99 | 0.14 | -1.84 | 29,29,29,29 | 0 |
| 84 | OHX | h | 401 | 7/7 | 0.97 | 0.09 | -1.85 | 203,206,208,210 | 0 |
| 84 | OHX | A | 1914 | 7/7 | 0.99 | 0.11 | -1.85 | 109,110,111,112 | 0 |
| 84 | OHX | 6 | 1922 | 7/7 | 0.99 | 0.10 | -1.85 | 111,112,113,114 | 0 |
| 87 | ZN | AQ | 501 | 1/1 | 0.97 | 0.08 | -1.86 | 77,77,77,77 | 0 |
| 84 | OHX | 6 | 1952 | 7/7 | 0.96 | 0.13 | -1.87 | 183,184,185,186 | 0 |
| 87 | ZN | AN | 500 | 1/1 | 1.00 | 0.11 | -1.88 | 43,43,43,43 | 0 |
| 85 | MG | 1 | 3887 | 1/1 | 0.86 | 0.12 | -1.90 | 49,49,49,49 | 0 |
| 84 | OHX | 1 | 3449 | 7/7 | 0.98 | 0.10 | -1.91 | 119,120,121,121 | 0 |
| 85 | MG | AR | 3868 | 1/1 | 0.96 | 0.13 | -1.91 | 33,33,33,33 | 0 |
| 87 | ZN | DL | 103 | 1/1 | 1.00 | 0.12 | -1.92 | 37,37,37,37 | 0 |
| 84 | OHX | 6 | 1928 | 7/7 | 0.98 | 0.09 | -1.92 | 150,151,152,152 | 0 |
| 84 | OHX | A | 1966 | 7/7 | 0.95 | 0.14 | -1.93 | 194,195,196,197 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 84 | OHX | 1 | 3492 | 7/7 | 0.96 | 0.15 | -1.93 | 127,128,128,128 | 0 |
| 87 | ZN | DR | 501 | 1/1 | 0.98 | 0.07 | -1.94 | 73,73,73,73 | 0 |
| 85 | MG | AR | 3777 | 1/1 | 0.96 | 0.14 | -1.94 | 50,50,50,50 | 0 |
| 84 | OHX | AR | 3451 | 7/7 | 0.98 | 0.15 | -1.95 | 104,105,106,106 | 0 |
| 85 | MG | 1 | 3756 | 1/1 | 0.96 | 0.15 | -1.96 | 22,22,22,22 | 0 |
| 84 | OHX | 1 | 3536 | 7/7 | 0.88 | 0.17 | -1.97 | 221,221,223,224 | 0 |
| 84 | OHX | 3 | 203 | 7/7 | 0.96 | 0.14 | -1.97 | 143,144,145,145 | 0 |
| 84 | OHX | AR | 3470 | 7/7 | 0.98 | 0.09 | -1.99 | 125,127,127,128 | 0 |
| 85 | MG | AR | 4165 | 1/1 | 0.97 | 0.07 | -2.00 | 88,88,88,88 | 0 |
| 84 | OHX | AR | 3488 | 7/7 | 0.97 | 0.13 | -2.00 | 129,130,130,131 | 0 |
| 84 | OHX | 1 | 3454 | 7/7 | 0.98 | 0.14 | -2.01 | 111,112,113,113 | 0 |
| 84 | OHX | CE | 402 | 7/7 | 0.97 | 0.12 | -2.01 | 142,143,144,144 | 0 |
| 84 | OHX | 1 | 3629 | 7/7 | 0.96 | 0.14 | -2.01 | 161,162,162,163 | 0 |
| 84 | OHX | AR | 3449 | 7/7 | 0.99 | 0.12 | -2.02 | 98,99,99,100 | 0 |
| 85 | MG | r | 302 | 1/1 | 0.98 | 0.10 | -2.02 | 40,40,40,40 | 0 |
| 84 | OHX | 6 | 1926 | 7/7 | 0.99 | 0.10 | -2.03 | 122,123,124,124 | 0 |
| 84 | OHX | A | 1933 | 7/7 | 0.97 | 0.12 | -2.04 | 154,155,156,157 | 0 |
| 84 | OHX | AR | 3527 | 7/7 | 0.98 | 0.10 | -2.04 | 138,139,140,141 | 0 |
| 84 | OHX | AR | 3525 | 7/7 | 0.97 | 0.13 | -2.05 | 150,151,151,152 | 0 |
| 84 | OHX | 1 | 3623 | 7/7 | 0.93 | 0.10 | -2.08 | 224,225,226,226 | 0 |
| 84 | OHX | 1 | 3535 | 7/7 | 0.96 | 0.10 | -2.09 | 196,198,199,200 | 0 |
| 85 | MG | AR | 4189 | 1/1 | 0.98 | 0.14 | -2.11 | 32,32,32,32 | 0 |
| 84 | OHX | AR | 3562 | 7/7 | 0.98 | 0.07 | -2.11 | 173,174,175,176 | 0 |
| 84 | OHX | 3 | 201 | 7/7 | 0.99 | 0.10 | -2.11 | 106,107,108,108 | 0 |
| 84 | OHX | 1 | 3447 | 7/7 | 0.99 | 0.14 | -2.11 | 95,95,95,95 | 0 |
| 84 | OHX | A | 1955 | 7/7 | 0.97 | 0.11 | -2.12 | 145,148,150,150 | 0 |
| 84 | OHX | AR | 3443 | 7/7 | 0.98 | 0.14 | -2.12 | 98,99,100,101 | 0 |
| 84 | OHX | CL | 301 | 7/7 | 0.97 | 0.10 | -2.13 | 165,166,167,168 | 0 |
| 84 | OHX | AR | 3586 | 7/7 | 0.93 | 0.14 | -2.14 | 182,184,185,185 | 0 |
| 84 | OHX | 1 | 3677 | 7/7 | 0.96 | 0.14 | -2.15 | 170,171,171,171 | 0 |
| 84 | OHX | AK | 103 | 7/7 | 0.98 | 0.12 | -2.15 | 145,146,146,146 | 0 |
| 85 | MG | 6 | 2142 | 1/1 | 0.86 | 0.10 | -2.16 | 72,72,72,72 | 0 |
| 84 | OHX | A | 1949 | 7/7 | 0.96 | 0.11 | -2.16 | 165,167,169,169 | 0 |
| 84 | OHX | 6 | 1910 | 7/7 | 0.99 | 0.14 | -2.16 | 93,93,93,93 | 0 |
| 84 | OHX | 6 | 1951 | 7/7 | 0.97 | 0.14 | -2.19 | 165,167,169,170 | 0 |
| 85 | MG | 1 | 4116 | 1/1 | 0.94 | 0.12 | -2.20 | 81,81,81,81 | 0 |
| 85 | MG | 1 | 4222 | 1/1 | 0.97 | 0.14 | -2.21 | 30,30,30,30 | 0 |
| 84 | OHX | A | 1937 | 7/7 | 0.97 | 0.14 | -2.21 | 152,154,157,157 | 0 |
| 84 | OHX | AR | 3493 | 7/7 | 0.98 | 0.12 | -2.23 | 137,139,139,140 | 0 |
| 84 | OHX | 1 | 3532 | 7/7 | 0.98 | 0.13 | -2.24 | 133,133,134,134 | 0 |
| 84 | OHX | AR | 3462 | 7/7 | 0.99 | 0.11 | -2.24 | 106,107,108,108 | 0 |
| 85 | MG | CE | 401 | 1/1 | 0.96 | 0.14 | -2.26 | 30,30,30,30 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 84 | OHX | A | 1928 | 7/7 | 0.96 | 0.13 | -2.26 | 156,158,159,159 | 0 |
| 84 | OHX | AR | 3603 | 7/7 | 0.92 | 0.13 | -2.26 | 182,183,184,185 | 0 |
| 84 | OHX | 6 | 1967 | 7/7 | 0.96 | 0.13 | -2.26 | 157,159,160,160 | 0 |
| 85 | MG | 6 | 2187 | 1/1 | 0.98 | 0.12 | -2.26 | 82,82,82,82 | 0 |
| 84 | OHX | 1 | 3439 | 7/7 | 0.99 | 0.11 | -2.26 | 102,103,103,104 | 0 |
| 85 | MG | AR | 3809 | 1/1 | 0.93 | 0.12 | -2.30 | 86,86,86,86 | 0 |
| 85 | MG | 1 | 4046 | 1/1 | 0.98 | 0.09 | -2.31 | 54,54,54,54 | 0 |
| 84 | OHX | A | 1944 | 7/7 | 0.97 | 0.11 | -2.31 | 161,163,165,165 | 0 |
| 84 | OHX | A | 1916 | 7/7 | 0.98 | 0.11 | -2.33 | 128,130,131,131 | 0 |
| 84 | OHX | 1 | 3450 | 7/7 | 0.98 | 0.12 | -2.35 | 116,117,118,118 | 0 |
| 84 | OHX | A | 1904 | 7/7 | 0.99 | 0.12 | -2.37 | 107,107,108,108 | 0 |
| 84 | OHX | AR | 3421 | 7/7 | 0.99 | 0.12 | -2.40 | 89,89,89,89 | 0 |
| 84 | OHX | A | 1917 | 7/7 | 0.99 | 0.12 | -2.40 | 126,128,129,130 | 0 |
| 87 | ZN | g | 501 | 1/1 | 0.96 | 0.04 | -2.41 | 143,143,143,143 | 0 |
| 84 | OHX | AR | 3480 | 7/7 | 0.97 | 0.12 | -2.42 | 132,132,132,133 | 0 |
| 84 | OHX | AR | 3469 | 7/7 | 0.98 | 0.10 | -2.43 | 122,124,125,125 | 0 |
| 84 | OHX | AR | 3498 | 7/7 | 0.98 | 0.09 | -2.43 | 143,144,145,146 | 0 |
| 85 | MG | 1 | 4218 | 1/1 | 0.98 | 0.07 | -2.44 | 84,84,84,84 | 0 |
| 84 | OHX | 1 | 3457 | 7/7 | 0.99 | 0.14 | -2.45 | 108,108,109,109 | 0 |
| 85 | MG | AR | 3942 | 1/1 | 0.94 | 0.10 | -2.46 | 45,45,45,45 | 0 |
| 84 | OHX | AR | 3438 | 7/7 | 0.99 | 0.12 | -2.46 | 89,89,89,90 | 0 |
| 84 | OHX | 1 | 3480 | 7/7 | 0.98 | 0.13 | -2.49 | 141,141,142,142 | 0 |
| 84 | OHX | 6 | 1927 | 7/7 | 0.97 | 0.16 | -2.49 | 128,128,130,130 | 0 |
| 85 | MG | AR | 3929 | 1/1 | 0.98 | 0.13 | -2.50 | 75,75,75,75 | 0 |
| 84 | OHX | 1 | 3498 | 7/7 | 0.97 | 0.11 | -2.50 | 150,150,151,152 | 0 |
| 84 | OHX | 1 | 3479 | 7/7 | 0.98 | 0.15 | -2.51 | 136,137,138,138 | 0 |
| 84 | OHX | AR | 3467 | 7/7 | 0.97 | 0.13 | -2.51 | 137,138,138,139 | 0 |
| 84 | OHX | 6 | 1920 | 7/7 | 0.98 | 0.12 | -2.51 | 124,126,127,128 | 0 |
| 84 | OHX | 6 | 1956 | 7/7 | 0.98 | 0.09 | -2.52 | 192,194,195,196 | 0 |
| 84 | OHX | 1 | 3464 | 7/7 | 0.98 | 0.11 | -2.53 | 136,137,138,139 | 0 |
| 84 | OHX | A | 1948 | 7/7 | 0.96 | 0.09 | -2.54 | 166,169,170,170 | 0 |
| 84 | OHX | AR | 3472 | 7/7 | 0.96 | 0.13 | -2.54 | 129,130,130,130 | 0 |
| 84 | OHX | 1 | 3423 | 7/7 | 0.99 | 0.15 | -2.56 | 91,92,92,92 | 0 |
| 84 | OHX | 1 | 3467 | 7/7 | 0.97 | 0.13 | -2.59 | 124,125,126,126 | 0 |
| 84 | OHX | AR | 3630 | 7/7 | 0.96 | 0.10 | -2.59 | 172,173,174,175 | 0 |
| 84 | OHX | AR | 3516 | 7/7 | 0.96 | 0.09 | -2.60 | 174,176,178,178 | 0 |
| 87 | ZN | e1 | 501 | 1/1 | 0.81 | 0.09 | -2.61 | 176,176,176,176 | 0 |
| 84 | OHX | AR | 3431 | 7/7 | 0.99 | 0.14 | -2.62 | 86,86,86,86 | 0 |
| 84 | OHX | A | 1956 | 7/7 | 0.97 | 0.13 | -2.64 | 171,173,174,175 | 0 |
| 84 | OHX | 1 | 3689 | 7/7 | 0.97 | 0.14 | -2.64 | 140,141,142,142 | 0 |
| 84 | OHX | 1 | 3563 | 7/7 | 0.97 | 0.15 | -2.66 | 151,152,152,152 | 0 |
| 84 | OHX | AR | 3511 | 7/7 | 0.98 | 0.15 | -2.68 | 96,96,96,97 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 84 | OHX | A | 1915 | 7/7 | 0.98 | 0.09 | -2.72 | 149,151,152,154 | 0 |
| 84 | OHX | 1 | 3429 | 7/7 | 0.99 | 0.13 | -2.72 | 89,89,90,90 | 0 |
| 84 | OHX | 6 | 1947 | 7/7 | 0.96 | 0.12 | -2.72 | 142,144,145,145 | 0 |
| 84 | OHX | 1 | 3472 | 7/7 | 0.99 | 0.12 | -2.73 | 114,115,115,116 | 0 |
| 84 | OHX | AS | 203 | 7/7 | 0.98 | 0.11 | -2.74 | 118,119,120,120 | 0 |
| 84 | OHX | A | 1919 | 7/7 | 0.99 | 0.10 | -2.75 | 113,115,116,116 | 0 |
| 84 | OHX | AR | 3450 | 7/7 | 0.98 | 0.11 | -2.77 | 109,110,112,113 | 0 |
| 84 | OHX | DH | 201 | 7/7 | 0.96 | 0.13 | -2.80 | 155,156,157,157 | 0 |
| 84 | OHX | A | 1961 | 7/7 | 0.97 | 0.13 | -2.81 | 175,176,179,180 | 0 |
| 84 | OHX | AR | 3454 | 7/7 | 0.98 | 0.12 | -2.86 | 120,120,121,121 | 0 |
| 84 | OHX | A | 1974 | 7/7 | 0.95 | 0.10 | -2.86 | 196,198,200,201 | 0 |
| 85 | MG | AR | 4006 | 1/1 | 0.97 | 0.10 | -2.86 | 33,33,33,33 | 0 |
| 84 | OHX | A | 1912 | 7/7 | 0.98 | 0.09 | -2.91 | 132,133,135,136 | 0 |
| 84 | OHX | AT | 210 | 7/7 | 0.97 | 0.11 | -2.94 | 164,164,165,165 | 0 |
| 84 | OHX | A | 2008 | 7/7 | 0.97 | 0.13 | -2.94 | 156,158,159,159 | 0 |
| 84 | OHX | AR | 3461 | 7/7 | 0.99 | 0.11 | -2.95 | 108,109,109,110 | 0 |
| 84 | OHX | 6 | 1938 | 7/7 | 0.97 | 0.14 | -2.96 | 145,146,148,148 | 0 |
| 85 | MG | j | 301 | 1/1 | 0.98 | 0.13 | -2.97 | 26,26,26,26 | 0 |
| 84 | OHX | 1 | 3560 | 7/7 | 0.98 | 0.13 | -2.98 | 155,156,158,158 | 0 |
| 84 | OHX | AR | 3522 | 7/7 | 0.97 | 0.14 | -3.00 | 134,135,136,136 | 0 |
| 84 | OHX | AR | 3435 | 7/7 | 0.99 | 0.11 | -3.01 | 96,96,96,96 | 0 |
| 84 | OHX | AR | 3481 | 7/7 | 0.97 | 0.11 | -3.05 | 132,132,133,133 | 0 |
| 84 | OHX | AR | 3510 | 7/7 | 0.97 | 0.10 | -3.06 | 154,155,156,157 | 0 |
| 84 | OHX | 1 | 3415 | 7/7 | 0.99 | 0.15 | -3.06 | 89,90,90,90 | 0 |
| 84 | OHX | AS | 207 | 7/7 | 0.98 | 0.11 | -3.08 | 163,165,166,166 | 0 |
| 85 | MG | 1 | 3993 | 1/1 | 0.98 | 0.10 | -3.08 | 27,27,27,27 | 0 |
| 85 | MG | i | 201 | 1/1 | 0.97 | 0.06 | -3.09 | 57,57,57,57 | 0 |
| 84 | OHX | 1 | 3486 | 7/7 | 0.97 | 0.12 | -3.11 | 146,146,147,147 | 0 |
| 84 | OHX | 1 | 3514 | 7/7 | 0.97 | 0.13 | -3.14 | 148,148,149,149 | 0 |
| 84 | OHX | AR | 3460 | 7/7 | 0.97 | 0.12 | -3.14 | 109,109,110,110 | 0 |
| 85 | MG | AR | 3940 | 1/1 | 0.97 | 0.10 | -3.16 | 34,34,34,34 | 0 |
| 84 | OHX | AR | 3502 | 7/7 | 0.98 | 0.11 | -3.17 | 131,132,132,133 | 0 |
| 85 | MG | 1 | 3850 | 1/1 | 1.00 | 0.12 | -3.19 | 29,29,29,29 | 0 |
| 84 | OHX | A | 1922 | 7/7 | 0.98 | 0.10 | -3.22 | 138,140,141,141 | 0 |
| 84 | OHX | AR | 3430 | 7/7 | 0.97 | 0.15 | -3.22 | 137,137,138,138 | 0 |
| 85 | MG | 1 | 4166 | 1/1 | 1.00 | 0.12 | -3.26 | 30,30,30,30 | 0 |
| 87 | ZN | c | 101 | 1/1 | 0.79 | 0.21 | -3.29 | 197,197,197,197 | 0 |
| 84 | OHX | 1 | 3725 | 7/7 | 0.94 | 0.08 | -3.31 | 203,204,205,206 | 0 |
| 84 | OHX | AR | 3471 | 7/7 | 0.98 | 0.12 | -3.33 | 127,127,128,128 | 0 |
| 84 | OHX | AR | 3610 | 7/7 | 0.97 | 0.13 | -3.38 | 139,140,140,140 | 0 |
| 84 | OHX | 6 | 1918 | 7/7 | 0.99 | 0.11 | -3.38 | 103,104,105,105 | 0 |
| 84 | OHX | 1 | 3483 | 7/7 | 0.98 | 0.10 | -3.39 | 118,119,120,121 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 84 | OHX | 1 | 3538 | 7/7 | 0.98 | 0.14 | -3.39 | 135,135,137,137 | 0 |
| 84 | OHX | A | 1938 | 7/7 | 0.98 | 0.14 | -3.40 | 138,139,140,141 | 0 |
| 84 | OHX | AR | 3552 | 7/7 | 0.98 | 0.12 | -3.41 | 148,148,149,149 | 0 |
| 84 | OHX | 1 | 3465 | 7/7 | 0.99 | 0.10 | -3.45 | 113,114,114,114 | 0 |
| 84 | OHX | 1 | 3500 | 7/7 | 0.97 | 0.07 | -3.46 | 156,157,159,159 | 0 |
| 84 | OHX | AR | 3478 | 7/7 | 0.98 | 0.12 | -3.46 | 102,103,103,104 | 0 |
| 84 | OHX | AR | 3452 | 7/7 | 0.98 | 0.11 | -3.48 | 108,109,110,111 | 0 |
| 84 | OHX | 1 | 3453 | 7/7 | 0.99 | 0.09 | -3.50 | 130,132,133,133 | 0 |
| 84 | OHX | 6 | 1915 | 7/7 | 0.98 | 0.12 | -3.54 | 100,101,102,102 | 0 |
| 84 | OHX | AR | 3428 | 7/7 | 0.99 | 0.10 | -3.56 | 97,97,98,98 | 0 |
| 84 | OHX | AR | 3512 | 7/7 | 0.98 | 0.10 | -3.58 | 132,132,132,133 | 0 |
| 84 | OHX | 1 | 3431 | 7/7 | 0.99 | 0.12 | -3.60 | 95,95,95,95 | 0 |
| 84 | OHX | 1 | 3685 | 7/7 | 0.96 | 0.16 | -3.60 | 173,173,175,175 | 0 |
| 84 | OHX | 1 | 3468 | 7/7 | 0.98 | 0.14 | -3.61 | 104,104,104,105 | 0 |
| 84 | OHX | A | 2034 | 7/7 | 0.84 | 0.14 | -3.64 | 277,279,281,282 | 0 |
| 84 | OHX | AR | 3457 | 7/7 | 0.98 | 0.13 | -3.65 | 107,107,108,108 | 0 |
| 84 | OHX | AR | 3410 | 7/7 | 0.99 | 0.13 | -3.68 | 86,86,86,86 | 0 |
| 84 | OHX | CG | 301 | 7/7 | 0.93 | 0.13 | -3.75 | 191,193,193,195 | 0 |
| 85 | MG | 1 | 3938 | 1/1 | 0.92 | 0.11 | -3.76 | 41,41,41,41 | 0 |
| 84 | OHX | AR | 3600 | 7/7 | 0.95 | 0.13 | -3.81 | 172,173,173,174 | 0 |
| 84 | OHX | 1 | 3502 | 7/7 | 0.99 | 0.10 | -3.83 | 100,101,102,102 | 0 |
| 84 | OHX | 6 | 1986 | 7/7 | 0.95 | 0.12 | -3.85 | 157,157,159,159 | 0 |
| 85 | MG | AR | 4105 | 1/1 | 0.99 | 0.08 | -3.87 | 41,41,41,41 | 0 |
| 85 | MG | 1 | 3931 | 1/1 | 0.99 | 0.12 | -3.88 | 31,31,31,31 | 0 |
| 84 | OHX | 6 | 1942 | 7/7 | 0.98 | 0.09 | -3.97 | 142,143,144,145 | 0 |
| 84 | OHX | 1 | 3519 | 7/7 | 0.99 | 0.10 | -3.98 | 112,112,113,113 | 0 |
| 84 | OHX | A | 1920 | 7/7 | 0.97 | 0.13 | -4.08 | 141,142,143,144 | 0 |
| 84 | OHX | AR | 3537 | 7/7 | 0.98 | 0.11 | -4.12 | 133,134,135,135 | 0 |
| 84 | OHX | A | 1923 | 7/7 | 0.98 | 0.09 | -4.12 | 137,138,140,140 | 0 |
| 84 | OHX | AR | 3464 | 7/7 | 0.97 | 0.13 | -4.12 | 117,118,118,118 | 0 |
| 84 | OHX | A | 1924 | 7/7 | 0.98 | 0.10 | -4.15 | 153,154,155,156 | 0 |
| 84 | OHX | A | 1992 | 7/7 | 0.96 | 0.13 | -4.16 | 167,169,170,171 | 0 |
| 84 | OHX | 1 | 3549 | 7/7 | 0.96 | 0.13 | -4.21 | 190,190,191,192 | 0 |
| 84 | OHX | 6 | 1930 | 7/7 | 0.98 | 0.12 | -4.32 | 114,115,116,117 | 0 |
| 84 | OHX | AR | 3531 | 7/7 | 0.98 | 0.10 | -4.34 | 123,124,124,124 | 0 |
| 84 | OHX | 6 | 1946 | 7/7 | 0.97 | 0.12 | -4.35 | 160,161,163,164 | 0 |
| 84 | OHX | 6 | 1959 | 7/7 | 0.98 | 0.11 | -4.47 | 154,155,156,157 | 0 |
| 84 | OHX | AR | 3491 | 7/7 | 0.98 | 0.10 | -4.61 | 130,131,132,132 | 0 |
| 84 | OHX | AR | 3448 | 7/7 | 0.98 | 0.12 | -4.69 | 109,110,110,110 | 0 |
| 84 | OHX | 1 | 3489 | 7/7 | 0.99 | 0.11 | -4.75 | 114,115,116,117 | 0 |
| 84 | OHX | 1 | 3459 | 7/7 | 0.99 | 0.09 | -4.75 | 134,134,135,136 | 0 |
| 84 | OHX | AR | 3486 | 7/7 | 0.99 | 0.09 | -4.86 | 118,119,120,121 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|--------|-----------------------------|-------|
| 84 | OHX | A | 1939 | 7/7 | 0.99 | 0.08 | -4.94 | 153,155,156,157 | 0 |
| 84 | OHX | AR | 3429 | 7/7 | 0.98 | 0.09 | -4.94 | 105,105,106,106 | 0 |
| 84 | OHX | AR | 3557 | 7/7 | 0.98 | 0.12 | -5.14 | 144,145,146,146 | 0 |
| 84 | OHX | 1 | 3506 | 7/7 | 0.98 | 0.09 | -5.17 | 159,160,161,162 | 0 |
| 84 | OHX | 1 | 3463 | 7/7 | 0.99 | 0.08 | -5.19 | 108,109,109,109 | 0 |
| 84 | OHX | AR | 3444 | 7/7 | 0.99 | 0.10 | -5.40 | 101,102,102,103 | 0 |
| 84 | OHX | AR | 3482 | 7/7 | 0.99 | 0.10 | -5.57 | 116,117,117,117 | 0 |
| 84 | OHX | AR | 3490 | 7/7 | 0.99 | 0.09 | -5.63 | 108,108,109,110 | 0 |
| 84 | OHX | 1 | 3478 | 7/7 | 0.98 | 0.11 | -5.65 | 133,134,135,135 | 0 |
| 84 | OHX | 1 | 3421 | 7/7 | 0.99 | 0.11 | -6.16 | 84,84,84,84 | 0 |
| 84 | OHX | 6 | 1934 | 7/7 | 0.99 | 0.09 | -6.29 | 141,141,143,144 | 0 |
| 84 | OHX | 6 | 1917 | 7/7 | 0.99 | 0.10 | -6.49 | 113,114,116,117 | 0 |
| 84 | OHX | 1 | 3490 | 7/7 | 0.98 | 0.10 | -6.83 | 134,135,136,136 | 0 |
| 84 | OHX | 6 | 1948 | 7/7 | 0.98 | 0.10 | -6.93 | 145,147,148,148 | 0 |
| 84 | OHX | AR | 3501 | 7/7 | 0.99 | 0.11 | -7.27 | 118,118,120,120 | 0 |
| 84 | OHX | 1 | 3591 | 7/7 | 0.97 | 0.12 | -7.50 | 185,186,187,188 | 0 |
| 84 | OHX | AR | 3425 | 7/7 | 0.99 | 0.10 | -9.09 | 85,85,85,85 | 0 |
| 84 | OHX | AT | 205 | 7/7 | 0.98 | 0.09 | -9.16 | 151,151,151,151 | 0 |
| 85 | MG | AR | 3761 | 1/1 | 0.96 | 0.10 | -10.46 | 41,41,41,41 | 0 |
| 84 | OHX | AR | 3737 | 7/7 | 0.80 | 0.69 | - | 260,261,262,262 | 0 |
| 85 | MG | 6 | 2105 | 1/1 | 0.96 | 0.34 | - | 24,24,24,24 | 0 |
| 85 | MG | AR | 3978 | 1/1 | 0.96 | 0.26 | - | 20,20,20,20 | 0 |
| 85 | MG | 1 | 3984 | 1/1 | 0.86 | 0.31 | - | 33,33,33,33 | 0 |
| 85 | MG | 6 | 2121 | 1/1 | 0.87 | 0.22 | - | 71,71,71,71 | 0 |
| 85 | MG | A | 2049 | 1/1 | 0.98 | 0.34 | - | 35,35,35,35 | 0 |
| 84 | OHX | AR | 3706 | 7/7 | 0.90 | 0.22 | - | 209,210,211,212 | 0 |
| 85 | MG | AR | 3764 | 1/1 | 0.92 | 0.18 | - | 27,27,27,27 | 0 |
| 85 | MG | AR | 4101 | 1/1 | 0.70 | 0.46 | - | 48,48,48,48 | 0 |
| 84 | OHX | 1 | 3446 | 7/7 | 0.98 | 0.16 | - | 107,108,109,110 | 0 |
| 85 | MG | 1 | 3923 | 1/1 | 0.96 | 0.50 | - | 7,7,7,7 | 0 |
| 85 | MG | 1 | 3766 | 1/1 | 0.89 | 0.29 | - | 23,23,23,23 | 0 |
| 85 | MG | AR | 3941 | 1/1 | 0.94 | 0.08 | - | 46,46,46,46 | 0 |
| 85 | MG | AR | 4087 | 1/1 | 0.96 | 0.35 | - | 31,31,31,31 | 0 |
| 85 | MG | 1 | 4030 | 1/1 | 0.81 | 0.44 | - | 45,45,45,45 | 0 |
| 85 | MG | 6 | 2086 | 1/1 | 0.96 | 0.24 | - | 49,49,49,49 | 0 |
| 85 | MG | AR | 4072 | 1/1 | 0.73 | 0.36 | - | 71,71,71,71 | 0 |
| 85 | MG | AR | 4107 | 1/1 | 0.89 | 0.26 | - | 79,79,79,79 | 0 |
| 85 | MG | 6 | 2143 | 1/1 | 0.93 | 0.18 | - | 90,90,90,90 | 0 |
| 84 | OHX | 1 | 3408 | 7/7 | 0.99 | 0.12 | - | 89,89,89,89 | 0 |
| 85 | MG | AR | 3917 | 1/1 | 0.98 | 0.33 | - | 29,29,29,29 | 0 |
| 85 | MG | 6 | 2181 | 1/1 | 0.52 | 0.49 | - | 78,78,78,78 | 0 |
| 85 | MG | 6 | 2175 | 1/1 | 0.93 | 0.19 | - | 41,41,41,41 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 85 | MG | 6 | 2084 | 1/1 | 0.93 | 0.27 | - | 35,35,35,35 | 0 |
| 85 | MG | 6 | 2166 | 1/1 | 0.80 | 0.16 | - | 36,36,36,36 | 0 |
| 85 | MG | 1 | 4049 | 1/1 | 0.95 | 0.18 | - | 36,36,36,36 | 0 |
| 85 | MG | A | 2051 | 1/1 | 0.93 | 0.26 | - | 62,62,62,62 | 0 |
| 84 | OHX | AR | 3596 | 7/7 | 0.96 | 0.30 | - | 208,209,210,211 | 0 |
| 85 | MG | AS | 213 | 1/1 | 0.97 | 0.23 | - | 40,40,40,40 | 0 |
| 85 | MG | AR | 4089 | 1/1 | 0.97 | 0.39 | - | 15,15,15,15 | 0 |
| 85 | MG | AR | 4167 | 1/1 | 0.68 | 0.51 | - | 72,72,72,72 | 0 |
| 84 | OHX | AR | 3649 | 7/7 | 0.96 | 0.30 | - | 207,208,208,208 | 0 |
| 85 | MG | 1 | 4178 | 1/1 | 0.90 | 0.20 | - | 42,42,42,42 | 0 |
| 85 | MG | AR | 4192 | 1/1 | 0.94 | 0.18 | - | 44,44,44,44 | 0 |
| 84 | OHX | 6 | 1964 | 7/7 | 0.93 | 0.20 | - | 175,175,177,177 | 0 |
| 85 | MG | 1 | 4205 | 1/1 | 0.97 | 0.53 | - | 26,26,26,26 | 0 |
| 85 | MG | 1 | 3809 | 1/1 | 0.90 | 0.32 | - | 23,23,23,23 | 0 |
| 84 | OHX | AR | 3446 | 7/7 | 0.99 | 0.09 | - | 99,100,100,101 | 0 |
| 85 | MG | AR | 4094 | 1/1 | 0.96 | 0.13 | - | 38,38,38,38 | 0 |
| 85 | MG | A | 2044 | 1/1 | 0.95 | 0.52 | - | 25,25,25,25 | 0 |
| 85 | MG | AR | 4048 | 1/1 | 0.87 | 0.16 | - | 33,33,33,33 | 0 |
| 84 | OHX | 1 | 3645 | 7/7 | 0.89 | 0.25 | - | 220,221,221,221 | 0 |
| 85 | MG | 1 | 4153 | 1/1 | 0.91 | 0.21 | - | 39,39,39,39 | 0 |
| 85 | MG | 1 | 4047 | 1/1 | 0.89 | 0.72 | - | 39,39,39,39 | 0 |
| 85 | MG | 6 | 2124 | 1/1 | 0.92 | 0.11 | - | 62,62,62,62 | 0 |
| 85 | MG | AR | 3878 | 1/1 | 0.98 | 0.27 | - | 12,12,12,12 | 0 |
| 85 | MG | 1 | 4207 | 1/1 | 0.89 | 0.31 | - | 44,44,44,44 | 0 |
| 84 | OHX | 6 | 2055 | 7/7 | 0.86 | 0.18 | - | 234,235,236,236 | 0 |
| 85 | MG | 1 | 4037 | 1/1 | 0.98 | 0.19 | - | 61,61,61,61 | 0 |
| 85 | MG | 1 | 4169 | 1/1 | 0.89 | 0.22 | - | 39,39,39,39 | 0 |
| 85 | MG | AR | 4108 | 1/1 | 0.92 | 0.17 | - | 25,25,25,25 | 0 |
| 85 | MG | 1 | 4185 | 1/1 | 0.84 | 0.56 | - | 48,48,48,48 | 0 |
| 85 | MG | AR | 3849 | 1/1 | 0.86 | 0.59 | - | 18,18,18,18 | 0 |
| 85 | MG | 1 | 4089 | 1/1 | 0.93 | 0.21 | - | 30,30,30,30 | 0 |
| 84 | OHX | 1 | 3669 | 7/7 | 0.96 | 0.23 | - | 125,126,127,127 | 0 |
| 84 | OHX | 1 | 3604 | 7/7 | 0.96 | 0.08 | - | 204,205,206,206 | 0 |
| 85 | MG | AR | 3865 | 1/1 | 0.98 | 0.27 | - | 23,23,23,23 | 0 |
| 85 | MG | CR | 204 | 1/1 | 0.94 | 0.21 | - | 46,46,46,46 | 0 |
| 85 | MG | 1 | 3862 | 1/1 | 0.94 | 0.34 | - | 18,18,18,18 | 0 |
| 85 | MG | 1 | 4068 | 1/1 | 0.95 | 0.20 | - | 39,39,39,39 | 0 |
| 85 | MG | 1 | 3965 | 1/1 | 0.94 | 0.12 | - | 32,32,32,32 | 0 |
| 85 | MG | AS | 223 | 1/1 | 0.89 | 0.23 | - | 59,59,59,59 | 0 |
| 84 | OHX | 1 | 3671 | 7/7 | 0.89 | 0.45 | - | 212,213,214,214 | 0 |
| 85 | MG | AR | 3740 | 1/1 | 0.88 | 0.45 | - | 46,46,46,46 | 0 |
| 85 | MG | 1 | 4127 | 1/1 | 0.93 | 0.16 | - | 58,58,58,58 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 85 | MG | A | 2133 | 1/1 | 0.92 | 0.40 | - | 54,54,54,54 | 0 |
| 85 | MG | A | 2110 | 1/1 | 0.59 | 0.38 | - | 108,108,108,108 | 0 |
| 85 | MG | 3 | 209 | 1/1 | 0.97 | 0.26 | - | 46,46,46,46 | 0 |
| 85 | MG | 1 | 3790 | 1/1 | 0.96 | 0.52 | - | 15,15,15,15 | 0 |
| 85 | MG | 1 | 3955 | 1/1 | 0.75 | 0.28 | - | 52,52,52,52 | 0 |
| 85 | MG | AR | 3785 | 1/1 | 0.97 | 0.29 | - | 29,29,29,29 | 0 |
| 85 | MG | AR | 4005 | 1/1 | 0.96 | 0.35 | - | 24,24,24,24 | 0 |
| 85 | MG | AS | 227 | 1/1 | 0.94 | 0.51 | - | 43,43,43,43 | 0 |
| 85 | MG | 1 | 3921 | 1/1 | 0.96 | 0.23 | - | 45,45,45,45 | 0 |
| 85 | MG | AR | 3953 | 1/1 | 0.89 | 0.21 | - | 35,35,35,35 | 0 |
| 85 | MG | 1 | 3920 | 1/1 | 0.94 | 0.30 | - | 29,29,29,29 | 0 |
| 85 | MG | 4 | 226 | 1/1 | 0.94 | 0.10 | - | 54,54,54,54 | 0 |
| 85 | MG | 6 | 2157 | 1/1 | 0.91 | 0.26 | - | 45,45,45,45 | 0 |
| 85 | MG | 1 | 4029 | 1/1 | 0.86 | 0.49 | - | 42,42,42,42 | 0 |
| 84 | OHX | 6 | 2046 | 7/7 | 0.91 | 0.17 | - | 244,245,247,248 | 0 |
| 85 | MG | A | 2147 | 1/1 | 0.76 | 0.20 | - | 106,106,106,106 | 0 |
| 85 | MG | A | 2083 | 1/1 | 0.96 | 0.37 | - | 62,62,62,62 | 0 |
| 84 | OHX | AR | 3716 | 7/7 | 0.80 | 0.35 | - | 292,293,293,294 | 0 |
| 84 | OHX | 4 | 211 | 7/7 | 0.91 | 0.24 | - | 225,225,226,226 | 0 |
| 85 | MG | AR | 4099 | 1/1 | 0.94 | 0.15 | - | 44,44,44,44 | 0 |
| 85 | MG | AR | 4079 | 1/1 | 0.92 | 0.33 | - | 36,36,36,36 | 0 |
| 85 | MG | A | 2067 | 1/1 | 0.93 | 0.58 | - | 32,32,32,32 | 0 |
| 84 | OHX | 1 | 3661 | 7/7 | 0.91 | 0.56 | - | 251,252,253,253 | 0 |
| 85 | MG | 1 | 3911 | 1/1 | 0.96 | 0.33 | - | 20,20,20,20 | 0 |
| 85 | MG | AR | 4172 | 1/1 | 0.86 | 0.32 | - | 25,25,25,25 | 0 |
| 85 | MG | 1 | 4036 | 1/1 | 0.92 | 0.25 | - | 35,35,35,35 | 0 |
| 85 | MG | 6 | 2065 | 1/1 | 0.76 | 0.46 | - | 32,32,32,32 | 0 |
| 85 | MG | k | 404 | 1/1 | 0.96 | 0.44 | - | 71,71,71,71 | 0 |
| 85 | MG | 6 | 2151 | 1/1 | 0.91 | 0.72 | - | 87,87,87,87 | 0 |
| 85 | MG | AR | 3820 | 1/1 | 0.76 | 0.64 | - | 55,55,55,55 | 0 |
| 85 | MG | 4 | 228 | 1/1 | 0.95 | 0.58 | - | 42,42,42,42 | 0 |
| 85 | MG | 1 | 3770 | 1/1 | 0.97 | 0.47 | - | 11,11,11,11 | 0 |
| 85 | MG | 6 | 2119 | 1/1 | 0.97 | 0.35 | - | 31,31,31,31 | 0 |
| 85 | MG | AR | 4120 | 1/1 | 0.93 | 0.22 | - | 32,32,32,32 | 0 |
| 85 | MG | 1 | 3969 | 1/1 | 0.90 | 0.12 | - | 45,45,45,45 | 0 |
| 85 | MG | AR | 4133 | 1/1 | 0.97 | 0.13 | - | 35,35,35,35 | 0 |
| 85 | MG | 1 | 3831 | 1/1 | 0.92 | 0.27 | - | 42,42,42,42 | 0 |
| 85 | MG | 1 | 3919 | 1/1 | 0.95 | 0.66 | - | 30,30,30,30 | 0 |
| 85 | MG | AR | 3965 | 1/1 | 0.69 | 0.33 | - | 54,54,54,54 | 0 |
| 85 | MG | 6 | 2148 | 1/1 | 0.59 | 0.21 | - | 69,69,69,69 | 0 |
| 85 | MG | A | 2070 | 1/1 | 0.95 | 0.49 | - | 59,59,59,59 | 0 |
| 85 | MG | AR | 3788 | 1/1 | 0.89 | 0.42 | - | 45,45,45,45 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 85 | MG | AR | 4064 | 1/1 | 0.93 | 0.21 | - | 30,30,30,30 | 0 |
| 85 | MG | 6 | 2139 | 1/1 | 0.70 | 0.31 | - | 75,75,75,75 | 0 |
| 85 | MG | 1 | 3816 | 1/1 | 0.98 | 0.36 | - | 28,28,28,28 | 0 |
| 85 | MG | 1 | 3983 | 1/1 | 0.86 | 0.38 | - | 59,59,59,59 | 0 |
| 84 | OHX | 1 | 3624 | 7/7 | 0.96 | 0.20 | - | 171,172,173,174 | 0 |
| 85 | MG | 6 | 2194 | 1/1 | 0.85 | 0.45 | - | 34,34,34,34 | 0 |
| 85 | MG | 1 | 3805 | 1/1 | 0.97 | 0.19 | - | 60,60,60,60 | 0 |
| 85 | MG | AS | 214 | 1/1 | 0.85 | 0.26 | - | 68,68,68,68 | 0 |
| 85 | MG | 1 | 3795 | 1/1 | 0.85 | 0.32 | - | 37,37,37,37 | 0 |
| 85 | MG | 1 | 4054 | 1/1 | 0.99 | 0.14 | - | 40,40,40,40 | 0 |
| 84 | OHX | A | 2011 | 7/7 | 0.94 | 0.17 | - | 208,209,211,211 | 0 |
| 84 | OHX | 1 | 3436 | 7/7 | 0.99 | 0.11 | - | 101,102,104,104 | 0 |
| 84 | OHX | AR | 3432 | 7/7 | 0.99 | 0.13 | - | 91,91,91,91 | 0 |
| 85 | MG | AR | 4236 | 1/1 | 0.98 | 0.32 | - | 22,22,22,22 | 0 |
| 85 | MG | A | 2122 | 1/1 | 0.93 | 0.41 | - | 42,42,42,42 | 0 |
| 84 | OHX | 6 | 2022 | 7/7 | 0.92 | 0.11 | - | 235,235,238,239 | 0 |
| 85 | MG | AR | 3918 | 1/1 | 0.94 | 0.40 | - | 21,21,21,21 | 0 |
| 85 | MG | 6 | 2078 | 1/1 | 0.95 | 0.43 | - | 25,25,25,25 | 0 |
| 85 | MG | AR | 3958 | 1/1 | 0.55 | 0.59 | - | 90,90,90,90 | 0 |
| 85 | MG | CO | 202 | 1/1 | 0.67 | 0.78 | - | 57,57,57,57 | 0 |
| 84 | OHX | 6 | 2051 | 7/7 | 0.80 | 0.36 | - | 228,229,230,231 | 0 |
| 85 | MG | 1 | 3734 | 1/1 | 0.95 | 0.32 | - | 27,27,27,27 | 0 |
| 84 | OHX | 1 | 3564 | 7/7 | 0.93 | 0.18 | - | 173,175,175,175 | 0 |
| 85 | MG | 1 | 4006 | 1/1 | 0.92 | 0.23 | - | 33,33,33,33 | 0 |
| 85 | MG | 1 | 4010 | 1/1 | 0.56 | 0.61 | - | 44,44,44,44 | 0 |
| 85 | MG | AR | 4017 | 1/1 | 0.96 | 0.17 | - | 27,27,27,27 | 0 |
| 84 | OHX | 1 | 3697 | 7/7 | 0.92 | 0.22 | - | 238,240,241,241 | 0 |
| 85 | MG | 1 | 3763 | 1/1 | 0.94 | 0.31 | - | 34,34,34,34 | 0 |
| 84 | OHX | AR | 3676 | 7/7 | 0.92 | 0.29 | - | 196,197,198,198 | 0 |
| 85 | MG | AR | 3982 | 1/1 | 0.91 | 0.26 | - | 35,35,35,35 | 0 |
| 84 | OHX | AR | 3651 | 7/7 | 0.95 | 0.22 | - | 229,230,231,231 | 0 |
| 85 | MG | AP | 503 | 1/1 | 0.61 | 0.19 | - | 61,61,61,61 | 0 |
| 85 | MG | 1 | 3735 | 1/1 | 0.93 | 0.23 | - | 39,39,39,39 | 0 |
| 85 | MG | 1 | 3941 | 1/1 | 0.83 | 0.30 | - | 36,36,36,36 | 0 |
| 85 | MG | AR | 4238 | 1/1 | 0.97 | 0.48 | - | 27,27,27,27 | 0 |
| 85 | MG | d3 | 201 | 1/1 | 0.96 | 0.13 | - | 48,48,48,48 | 0 |
| 85 | MG | AR | 4122 | 1/1 | 0.75 | 0.43 | - | 70,70,70,70 | 0 |
| 85 | MG | A | 2112 | 1/1 | 0.61 | 0.41 | - | 77,77,77,77 | 0 |
| 85 | MG | AR | 3844 | 1/1 | 0.92 | 0.26 | - | 25,25,25,25 | 0 |
| 85 | MG | 1 | 4118 | 1/1 | 0.98 | 0.23 | - | 87,87,87,87 | 0 |
| 85 | MG | 1 | 3760 | 1/1 | 0.94 | 0.62 | - | 26,26,26,26 | 0 |
| 85 | MG | 1 | 4144 | 1/1 | 0.94 | 0.20 | - | 59,59,59,59 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 85 | MG | 6 | 2080 | 1/1 | 0.94 | 0.15 | - | 53,53,53,53 | 0 |
| 85 | MG | 4 | 214 | 1/1 | 0.95 | 0.46 | - | 18,18,18,18 | 0 |
| 85 | MG | 1 | 3761 | 1/1 | 0.87 | 0.42 | - | 44,44,44,44 | 0 |
| 85 | MG | 1 | 3932 | 1/1 | 0.98 | 0.25 | - | 24,24,24,24 | 0 |
| 85 | MG | 1 | 4187 | 1/1 | 1.00 | 0.10 | - | 55,55,55,55 | 0 |
| 84 | OHX | AR | 3682 | 7/7 | 0.89 | 0.42 | - | 213,214,214,215 | 0 |
| 85 | MG | b | 101 | 1/1 | 0.87 | 0.22 | - | 57,57,57,57 | 0 |
| 84 | OHX | AR | 3735 | 7/7 | 0.86 | 0.31 | - | 246,247,248,248 | 0 |
| 85 | MG | 1 | 4020 | 1/1 | 0.96 | 0.12 | - | 38,38,38,38 | 0 |
| 85 | MG | AR | 3808 | 1/1 | 0.86 | 0.24 | - | 33,33,33,33 | 0 |
| 85 | MG | 1 | 4139 | 1/1 | 0.96 | 0.18 | - | 29,29,29,29 | 0 |
| 84 | OHX | CM | 201 | 7/7 | 0.88 | 0.22 | - | 247,248,249,250 | 0 |
| 85 | MG | A | 2063 | 1/1 | 0.97 | 0.42 | - | 36,36,36,36 | 0 |
| 85 | MG | 1 | 3940 | 1/1 | 0.93 | 0.21 | - | 21,21,21,21 | 0 |
| 85 | MG | 1 | 4199 | 1/1 | 0.88 | 0.62 | - | 25,25,25,25 | 0 |
| 84 | OHX | AR | 3558 | 7/7 | 0.95 | 0.22 | - | 159,160,160,160 | 0 |
| 84 | OHX | AR | 3476 | 7/7 | 0.98 | 0.12 | - | 127,128,129,130 | 0 |
| 84 | OHX | A | 2037 | 7/7 | 0.93 | 0.28 | - | 238,240,241,241 | 0 |
| 85 | MG | AR | 3976 | 1/1 | 0.83 | 0.41 | - | 42,42,42,42 | 0 |
| 84 | OHX | A | 2025 | 7/7 | 0.85 | 0.24 | - | 249,252,253,253 | 0 |
| 85 | MG | A | 2132 | 1/1 | 0.91 | 0.27 | - | 71,71,71,71 | 0 |
| 84 | OHX | 6 | 1912 | 7/7 | 0.99 | 0.09 | - | 107,108,110,110 | 0 |
| 85 | MG | 1 | 3867 | 1/1 | 0.95 | 0.37 | - | 26,26,26,26 | 0 |
| 85 | MG | AR | 3751 | 1/1 | 0.98 | 0.21 | - | 29,29,29,29 | 0 |
| 85 | MG | AR | 4036 | 1/1 | 0.77 | 0.25 | - | 68,68,68,68 | 0 |
| 84 | OHX | 1 | 3598 | 7/7 | 0.96 | 0.14 | - | 173,173,174,175 | 0 |
| 84 | OHX | 1 | 3455 | 7/7 | 0.98 | 0.13 | - | 104,104,105,105 | 0 |
| 85 | MG | 1 | 3879 | 1/1 | 0.93 | 0.29 | - | 47,47,47,47 | 0 |
| 85 | MG | AR | 3990 | 1/1 | 0.81 | 0.41 | - | 37,37,37,37 | 0 |
| 85 | MG | AR | 4044 | 1/1 | 0.93 | 0.25 | - | 51,51,51,51 | 0 |
| 85 | MG | AR | 4035 | 1/1 | 0.92 | 0.20 | - | 39,39,39,39 | 0 |
| 85 | MG | 4 | 216 | 1/1 | 0.96 | 0.20 | - | 42,42,42,42 | 0 |
| 85 | MG | 1 | 4038 | 1/1 | 0.83 | 0.34 | - | 33,33,33,33 | 0 |
| 85 | MG | 1 | 4181 | 1/1 | 0.84 | 0.23 | - | 50,50,50,50 | 0 |
| 85 | MG | A | 2139 | 1/1 | 0.72 | 0.33 | - | 86,86,86,86 | 0 |
| 85 | MG | 1 | 4152 | 1/1 | 0.88 | 0.20 | - | 40,40,40,40 | 0 |
| 85 | MG | AS | 212 | 1/1 | 0.95 | 0.38 | - | 13,13,13,13 | 0 |
| 85 | MG | A | 2129 | 1/1 | 0.69 | 0.45 | - | 58,58,58,58 | 0 |
| 85 | MG | 3 | 218 | 1/1 | 0.78 | 0.31 | - | 49,49,49,49 | 0 |
| 84 | OHX | c3 | 201 | 7/7 | 0.89 | 0.25 | - | 212,213,214,215 | 0 |
| 85 | MG | 1 | 4074 | 1/1 | 0.96 | 0.16 | - | 45,45,45,45 | 0 |
| 84 | OHX | AR | 3664 | 7/7 | 0.74 | 0.30 | - | 287,287,288,288 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | OHX | 6 | 1931 | 7/7 | 0.97 | 0.12 | - | 151,152,153,153 | 0 |
| 85 | MG | 6 | 2089 | 1/1 | 0.93 | 0.25 | - | 34,34,34,34 | 0 |
| 85 | MG | A | 2126 | 1/1 | 0.93 | 0.16 | - | 48,48,48,48 | 0 |
| 85 | MG | 1 | 4212 | 1/1 | 0.99 | 0.32 | - | 27,27,27,27 | 0 |
| 84 | OHX | 4 | 202 | 7/7 | 0.97 | 0.11 | - | 157,158,158,158 | 0 |
| 85 | MG | AR | 3803 | 1/1 | 0.84 | 0.21 | - | 54,54,54,54 | 0 |
| 85 | MG | 1 | 3926 | 1/1 | 0.96 | 0.54 | - | 21,21,21,21 | 0 |
| 85 | MG | 1 | 3961 | 1/1 | 0.88 | 0.35 | - | 26,26,26,26 | 0 |
| 85 | MG | 1 | 4132 | 1/1 | 0.95 | 0.37 | - | 42,42,42,42 | 0 |
| 85 | MG | A | 2097 | 1/1 | 0.92 | 0.32 | - | 55,55,55,55 | 0 |
| 85 | MG | l | 402 | 1/1 | 0.65 | 0.45 | - | 32,32,32,32 | 0 |
| 85 | MG | AR | 4093 | 1/1 | 0.82 | 0.34 | - | 46,46,46,46 | 0 |
| 85 | MG | AS | 216 | 1/1 | 0.80 | 0.68 | - | 41,41,41,41 | 0 |
| 85 | MG | A | 2069 | 1/1 | 0.85 | 0.29 | - | 36,36,36,36 | 0 |
| 85 | MG | AR | 4007 | 1/1 | 0.97 | 0.11 | - | 23,23,23,23 | 0 |
| 85 | MG | A | 2102 | 1/1 | 0.97 | 0.32 | - | 52,52,52,52 | 0 |
| 85 | MG | A | 2077 | 1/1 | 0.96 | 0.19 | - | 25,25,25,25 | 0 |
| 84 | OHX | 1 | 3570 | 7/7 | 0.94 | 0.15 | - | 202,203,204,205 | 0 |
| 84 | OHX | 1 | 3653 | 7/7 | 0.93 | 0.42 | - | 193,195,196,196 | 0 |
| 85 | MG | 1 | 4028 | 1/1 | 0.91 | 0.28 | - | 24,24,24,24 | 0 |
| 85 | MG | 1 | 3933 | 1/1 | 0.90 | 0.23 | - | 37,37,37,37 | 0 |
| 85 | MG | z | 203 | 1/1 | 0.87 | 0.20 | - | 45,45,45,45 | 0 |
| 85 | MG | 1 | 3975 | 1/1 | 0.89 | 0.17 | - | 43,43,43,43 | 0 |
| 85 | MG | AR | 3871 | 1/1 | 0.96 | 0.50 | - | 20,20,20,20 | 0 |
| 85 | MG | 6 | 2101 | 1/1 | 0.97 | 0.28 | - | 37,37,37,37 | 0 |
| 85 | MG | AR | 4149 | 1/1 | 0.97 | 0.13 | - | 28,28,28,28 | 0 |
| 85 | MG | 1 | 3967 | 1/1 | 0.94 | 0.16 | - | 47,47,47,47 | 0 |
| 85 | MG | AR | 3873 | 1/1 | 0.96 | 0.31 | - | 23,23,23,23 | 0 |
| 85 | MG | AR | 4054 | 1/1 | 0.94 | 0.24 | - | 33,33,33,33 | 0 |
| 85 | MG | DC | 203 | 1/1 | 0.84 | 0.25 | - | 35,35,35,35 | 0 |
| 85 | MG | 1 | 3799 | 1/1 | 0.95 | 0.29 | - | 28,28,28,28 | 0 |
| 85 | MG | 1 | 4016 | 1/1 | 0.94 | 0.17 | - | 11,11,11,11 | 0 |
| 85 | MG | 4 | 227 | 1/1 | 0.92 | 0.22 | - | 42,42,42,42 | 0 |
| 85 | MG | AR | 4156 | 1/1 | 0.82 | 0.49 | - | 71,71,71,71 | 0 |
| 84 | OHX | 6 | 1939 | 7/7 | 0.98 | 0.11 | - | 131,133,134,135 | 0 |
| 85 | MG | 1 | 3982 | 1/1 | 0.38 | 0.26 | - | 98,98,98,98 | 0 |
| 85 | MG | CF | 403 | 1/1 | 0.87 | 0.29 | - | 30,30,30,30 | 0 |
| 84 | OHX | 1 | 3525 | 7/7 | 0.98 | 0.10 | - | 151,152,153,154 | 0 |
| 84 | OHX | AR | 3678 | 7/7 | 0.91 | 0.53 | - | 238,238,239,239 | 0 |
| 84 | OHX | AR | 3629 | 7/7 | 0.92 | 0.31 | - | 209,210,211,212 | 0 |
| 85 | MG | o | 303 | 1/1 | 0.88 | 0.21 | - | 38,38,38,38 | 0 |
| 85 | MG | 1 | 4072 | 1/1 | 0.93 | 0.23 | - | 55,55,55,55 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 85 | MG | 1 | 4154 | 1/1 | 0.95 | 0.20 | - | 92,92,92,92 | 0 |
| 85 | MG | AR | 3818 | 1/1 | 0.88 | 0.27 | - | 45,45,45,45 | 0 |
| 85 | MG | 1 | 3950 | 1/1 | 0.84 | 0.11 | - | 70,70,70,70 | 0 |
| 85 | MG | 1 | 4134 | 1/1 | 0.85 | 0.19 | - | 50,50,50,50 | 0 |
| 85 | MG | AR | 4211 | 1/1 | 0.80 | 0.23 | - | 86,86,86,86 | 0 |
| 85 | MG | A | 2071 | 1/1 | 0.94 | 0.32 | - | 45,45,45,45 | 0 |
| 84 | OHX | AR | 3598 | 7/7 | 0.91 | 0.17 | - | 205,206,207,208 | 0 |
| 85 | MG | AR | 3956 | 1/1 | 0.91 | 0.20 | - | 41,41,41,41 | 0 |
| 85 | MG | AR | 4043 | 1/1 | 0.85 | 0.33 | - | 48,48,48,48 | 0 |
| 85 | MG | AR | 3843 | 1/1 | 0.98 | 0.24 | - | 13,13,13,13 | 0 |
| 85 | MG | AR | 3977 | 1/1 | 0.92 | 0.55 | - | 26,26,26,26 | 0 |
| 85 | MG | A | 2114 | 1/1 | 0.91 | 0.36 | - | 41,41,41,41 | 0 |
| 85 | MG | 1 | 3959 | 1/1 | 0.94 | 0.23 | - | 54,54,54,54 | 0 |
| 85 | MG | 6 | 2131 | 1/1 | 0.96 | 0.38 | - | 32,32,32,32 | 0 |
| 85 | MG | AR | 4234 | 1/1 | 0.84 | 0.28 | - | 17,17,17,17 | 0 |
| 85 | MG | 6 | 2095 | 1/1 | 0.93 | 0.58 | - | 32,32,32,32 | 0 |
| 85 | MG | 3 | 219 | 1/1 | 0.94 | 0.14 | - | 77,77,77,77 | 0 |
| 85 | MG | AR | 3989 | 1/1 | 0.93 | 0.33 | - | 85,85,85,85 | 0 |
| 85 | MG | 1 | 3750 | 1/1 | 0.97 | 0.08 | - | 70,70,70,70 | 0 |
| 85 | MG | A | 2145 | 1/1 | 0.99 | 0.21 | - | 83,83,83,83 | 0 |
| 85 | MG | 3 | 215 | 1/1 | 0.93 | 0.23 | - | 39,39,39,39 | 0 |
| 85 | MG | 1 | 3952 | 1/1 | 0.92 | 0.16 | - | 34,34,34,34 | 0 |
| 85 | MG | 1 | 3749 | 1/1 | 0.87 | 0.35 | - | 38,38,38,38 | 0 |
| 85 | MG | AR | 3987 | 1/1 | 0.98 | 0.33 | - | 50,50,50,50 | 0 |
| 85 | MG | 1 | 4053 | 1/1 | 0.95 | 0.18 | - | 32,32,32,32 | 0 |
| 85 | MG | 6 | 2134 | 1/1 | 0.84 | 0.21 | - | 43,43,43,43 | 0 |
| 85 | MG | AR | 3921 | 1/1 | 0.95 | 0.27 | - | 10,10,10,10 | 0 |
| 85 | MG | 6 | 2102 | 1/1 | 0.94 | 0.30 | - | 14,14,14,14 | 0 |
| 85 | MG | 1 | 4122 | 1/1 | 0.95 | 0.49 | - | 45,45,45,45 | 0 |
| 84 | OHX | AR | 3720 | 7/7 | 0.70 | 0.34 | - | 267,269,269,270 | 0 |
| 85 | MG | AR | 3833 | 1/1 | 0.96 | 0.15 | - | 37,37,37,37 | 0 |
| 84 | OHX | AR | 3727 | 7/7 | 0.82 | 0.34 | - | 277,279,280,280 | 0 |
| 85 | MG | 1 | 4145 | 1/1 | 0.95 | 0.18 | - | 48,48,48,48 | 0 |
| 85 | MG | AR | 3841 | 1/1 | 0.99 | 0.32 | - | 25,25,25,25 | 0 |
| 85 | MG | AR | 4207 | 1/1 | 1.00 | 0.14 | - | 50,50,50,50 | 0 |
| 85 | MG | 1 | 4045 | 1/1 | 0.92 | 0.11 | - | 62,62,62,62 | 0 |
| 85 | MG | AR | 3827 | 1/1 | 0.94 | 0.45 | - | 40,40,40,40 | 0 |
| 85 | MG | AR | 4216 | 1/1 | 0.94 | 0.30 | - | 67,67,67,67 | 0 |
| 85 | MG | AR | 3884 | 1/1 | 0.90 | 0.27 | - | 27,27,27,27 | 0 |
| 85 | MG | AR | 4231 | 1/1 | 0.97 | 0.34 | - | 9,9,9,9 | 0 |
| 85 | MG | AR | 4060 | 1/1 | 0.90 | 0.27 | - | 56,56,56,56 | 0 |
| 85 | MG | 1 | 3824 | 1/1 | 0.65 | 0.26 | - | 77,77,77,77 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 85 | MG | A | 2138 | 1/1 | 0.97 | 0.29 | - | 35,35,35,35 | 0 |
| 85 | MG | 1 | 4025 | 1/1 | 0.93 | 0.24 | - | 34,34,34,34 | 0 |
| 85 | MG | AR | 3778 | 1/1 | 0.94 | 0.37 | - | 42,42,42,42 | 0 |
| 85 | MG | A | 2098 | 1/1 | 0.78 | 0.44 | - | 72,72,72,72 | 0 |
| 85 | MG | 6 | 2160 | 1/1 | 0.91 | 0.24 | - | 121,121,121,121 | 0 |
| 84 | OHX | A | 2007 | 7/7 | 0.85 | 0.20 | - | 275,277,278,279 | 0 |
| 85 | MG | 1 | 3861 | 1/1 | 0.97 | 0.14 | - | 65,65,65,65 | 0 |
| 84 | OHX | 1 | 3670 | 7/7 | 0.90 | 0.30 | - | 215,215,217,217 | 0 |
| 85 | MG | 1 | 3827 | 1/1 | 0.97 | 0.27 | - | 21,21,21,21 | 0 |
| 85 | MG | AR | 4151 | 1/1 | 0.69 | 0.28 | - | 30,30,30,30 | 0 |
| 84 | OHX | A | 2005 | 7/7 | 0.90 | 0.45 | - | 204,206,207,207 | 0 |
| 85 | MG | AR | 3998 | 1/1 | 0.90 | 0.49 | - | 18,18,18,18 | 0 |
| 85 | MG | AR | 3920 | 1/1 | 0.96 | 0.34 | - | 19,19,19,19 | 0 |
| 85 | MG | 1 | 4160 | 1/1 | 0.93 | 0.26 | - | 40,40,40,40 | 0 |
| 85 | MG | A | 2094 | 1/1 | 0.62 | 0.28 | - | 110,110,110,110 | 0 |
| 85 | MG | 1 | 3864 | 1/1 | 0.82 | 0.50 | - | 33,33,33,33 | 0 |
| 85 | MG | AR | 4140 | 1/1 | 0.90 | 0.26 | - | 24,24,24,24 | 0 |
| 84 | OHX | 1 | 3674 | 7/7 | 0.87 | 0.36 | - | 212,212,213,213 | 0 |
| 85 | MG | AR | 3997 | 1/1 | 0.94 | 0.26 | - | 45,45,45,45 | 0 |
| 85 | MG | AR | 4113 | 1/1 | 0.96 | 0.30 | - | 17,17,17,17 | 0 |
| 84 | OHX | 6 | 2048 | 7/7 | 0.89 | 0.43 | - | 224,224,225,226 | 0 |
| 84 | OHX | 6 | 2018 | 7/7 | 0.96 | 0.27 | - | 186,187,188,189 | 0 |
| 85 | MG | 1 | 3895 | 1/1 | 0.90 | 0.27 | - | 29,29,29,29 | 0 |
| 85 | MG | AR | 4115 | 1/1 | 0.96 | 0.34 | - | 64,64,64,64 | 0 |
| 85 | MG | 1 | 3886 | 1/1 | 0.98 | 0.43 | - | 24,24,24,24 | 0 |
| 85 | MG | AR | 3960 | 1/1 | 0.94 | 0.15 | - | 17,17,17,17 | 0 |
| 85 | MG | AS | 220 | 1/1 | 0.82 | 0.21 | - | 42,42,42,42 | 0 |
| 85 | MG | 4 | 233 | 1/1 | 0.86 | 0.61 | - | 61,61,61,61 | 0 |
| 85 | MG | AR | 4130 | 1/1 | 0.89 | 0.17 | - | 19,19,19,19 | 0 |
| 85 | MG | 1 | 4100 | 1/1 | 0.83 | 0.30 | - | 87,87,87,87 | 0 |
| 85 | MG | AR | 4220 | 1/1 | 0.78 | 0.38 | - | 54,54,54,54 | 0 |
| 85 | MG | AR | 3972 | 1/1 | 0.93 | 0.30 | - | 38,38,38,38 | 0 |
| 84 | OHX | CF | 402 | 7/7 | 0.88 | 0.47 | - | 254,255,256,256 | 0 |
| 85 | MG | AR | 4132 | 1/1 | 0.98 | 0.08 | - | 36,36,36,36 | 0 |
| 85 | MG | AR | 3796 | 1/1 | 0.93 | 0.59 | - | 32,32,32,32 | 0 |
| 85 | MG | AR | 4016 | 1/1 | 0.91 | 0.45 | - | 104,104,104,104 | 0 |
| 84 | OHX | AR | 3468 | 7/7 | 0.98 | 0.11 | - | 111,112,113,114 | 0 |
| 84 | OHX | 1 | 3469 | 7/7 | 0.98 | 0.12 | - | 118,118,119,120 | 0 |
| 84 | OHX | 1 | 3513 | 7/7 | 0.97 | 0.13 | - | 140,141,142,142 | 0 |
| 85 | MG | 1 | 3935 | 1/1 | 0.96 | 0.24 | - | 24,24,24,24 | 0 |
| 85 | MG | AR | 3829 | 1/1 | 0.98 | 0.42 | - | 16,16,16,16 | 0 |
| 84 | OHX | 6 | 2020 | 7/7 | 0.95 | 0.23 | - | 177,178,179,179 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | OHX | AR | 3665 | 7/7 | 0.95 | 0.26 | - | 189,189,189,189 | 0 |
| 85 | MG | AR | 3780 | 1/1 | 0.95 | 0.27 | - | 20,20,20,20 | 0 |
| 85 | MG | AR | 4039 | 1/1 | 0.91 | 0.28 | - | 37,37,37,37 | 0 |
| 85 | MG | AR | 3859 | 1/1 | 0.94 | 0.27 | - | 28,28,28,28 | 0 |
| 85 | MG | AR | 4104 | 1/1 | 0.91 | 0.30 | - | 55,55,55,55 | 0 |
| 85 | MG | 1 | 3954 | 1/1 | 0.96 | 0.16 | - | 45,45,45,45 | 0 |
| 85 | MG | 1 | 3880 | 1/1 | 0.90 | 0.51 | - | 29,29,29,29 | 0 |
| 85 | MG | 1 | 3908 | 1/1 | 0.97 | 0.36 | - | 14,14,14,14 | 0 |
| 85 | MG | 3 | 211 | 1/1 | 0.97 | 0.30 | - | 33,33,33,33 | 0 |
| 84 | OHX | AR | 3419 | 7/7 | 0.99 | 0.13 | - | 94,94,95,95 | 0 |
| 85 | MG | AR | 3795 | 1/1 | 0.91 | 0.19 | - | 22,22,22,22 | 0 |
| 85 | MG | CU | 201 | 1/1 | 0.94 | 0.19 | - | 44,44,44,44 | 0 |
| 85 | MG | A | 2076 | 1/1 | 0.83 | 0.25 | - | 50,50,50,50 | 0 |
| 85 | MG | AR | 4144 | 1/1 | 0.96 | 0.15 | - | 35,35,35,35 | 0 |
| 85 | MG | 1 | 3939 | 1/1 | 0.86 | 0.32 | - | 29,29,29,29 | 0 |
| 84 | OHX | AR | 3647 | 7/7 | 0.92 | 0.31 | - | 203,204,205,205 | 0 |
| 85 | MG | AR | 4210 | 1/1 | 0.98 | 0.37 | - | 33,33,33,33 | 0 |
| 85 | MG | 6 | 2144 | 1/1 | 0.89 | 0.31 | - | 42,42,42,42 | 0 |
| 85 | MG | AR | 3893 | 1/1 | 0.73 | 0.58 | - | 40,40,40,40 | 0 |
| 85 | MG | A | 2058 | 1/1 | 0.96 | 0.48 | - | 27,27,27,27 | 0 |
| 85 | MG | 1 | 4121 | 1/1 | 0.91 | 0.28 | - | 32,32,32,32 | 0 |
| 85 | MG | 1 | 4073 | 1/1 | 0.70 | 0.30 | - | 79,79,79,79 | 0 |
| 84 | OHX | 1 | 3565 | 7/7 | 0.95 | 0.16 | - | 168,169,170,170 | 0 |
| 85 | MG | 1 | 4097 | 1/1 | 1.00 | 0.17 | - | 61,61,61,61 | 0 |
| 85 | MG | 6 | 2104 | 1/1 | 0.94 | 0.24 | - | 22,22,22,22 | 0 |
| 85 | MG | 1 | 4202 | 1/1 | 0.90 | 0.33 | - | 27,27,27,27 | 0 |
| 85 | MG | AR | 3904 | 1/1 | 0.97 | 0.73 | - | 11,11,11,11 | 0 |
| 85 | MG | 1 | 4003 | 1/1 | 0.85 | 0.41 | - | 46,46,46,46 | 0 |
| 85 | MG | 1 | 3787 | 1/1 | 0.98 | 0.28 | - | 15,15,15,15 | 0 |
| 85 | MG | AR | 4119 | 1/1 | 0.83 | 0.19 | - | 77,77,77,77 | 0 |
| 85 | MG | AR | 3742 | 1/1 | 0.93 | 0.34 | - | 29,29,29,29 | 0 |
| 85 | MG | 1 | 4043 | 1/1 | 0.90 | 0.35 | - | 40,40,40,40 | 0 |
| 85 | MG | AR | 4062 | 1/1 | 0.86 | 0.20 | - | 54,54,54,54 | 0 |
| 85 | MG | 1 | 3974 | 1/1 | 0.81 | 0.39 | - | 43,43,43,43 | 0 |
| 85 | MG | 1 | 4151 | 1/1 | 0.96 | 0.15 | - | 53,53,53,53 | 0 |
| 85 | MG | CR | 203 | 1/1 | 0.82 | 0.33 | - | 74,74,74,74 | 0 |
| 85 | MG | 4 | 223 | 1/1 | 0.97 | 0.26 | - | 44,44,44,44 | 0 |
| 85 | MG | AR | 3966 | 1/1 | 0.95 | 0.24 | - | 24,24,24,24 | 0 |
| 85 | MG | k | 403 | 1/1 | 0.99 | 0.21 | - | 24,24,24,24 | 0 |
| 85 | MG | 1 | 3878 | 1/1 | 0.98 | 0.18 | - | 36,36,36,36 | 0 |
| 85 | MG | AR | 3774 | 1/1 | 0.92 | 0.21 | - | 23,23,23,23 | 0 |
| 85 | MG | AR | 4069 | 1/1 | 0.93 | 0.20 | - | 53,53,53,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 85 | MG | A | 2103 | 1/1 | 0.71 | 0.43 | - | 64,64,64,64 | 0 |
| 85 | MG | 1 | 4014 | 1/1 | 0.78 | 0.16 | - | 46,46,46,46 | 0 |
| 84 | OHX | AR | 3625 | 7/7 | 0.94 | 0.19 | - | 216,216,218,219 | 0 |
| 85 | MG | AR | 4112 | 1/1 | 0.96 | 0.14 | - | 70,70,70,70 | 0 |
| 85 | MG | AR | 4034 | 1/1 | 0.91 | 0.25 | - | 42,42,42,42 | 0 |
| 85 | MG | AR | 3863 | 1/1 | 0.96 | 0.60 | - | 15,15,15,15 | 0 |
| 85 | MG | x | 207 | 1/1 | 0.97 | 0.15 | - | 17,17,17,17 | 0 |
| 85 | MG | AR | 3798 | 1/1 | 0.96 | 0.39 | - | 21,21,21,21 | 0 |
| 85 | MG | AR | 4222 | 1/1 | 0.98 | 0.15 | - | 27,27,27,27 | 0 |
| 85 | MG | AS | 225 | 1/1 | 0.96 | 0.15 | - | 67,67,67,67 | 0 |
| 84 | OHX | 1 | 3709 | 7/7 | 0.83 | 0.43 | - | 229,231,231,232 | 0 |
| 84 | OHX | 1 | 3606 | 7/7 | 0.88 | 0.28 | - | 193,194,194,195 | 0 |
| 85 | MG | AR | 3861 | 1/1 | 0.96 | 0.42 | - | 16,16,16,16 | 0 |
| 85 | MG | AR | 3823 | 1/1 | 0.93 | 0.56 | - | 15,15,15,15 | 0 |
| 84 | OHX | AR | 3566 | 7/7 | 0.95 | 0.17 | - | 205,206,207,207 | 0 |
| 85 | MG | AR | 3784 | 1/1 | 0.84 | 0.38 | - | 29,29,29,29 | 0 |
| 84 | OHX | 6 | 2021 | 7/7 | 0.93 | 0.32 | - | 210,210,212,213 | 0 |
| 85 | MG | AR | 4150 | 1/1 | 0.96 | 0.12 | - | 49,49,49,49 | 0 |
| 85 | MG | 6 | 2070 | 1/1 | 0.96 | 0.56 | - | 17,17,17,17 | 0 |
| 85 | MG | A | 2134 | 1/1 | 0.90 | 0.55 | - | 34,34,34,34 | 0 |
| 84 | OHX | A | 2022 | 7/7 | 0.93 | 0.29 | - | 229,230,232,233 | 0 |
| 85 | MG | 1 | 3997 | 1/1 | 0.93 | 0.30 | - | 37,37,37,37 | 0 |
| 85 | MG | A | 2121 | 1/1 | 0.93 | 0.08 | - | 66,66,66,66 | 0 |
| 85 | MG | AR | 3908 | 1/1 | 0.98 | 0.46 | - | 18,18,18,18 | 0 |
| 85 | MG | AR | 3754 | 1/1 | 0.98 | 0.14 | - | 35,35,35,35 | 0 |
| 85 | MG | 1 | 3854 | 1/1 | 0.96 | 0.40 | - | 13,13,13,13 | 0 |
| 85 | MG | 4 | 218 | 1/1 | 0.92 | 0.52 | - | 7,7,7,7 | 0 |
| 85 | MG | AR | 4134 | 1/1 | 0.97 | 0.28 | - | 10,10,10,10 | 0 |
| 85 | MG | 4 | 220 | 1/1 | 0.98 | 0.37 | - | 37,37,37,37 | 0 |
| 85 | MG | 1 | 3877 | 1/1 | 0.89 | 0.13 | - | 44,44,44,44 | 0 |
| 85 | MG | AR | 4042 | 1/1 | 0.89 | 0.26 | - | 20,20,20,20 | 0 |
| 85 | MG | 1 | 3978 | 1/1 | 0.83 | 0.30 | - | 32,32,32,32 | 0 |
| 85 | MG | AR | 4075 | 1/1 | 0.92 | 0.32 | - | 35,35,35,35 | 0 |
| 85 | MG | 1 | 4027 | 1/1 | 0.75 | 0.35 | - | 51,51,51,51 | 0 |
| 84 | OHX | 1 | 3649 | 7/7 | 0.90 | 0.20 | - | 247,248,249,250 | 0 |
| 85 | MG | AR | 3766 | 1/1 | 0.90 | 0.23 | - | 21,21,21,21 | 0 |
| 85 | MG | 1 | 4107 | 1/1 | 0.60 | 0.28 | - | 66,66,66,66 | 0 |
| 85 | MG | 1 | 3814 | 1/1 | 0.97 | 0.31 | - | 39,39,39,39 | 0 |
| 85 | MG | AR | 3993 | 1/1 | 0.89 | 0.21 | - | 62,62,62,62 | 0 |
| 85 | MG | s8 | 302 | 1/1 | 0.90 | 0.27 | - | 44,44,44,44 | 0 |
| 85 | MG | AR | 4077 | 1/1 | 0.81 | 0.34 | - | 49,49,49,49 | 0 |
| 85 | MG | 6 | 2152 | 1/1 | 0.77 | 0.30 | - | 57,57,57,57 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | OHX | A | 2036 | 7/7 | 0.88 | 0.13 | - | 274,277,278,279 | 0 |
| 85 | MG | AR | 4059 | 1/1 | 0.78 | 0.15 | - | 67,67,67,67 | 0 |
| 85 | MG | 6 | 2115 | 1/1 | 0.96 | 0.36 | - | 36,36,36,36 | 0 |
| 85 | MG | AR | 4051 | 1/1 | 0.99 | 0.12 | - | 62,62,62,62 | 0 |
| 85 | MG | AS | 228 | 1/1 | 0.67 | 0.25 | - | 48,48,48,48 | 0 |
| 84 | OHX | AR | 3623 | 7/7 | 0.94 | 0.17 | - | 186,187,188,188 | 0 |
| 84 | OHX | 1 | 3724 | 7/7 | 0.89 | 0.51 | - | 243,244,245,246 | 0 |
| 85 | MG | A | 2045 | 1/1 | 0.93 | 0.42 | - | 35,35,35,35 | 0 |
| 85 | MG | 1 | 4035 | 1/1 | 0.97 | 0.19 | - | 131,131,131,131 | 0 |
| 84 | OHX | 1 | 3524 | 7/7 | 0.97 | 0.23 | - | 164,164,166,167 | 0 |
| 85 | MG | 1 | 4196 | 1/1 | 0.96 | 0.36 | - | 35,35,35,35 | 0 |
| 85 | MG | 1 | 4203 | 1/1 | 0.93 | 0.52 | - | 34,34,34,34 | 0 |
| 85 | MG | 1 | 4150 | 1/1 | 0.86 | 1.02 | - | 73,73,73,73 | 0 |
| 85 | MG | AR | 4204 | 1/1 | 0.94 | 0.21 | - | 31,31,31,31 | 0 |
| 85 | MG | 1 | 4102 | 1/1 | 0.72 | 0.39 | - | 40,40,40,40 | 0 |
| 84 | OHX | AR | 3599 | 7/7 | 0.92 | 0.30 | - | 201,202,203,203 | 0 |
| 85 | MG | 1 | 4213 | 1/1 | 0.94 | 0.21 | - | 36,36,36,36 | 0 |
| 84 | OHX | A | 2032 | 7/7 | 0.91 | 0.19 | - | 234,236,237,239 | 0 |
| 85 | MG | 1 | 4125 | 1/1 | 0.94 | 0.20 | - | 58,58,58,58 | 0 |
| 85 | MG | A | 2146 | 1/1 | 0.88 | 0.61 | - | 29,29,29,29 | 0 |
| 85 | MG | 6 | 2179 | 1/1 | 0.79 | 0.30 | - | 52,52,52,52 | 0 |
| 84 | OHX | 6 | 1976 | 7/7 | 0.83 | 0.42 | - | 182,182,183,184 | 0 |
| 85 | MG | 1 | 3736 | 1/1 | 0.73 | 0.16 | - | 82,82,82,82 | 0 |
| 84 | OHX | AR | 3656 | 7/7 | 0.94 | 0.20 | - | 187,187,189,189 | 0 |
| 85 | MG | CR | 202 | 1/1 | 0.97 | 0.20 | - | 20,20,20,20 | 0 |
| 85 | MG | CK | 202 | 1/1 | 0.59 | 0.64 | - | 52,52,52,52 | 0 |
| 85 | MG | 1 | 4194 | 1/1 | 0.86 | 0.23 | - | 82,82,82,82 | 0 |
| 85 | MG | 6 | 2186 | 1/1 | 0.94 | 0.15 | - | 82,82,82,82 | 0 |
| 85 | MG | AR | 3791 | 1/1 | 0.91 | 0.47 | - | 32,32,32,32 | 0 |
| 85 | MG | 1 | 4214 | 1/1 | 0.95 | 0.18 | - | 50,50,50,50 | 0 |
| 84 | OHX | 1 | 3451 | 7/7 | 0.99 | 0.10 | - | 101,101,102,103 | 0 |
| 85 | MG | 1 | 3981 | 1/1 | 0.87 | 0.37 | - | 59,59,59,59 | 0 |
| 85 | MG | 1 | 4198 | 1/1 | 0.92 | 0.56 | - | 36,36,36,36 | 0 |
| 85 | MG | 1 | 3849 | 1/1 | 0.98 | 0.44 | - | 21,21,21,21 | 0 |
| 85 | MG | AT | 222 | 1/1 | 0.96 | 0.43 | - | 35,35,35,35 | 0 |
| 85 | MG | AR | 4217 | 1/1 | 0.68 | 0.24 | - | 65,65,65,65 | 0 |
| 85 | MG | 1 | 4033 | 1/1 | 0.89 | 0.25 | - | 57,57,57,57 | 0 |
| 85 | MG | AR | 4061 | 1/1 | 0.85 | 0.51 | - | 40,40,40,40 | 0 |
| 85 | MG | 1 | 3781 | 1/1 | 0.89 | 0.25 | - | 24,24,24,24 | 0 |
| 84 | OHX | AR | 3642 | 7/7 | 0.96 | 0.28 | - | 189,189,191,191 | 0 |
| 85 | MG | AS | 226 | 1/1 | 0.90 | 0.45 | - | 36,36,36,36 | 0 |
| 85 | MG | 1 | 4162 | 1/1 | 0.69 | 0.27 | - | 118,118,118,118 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 85 | MG | 6 | 2169 | 1/1 | 0.86 | 0.39 | - | 39,39,39,39 | 0 |
| 85 | MG | 1 | 4112 | 1/1 | 0.86 | 0.28 | - | 41,41,41,41 | 0 |
| 85 | MG | 6 | 2075 | 1/1 | 0.78 | 0.39 | - | 49,49,49,49 | 0 |
| 85 | MG | AR | 3760 | 1/1 | 0.96 | 0.39 | - | 21,21,21,21 | 0 |
| 85 | MG | 6 | 2178 | 1/1 | 0.95 | 0.24 | - | 26,26,26,26 | 0 |
| 85 | MG | 6 | 2168 | 1/1 | 0.77 | 0.40 | - | 50,50,50,50 | 0 |
| 85 | MG | AR | 4025 | 1/1 | 0.80 | 0.22 | - | 40,40,40,40 | 0 |
| 85 | MG | A | 2106 | 1/1 | 0.97 | 0.47 | - | 30,30,30,30 | 0 |
| 84 | OHX | 6 | 1943 | 7/7 | 0.97 | 0.11 | - | 147,149,150,150 | 0 |
| 85 | MG | A | 2113 | 1/1 | 0.89 | 0.25 | - | 35,35,35,35 | 0 |
| 85 | MG | AR | 4162 | 1/1 | 0.81 | 0.26 | - | 54,54,54,54 | 0 |
| 85 | MG | 4 | 224 | 1/1 | 0.85 | 0.22 | - | 51,51,51,51 | 0 |
| 85 | MG | AR | 3772 | 1/1 | 0.85 | 0.53 | - | 81,81,81,81 | 0 |
| 85 | MG | 1 | 4088 | 1/1 | 0.88 | 0.22 | - | 28,28,28,28 | 0 |
| 84 | OHX | 6 | 2041 | 7/7 | 0.89 | 0.37 | - | 209,209,210,211 | 0 |
| 85 | MG | AR | 4086 | 1/1 | 0.81 | 0.38 | - | 28,28,28,28 | 0 |
| 85 | MG | DR | 502 | 1/1 | 0.76 | 0.36 | - | 76,76,76,76 | 0 |
| 84 | OHX | AR | 3738 | 7/7 | 0.86 | 0.24 | - | 270,271,272,272 | 0 |
| 85 | MG | AR | 4232 | 1/1 | 0.97 | 0.26 | - | 33,33,33,33 | 0 |
| 85 | MG | AR | 3775 | 1/1 | 0.87 | 0.27 | - | 16,16,16,16 | 0 |
| 84 | OHX | 1 | 3543 | 7/7 | 0.95 | 0.14 | - | 166,166,167,167 | 0 |
| 85 | MG | 1 | 3876 | 1/1 | 0.91 | 0.38 | - | 39,39,39,39 | 0 |
| 85 | MG | 3 | 217 | 1/1 | 0.94 | 0.15 | - | 48,48,48,48 | 0 |
| 85 | MG | AR | 4243 | 1/1 | 0.98 | 0.43 | - | 22,22,22,22 | 0 |
| 85 | MG | AR | 3932 | 1/1 | 0.98 | 0.38 | - | 25,25,25,25 | 0 |
| 85 | MG | AR | 3790 | 1/1 | 0.98 | 0.28 | - | 17,17,17,17 | 0 |
| 85 | MG | AR | 4013 | 1/1 | 0.95 | 0.34 | - | 38,38,38,38 | 0 |
| 85 | MG | 1 | 4004 | 1/1 | 0.93 | 0.21 | - | 31,31,31,31 | 0 |
| 85 | MG | AR | 3759 | 1/1 | 0.85 | 0.29 | - | 103,103,103,103 | 0 |
| 85 | MG | 1 | 4079 | 1/1 | 0.82 | 0.48 | - | 47,47,47,47 | 0 |
| 85 | MG | AR | 3781 | 1/1 | 0.96 | 0.34 | - | 11,11,11,11 | 0 |
| 84 | OHX | 1 | 3460 | 7/7 | 0.99 | 0.12 | - | 112,114,115,116 | 0 |
| 84 | OHX | AR | 3548 | 7/7 | 0.98 | 0.18 | - | 165,166,166,166 | 0 |
| 85 | MG | 1 | 4128 | 1/1 | 0.93 | 0.19 | - | 27,27,27,27 | 0 |
| 85 | MG | AR | 3996 | 1/1 | 0.76 | 0.33 | - | 38,38,38,38 | 0 |
| 85 | MG | AR | 3832 | 1/1 | 0.88 | 0.18 | - | 46,46,46,46 | 0 |
| 85 | MG | AR | 4202 | 1/1 | 0.74 | 0.51 | - | 72,72,72,72 | 0 |
| 85 | MG | AR | 4190 | 1/1 | 0.99 | 0.24 | - | 107,107,107,107 | 0 |
| 85 | MG | AR | 3804 | 1/1 | 0.72 | 0.45 | - | 36,36,36,36 | 0 |
| 84 | OHX | AR | 3574 | 7/7 | 0.97 | 0.27 | - | 171,172,173,173 | 0 |
| 84 | OHX | 1 | 3719 | 7/7 | 0.88 | 0.38 | - | 264,264,265,265 | 0 |
| 85 | MG | AR | 4020 | 1/1 | 0.92 | 0.14 | - | 69,69,69,69 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 85 | MG | AR | 3789 | 1/1 | 0.95 | 0.24 | - | 36,36,36,36 | 0 |
| 85 | MG | 1 | 3875 | 1/1 | 0.87 | 0.26 | - | 18,18,18,18 | 0 |
| 85 | MG | A | 2120 | 1/1 | 0.98 | 0.08 | - | 74,74,74,74 | 0 |
| 84 | OHX | 1 | 3573 | 7/7 | 0.97 | 0.10 | - | 196,196,197,197 | 0 |
| 85 | MG | 1 | 4143 | 1/1 | 0.99 | 0.07 | - | 53,53,53,53 | 0 |
| 85 | MG | 3 | 210 | 1/1 | 0.94 | 0.25 | - | 41,41,41,41 | 0 |
| 85 | MG | 1 | 4098 | 1/1 | 0.95 | 0.19 | - | 33,33,33,33 | 0 |
| 85 | MG | l2 | 202 | 1/1 | 0.86 | 0.23 | - | 48,48,48,48 | 0 |
| 85 | MG | 1 | 4123 | 1/1 | 0.92 | 0.23 | - | 41,41,41,41 | 0 |
| 84 | OHX | 1 | 3600 | 7/7 | 0.86 | 0.45 | - | 258,258,259,259 | 0 |
| 84 | OHX | AR | 3495 | 7/7 | 0.96 | 0.14 | - | 163,165,166,166 | 0 |
| 85 | MG | 6 | 2192 | 1/1 | 0.94 | 0.63 | - | 54,54,54,54 | 0 |
| 85 | MG | 1 | 3999 | 1/1 | 0.94 | 0.29 | - | 38,38,38,38 | 0 |
| 84 | OHX | O | 201 | 7/7 | 0.88 | 0.17 | - | 249,252,253,253 | 0 |
| 85 | MG | 1 | 3916 | 1/1 | 0.96 | 0.51 | - | 14,14,14,14 | 0 |
| 84 | OHX | 6 | 1936 | 7/7 | 0.96 | 0.18 | - | 145,146,146,146 | 0 |
| 84 | OHX | AT | 213 | 7/7 | 0.96 | 0.11 | - | 175,176,176,177 | 0 |
| 85 | MG | AR | 4237 | 1/1 | 0.87 | 0.31 | - | 26,26,26,26 | 0 |
| 85 | MG | 6 | 2077 | 1/1 | 0.98 | 0.56 | - | 51,51,51,51 | 0 |
| 84 | OHX | AR | 3718 | 7/7 | 0.76 | 0.34 | - | 255,256,257,257 | 0 |
| 85 | MG | 1 | 4011 | 1/1 | 0.92 | 0.18 | - | 38,38,38,38 | 0 |
| 85 | MG | AR | 4143 | 1/1 | 0.92 | 0.25 | - | 38,38,38,38 | 0 |
| 85 | MG | 1 | 3995 | 1/1 | 0.95 | 0.27 | - | 54,54,54,54 | 0 |
| 85 | MG | AR | 4003 | 1/1 | 0.93 | 0.36 | - | 73,73,73,73 | 0 |
| 85 | MG | A | 2140 | 1/1 | 0.92 | 0.29 | - | 55,55,55,55 | 0 |
| 85 | MG | AR | 4110 | 1/1 | 1.00 | 0.11 | - | 45,45,45,45 | 0 |
| 85 | MG | AR | 4031 | 1/1 | 0.96 | 0.25 | - | 31,31,31,31 | 0 |
| 85 | MG | 4 | 222 | 1/1 | 0.85 | 0.45 | - | 61,61,61,61 | 0 |
| 85 | MG | 1 | 3811 | 1/1 | 0.94 | 0.21 | - | 42,42,42,42 | 0 |
| 85 | MG | 6 | 2197 | 1/1 | 0.87 | 0.31 | - | 57,57,57,57 | 0 |
| 85 | MG | 1 | 3980 | 1/1 | 0.93 | 0.26 | - | 19,19,19,19 | 0 |
| 84 | OHX | AR | 3615 | 7/7 | 0.95 | 0.24 | - | 169,170,171,171 | 0 |
| 85 | MG | AR | 4067 | 1/1 | 0.95 | 0.29 | - | 98,98,98,98 | 0 |
| 85 | MG | 6 | 2188 | 1/1 | 0.94 | 0.33 | - | 55,55,55,55 | 0 |
| 85 | MG | 1 | 3771 | 1/1 | 0.98 | 0.48 | - | 23,23,23,23 | 0 |
| 85 | MG | AR | 4229 | 1/1 | 0.96 | 0.46 | - | 23,23,23,23 | 0 |
| 85 | MG | AR | 3888 | 1/1 | 0.86 | 0.46 | - | 33,33,33,33 | 0 |
| 85 | MG | AR | 4198 | 1/1 | 0.96 | 0.24 | - | 34,34,34,34 | 0 |
| 85 | MG | 1 | 3966 | 1/1 | 0.61 | 0.21 | - | 62,62,62,62 | 0 |
| 85 | MG | 1 | 4083 | 1/1 | 0.98 | 0.11 | - | 34,34,34,34 | 0 |
| 85 | MG | 6 | 2158 | 1/1 | 0.95 | 0.19 | - | 64,64,64,64 | 0 |
| 85 | MG | AR | 3981 | 1/1 | 0.96 | 0.18 | - | 17,17,17,17 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 85 | MG | AR | 4100 | 1/1 | 0.84 | 0.35 | - | 67,67,67,67 | 0 |
| 85 | MG | AR | 4029 | 1/1 | 0.87 | 0.35 | - | 32,32,32,32 | 0 |
| 85 | MG | 6 | 2059 | 1/1 | 0.98 | 0.42 | - | 40,40,40,40 | 0 |
| 85 | MG | AR | 3799 | 1/1 | 0.97 | 0.17 | - | 83,83,83,83 | 0 |
| 85 | MG | AR | 3838 | 1/1 | 0.94 | 0.61 | - | 21,21,21,21 | 0 |
| 85 | MG | 1 | 3868 | 1/1 | 0.98 | 0.58 | - | 9,9,9,9 | 0 |
| 85 | MG | 1 | 4002 | 1/1 | 0.91 | 0.22 | - | 104,104,104,104 | 0 |
| 85 | MG | AR | 3828 | 1/1 | 0.92 | 0.30 | - | 47,47,47,47 | 0 |
| 85 | MG | 1 | 4070 | 1/1 | 0.83 | 0.30 | - | 37,37,37,37 | 0 |
| 85 | MG | 1 | 3778 | 1/1 | 0.94 | 0.19 | - | 20,20,20,20 | 0 |
| 85 | MG | AR | 4170 | 1/1 | 0.81 | 0.36 | - | 128,128,128,128 | 0 |
| 85 | MG | 1 | 3786 | 1/1 | 0.86 | 0.42 | - | 37,37,37,37 | 0 |
| 85 | MG | 1 | 4041 | 1/1 | 0.83 | 0.46 | - | 38,38,38,38 | 0 |
| 85 | MG | 1 | 4109 | 1/1 | 0.83 | 0.33 | - | 37,37,37,37 | 0 |
| 84 | OHX | A | 1981 | 7/7 | 0.94 | 0.10 | - | 231,234,235,236 | 0 |
| 85 | MG | 1 | 3828 | 1/1 | 0.98 | 0.41 | - | 29,29,29,29 | 0 |
| 85 | MG | AR | 3949 | 1/1 | 0.96 | 0.38 | - | 19,19,19,19 | 0 |
| 85 | MG | 1 | 3789 | 1/1 | 0.76 | 0.70 | - | 51,51,51,51 | 0 |
| 84 | OHX | AT | 208 | 7/7 | 0.97 | 0.12 | - | 154,154,155,155 | 0 |
| 84 | OHX | AR | 3636 | 7/7 | 0.96 | 0.17 | - | 187,188,188,189 | 0 |
| 85 | MG | A | 2096 | 1/1 | 0.98 | 0.26 | - | 51,51,51,51 | 0 |
| 85 | MG | 6 | 2090 | 1/1 | 0.89 | 0.42 | - | 45,45,45,45 | 0 |
| 84 | OHX | 1 | 3512 | 7/7 | 0.95 | 0.12 | - | 170,172,172,173 | 0 |
| 85 | MG | AR | 3883 | 1/1 | 0.99 | 0.34 | - | 12,12,12,12 | 0 |
| 85 | MG | AR | 3819 | 1/1 | 0.99 | 0.50 | - | 53,53,53,53 | 0 |
| 84 | OHX | AR | 3616 | 7/7 | 0.93 | 0.35 | - | 210,210,211,212 | 0 |
| 85 | MG | 6 | 2163 | 1/1 | 0.96 | 0.12 | - | 60,60,60,60 | 0 |
| 84 | OHX | AR | 3605 | 7/7 | 0.91 | 0.14 | - | 194,195,196,196 | 0 |
| 84 | OHX | 1 | 3630 | 7/7 | 0.93 | 0.19 | - | 199,200,200,201 | 0 |
| 85 | MG | AT | 227 | 1/1 | 0.81 | 0.36 | - | 73,73,73,73 | 0 |
| 84 | OHX | A | 2041 | 7/7 | 0.89 | 0.41 | - | 201,203,204,204 | 0 |
| 85 | MG | AR | 4004 | 1/1 | 0.95 | 0.33 | - | 27,27,27,27 | 0 |
| 85 | MG | AR | 3916 | 1/1 | 0.94 | 0.41 | - | 3,3,3,3 | 0 |
| 85 | MG | 1 | 4177 | 1/1 | 0.86 | 0.21 | - | 45,45,45,45 | 0 |
| 85 | MG | 1 | 3796 | 1/1 | 0.94 | 0.19 | - | 33,33,33,33 | 0 |
| 85 | MG | AR | 4193 | 1/1 | 0.78 | 0.56 | - | 62,62,62,62 | 0 |
| 85 | MG | 1 | 3893 | 1/1 | 0.98 | 0.28 | - | 38,38,38,38 | 0 |
| 85 | MG | AR | 4117 | 1/1 | 0.91 | 0.23 | - | 53,53,53,53 | 0 |
| 84 | OHX | 1 | 3556 | 7/7 | 0.92 | 0.19 | - | 180,181,182,183 | 0 |
| 84 | OHX | 6 | 1916 | 7/7 | 0.99 | 0.11 | - | 102,103,104,104 | 0 |
| 85 | MG | 6 | 2128 | 1/1 | 0.90 | 0.29 | - | 53,53,53,53 | 0 |
| 85 | MG | AR | 4153 | 1/1 | 0.87 | 0.26 | - | 52,52,52,52 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | OHX | A | 2000 | 7/7 | 0.91 | 0.22 | - | 194,195,196,197 | 0 |
| 84 | OHX | 6 | 1949 | 7/7 | 0.97 | 0.13 | - | 165,167,168,168 | 0 |
| 84 | OHX | 1 | 3633 | 7/7 | 0.91 | 0.17 | - | 193,194,195,197 | 0 |
| 85 | MG | 6 | 2072 | 1/1 | 0.92 | 0.23 | - | 36,36,36,36 | 0 |
| 84 | OHX | 1 | 3628 | 7/7 | 0.93 | 0.20 | - | 234,235,236,237 | 0 |
| 85 | MG | AR | 3793 | 1/1 | 0.97 | 0.55 | - | 23,23,23,23 | 0 |
| 85 | MG | 6 | 2088 | 1/1 | 0.94 | 0.38 | - | 30,30,30,30 | 0 |
| 85 | MG | AR | 4137 | 1/1 | 0.95 | 0.16 | - | 57,57,57,57 | 0 |
| 85 | MG | 1 | 4081 | 1/1 | 0.94 | 0.11 | - | 35,35,35,35 | 0 |
| 85 | MG | AR | 4041 | 1/1 | 0.90 | 0.12 | - | 47,47,47,47 | 0 |
| 85 | MG | s1 | 301 | 1/1 | 1.00 | 0.16 | - | 67,67,67,67 | 0 |
| 85 | MG | 1 | 3856 | 1/1 | 0.99 | 0.31 | - | 15,15,15,15 | 0 |
| 85 | MG | AR | 4125 | 1/1 | 0.84 | 0.22 | - | 62,62,62,62 | 0 |
| 85 | MG | AR | 3912 | 1/1 | 0.98 | 0.54 | - | 1,1,1,1 | 0 |
| 85 | MG | 1 | 3943 | 1/1 | 0.97 | 0.32 | - | 22,22,22,22 | 0 |
| 85 | MG | 1 | 4042 | 1/1 | 0.94 | 0.16 | - | 65,65,65,65 | 0 |
| 85 | MG | 1 | 4050 | 1/1 | 0.89 | 0.30 | - | 34,34,34,34 | 0 |
| 84 | OHX | AR | 3637 | 7/7 | 0.90 | 0.30 | - | 204,205,205,205 | 0 |
| 85 | MG | 1 | 3762 | 1/1 | 0.83 | 0.48 | - | 40,40,40,40 | 0 |
| 85 | MG | 1 | 4005 | 1/1 | 0.92 | 0.63 | - | 37,37,37,37 | 0 |
| 85 | MG | AR | 4123 | 1/1 | 0.91 | 0.25 | - | 39,39,39,39 | 0 |
| 84 | OHX | 3 | 202 | 7/7 | 0.96 | 0.13 | - | 176,177,177,178 | 0 |
| 85 | MG | AR | 4046 | 1/1 | 0.96 | 0.19 | - | 45,45,45,45 | 0 |
| 85 | MG | 1 | 3991 | 1/1 | 0.97 | 0.25 | - | 30,30,30,30 | 0 |
| 85 | MG | AR | 4160 | 1/1 | 0.97 | 0.26 | - | 31,31,31,31 | 0 |
| 85 | MG | A | 2135 | 1/1 | 0.73 | 0.61 | - | 50,50,50,50 | 0 |
| 85 | MG | 6 | 2141 | 1/1 | 0.96 | 0.21 | - | 56,56,56,56 | 0 |
| 85 | MG | AR | 3771 | 1/1 | 0.88 | 0.22 | - | 24,24,24,24 | 0 |
| 85 | MG | AR | 3955 | 1/1 | 0.86 | 0.25 | - | 32,32,32,32 | 0 |
| 85 | MG | AS | 221 | 1/1 | 0.84 | 0.20 | - | 36,36,36,36 | 0 |
| 85 | MG | 1 | 4009 | 1/1 | 0.94 | 0.40 | - | 41,41,41,41 | 0 |
| 85 | MG | 1 | 3990 | 1/1 | 0.95 | 0.41 | - | 36,36,36,36 | 0 |
| 85 | MG | AR | 3837 | 1/1 | 0.95 | 0.17 | - | 16,16,16,16 | 0 |
| 85 | MG | AR | 4103 | 1/1 | 0.93 | 0.16 | - | 35,35,35,35 | 0 |
| 85 | MG | DF | 201 | 1/1 | 0.94 | 0.31 | - | 30,30,30,30 | 0 |
| 85 | MG | 6 | 2114 | 1/1 | 0.95 | 0.36 | - | 28,28,28,28 | 0 |
| 85 | MG | AR | 4010 | 1/1 | 0.93 | 0.43 | - | 28,28,28,28 | 0 |
| 85 | MG | AR | 4126 | 1/1 | 0.89 | 0.29 | - | 73,73,73,73 | 0 |
| 84 | OHX | AR | 3670 | 7/7 | 0.83 | 0.29 | - | 229,230,230,231 | 0 |
| 85 | MG | AR | 3968 | 1/1 | 0.86 | 0.33 | - | 29,29,29,29 | 0 |
| 85 | MG | 1 | 3863 | 1/1 | 0.97 | 0.43 | - | 25,25,25,25 | 0 |
| 84 | OHX | AR | 3588 | 7/7 | 0.95 | 0.16 | - | 176,177,178,178 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | OHX | 1 | 3663 | 7/7 | 0.95 | 0.32 | - | 214,216,217,217 | 0 |
| 85 | MG | A | 2089 | 1/1 | 0.73 | 0.49 | - | 65,65,65,65 | 0 |
| 84 | OHX | AR | 3434 | 7/7 | 0.99 | 0.16 | - | 87,87,88,88 | 0 |
| 84 | OHX | A | 1952 | 7/7 | 0.96 | 0.26 | - | 181,183,185,185 | 0 |
| 85 | MG | AR | 4148 | 1/1 | 0.93 | 0.13 | - | 36,36,36,36 | 0 |
| 84 | OHX | z | 201 | 7/7 | 0.90 | 0.23 | - | 257,258,259,259 | 0 |
| 84 | OHX | AR | 3487 | 7/7 | 0.98 | 0.12 | - | 116,117,117,117 | 0 |
| 85 | MG | AR | 3928 | 1/1 | 0.94 | 0.26 | - | 10,10,10,10 | 0 |
| 85 | MG | AR | 3879 | 1/1 | 0.94 | 0.55 | - | 21,21,21,21 | 0 |
| 85 | MG | AR | 4129 | 1/1 | 0.96 | 0.32 | - | 21,21,21,21 | 0 |
| 85 | MG | 1 | 3897 | 1/1 | 0.91 | 0.38 | - | 13,13,13,13 | 0 |
| 85 | MG | 1 | 3836 | 1/1 | 0.98 | 0.24 | - | 17,17,17,17 | 0 |
| 85 | MG | 1 | 3802 | 1/1 | 0.94 | 0.21 | - | 32,32,32,32 | 0 |
| 85 | MG | 1 | 4210 | 1/1 | 0.95 | 0.32 | - | 32,32,32,32 | 0 |
| 85 | MG | AR | 3962 | 1/1 | 0.86 | 0.20 | - | 43,43,43,43 | 0 |
| 84 | OHX | 1 | 3616 | 7/7 | 0.96 | 0.22 | - | 177,177,178,178 | 0 |
| 85 | MG | 1 | 3794 | 1/1 | 0.96 | 0.22 | - | 31,31,31,31 | 0 |
| 84 | OHX | AR | 3628 | 7/7 | 0.92 | 0.27 | - | 209,210,211,211 | 0 |
| 85 | MG | AS | 222 | 1/1 | 0.98 | 0.23 | - | 13,13,13,13 | 0 |
| 85 | MG | AR | 3746 | 1/1 | 0.58 | 0.29 | - | 39,39,39,39 | 0 |
| 85 | MG | A | 2127 | 1/1 | 0.78 | 0.30 | - | 55,55,55,55 | 0 |
| 85 | MG | AS | 215 | 1/1 | 0.94 | 0.67 | - | 12,12,12,12 | 0 |
| 85 | MG | AS | 224 | 1/1 | 0.89 | 0.26 | - | 55,55,55,55 | 0 |
| 85 | MG | 1 | 3901 | 1/1 | 0.99 | 0.49 | - | 12,12,12,12 | 0 |
| 85 | MG | 1 | 3757 | 1/1 | 0.93 | 0.13 | - | 46,46,46,46 | 0 |
| 85 | MG | AR | 3821 | 1/1 | 0.98 | 0.35 | - | 26,26,26,26 | 0 |
| 85 | MG | 1 | 4031 | 1/1 | 0.82 | 0.41 | - | 38,38,38,38 | 0 |
| 85 | MG | 1 | 4012 | 1/1 | 0.94 | 0.20 | - | 26,26,26,26 | 0 |
| 85 | MG | AR | 4219 | 1/1 | 0.86 | 0.33 | - | 47,47,47,47 | 0 |
| 85 | MG | 1 | 4067 | 1/1 | 0.96 | 0.19 | - | 24,24,24,24 | 0 |
| 85 | MG | 1 | 4133 | 1/1 | 0.91 | 0.46 | - | 28,28,28,28 | 0 |
| 85 | MG | AR | 3800 | 1/1 | 0.98 | 0.28 | - | 22,22,22,22 | 0 |
| 85 | MG | AR | 4186 | 1/1 | 0.95 | 0.34 | - | 33,33,33,33 | 0 |
| 85 | MG | AR | 4154 | 1/1 | 0.89 | 0.10 | - | 50,50,50,50 | 0 |
| 85 | MG | AR | 4241 | 1/1 | 0.42 | 0.56 | - | 59,59,59,59 | 0 |
| 85 | MG | AR | 4194 | 1/1 | 0.92 | 0.27 | - | 47,47,47,47 | 0 |
| 85 | MG | AR | 3869 | 1/1 | 0.96 | 0.40 | - | 12,12,12,12 | 0 |
| 85 | MG | 1 | 4040 | 1/1 | 0.82 | 0.53 | - | 42,42,42,42 | 0 |
| 84 | OHX | A | 1960 | 7/7 | 0.94 | 0.15 | - | 225,226,227,228 | 0 |
| 84 | OHX | 1 | 3673 | 7/7 | 0.95 | 0.16 | - | 192,193,194,194 | 0 |
| 85 | MG | 1 | 4183 | 1/1 | 0.75 | 0.47 | - | 41,41,41,41 | 0 |
| 85 | MG | AR | 4027 | 1/1 | 0.97 | 0.26 | - | 33,33,33,33 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 85 | MG | AR | 4184 | 1/1 | 0.93 | 0.20 | - | 35,35,35,35 | 0 |
| 85 | MG | 1 | 3800 | 1/1 | 0.96 | 0.40 | - | 37,37,37,37 | 0 |
| 85 | MG | AR | 4124 | 1/1 | 0.93 | 0.17 | - | 54,54,54,54 | 0 |
| 85 | MG | 1 | 4167 | 1/1 | 0.99 | 0.15 | - | 52,52,52,52 | 0 |
| 84 | OHX | 1 | 3567 | 7/7 | 0.96 | 0.23 | - | 177,178,178,179 | 0 |
| 85 | MG | AR | 4203 | 1/1 | 0.90 | 0.35 | - | 37,37,37,37 | 0 |
| 84 | OHX | AR | 3657 | 7/7 | 0.93 | 0.34 | - | 207,207,209,209 | 0 |
| 84 | OHX | 6 | 1905 | 7/7 | 0.99 | 0.20 | - | 100,100,101,101 | 0 |
| 85 | MG | AR | 4012 | 1/1 | 0.86 | 0.24 | - | 50,50,50,50 | 0 |
| 85 | MG | 1 | 3751 | 1/1 | 0.88 | 0.16 | - | 50,50,50,50 | 0 |
| 85 | MG | AR | 3970 | 1/1 | 0.93 | 0.22 | - | 53,53,53,53 | 0 |
| 85 | MG | A | 2068 | 1/1 | 0.83 | 0.46 | - | 68,68,68,68 | 0 |
| 85 | MG | 1 | 4001 | 1/1 | 0.80 | 0.32 | - | 65,65,65,65 | 0 |
| 85 | MG | AR | 4208 | 1/1 | 0.92 | 0.24 | - | 62,62,62,62 | 0 |
| 85 | MG | A | 2046 | 1/1 | 0.59 | 0.20 | - | 56,56,56,56 | 0 |
| 84 | OHX | A | 1978 | 7/7 | 0.94 | 0.14 | - | 210,212,214,214 | 0 |
| 85 | MG | A | 2148 | 1/1 | 0.87 | 0.43 | - | 103,103,103,103 | 0 |
| 85 | MG | AR | 4214 | 1/1 | 0.78 | 0.43 | - | 61,61,61,61 | 0 |
| 85 | MG | A | 2073 | 1/1 | 0.61 | 0.41 | - | 65,65,65,65 | 0 |
| 85 | MG | AR | 3903 | 1/1 | 0.98 | 0.41 | - | 5,5,5,5 | 0 |
| 85 | MG | 1 | 4193 | 1/1 | 0.96 | 0.37 | - | 9,9,9,9 | 0 |
| 84 | OHX | 6 | 1992 | 7/7 | 0.94 | 0.22 | - | 185,186,187,188 | 0 |
| 85 | MG | AR | 3986 | 1/1 | 0.84 | 0.86 | - | 41,41,41,41 | 0 |
| 85 | MG | 6 | 2100 | 1/1 | 0.97 | 0.44 | - | 16,16,16,16 | 0 |
| 85 | MG | 1 | 3971 | 1/1 | 0.98 | 0.18 | - | 63,63,63,63 | 0 |
| 85 | MG | 1 | 4093 | 1/1 | 0.92 | 0.47 | - | 16,16,16,16 | 0 |
| 84 | OHX | 6 | 1935 | 7/7 | 0.98 | 0.12 | - | 136,137,138,139 | 0 |
| 85 | MG | 1 | 3767 | 1/1 | 0.90 | 0.12 | - | 34,34,34,34 | 0 |
| 85 | MG | 1 | 3907 | 1/1 | 0.95 | 0.38 | - | 13,13,13,13 | 0 |
| 85 | MG | 6 | 2116 | 1/1 | 0.91 | 0.42 | - | 41,41,41,41 | 0 |
| 85 | MG | 1 | 3823 | 1/1 | 0.96 | 0.20 | - | 51,51,51,51 | 0 |
| 85 | MG | AR | 3770 | 1/1 | 0.87 | 0.36 | - | 36,36,36,36 | 0 |
| 85 | MG | 1 | 3977 | 1/1 | 0.89 | 0.36 | - | 21,21,21,21 | 0 |
| 85 | MG | 6 | 2171 | 1/1 | 0.95 | 0.23 | - | 34,34,34,34 | 0 |
| 85 | MG | 1 | 4082 | 1/1 | 0.97 | 0.13 | - | 22,22,22,22 | 0 |
| 84 | OHX | AR | 3551 | 7/7 | 0.97 | 0.19 | - | 161,162,163,164 | 0 |
| 84 | OHX | 1 | 3648 | 7/7 | 0.90 | 0.27 | - | 258,259,260,260 | 0 |
| 85 | MG | 1 | 3942 | 1/1 | 0.97 | 0.37 | - | 20,20,20,20 | 0 |
| 85 | MG | 1 | 4159 | 1/1 | 0.93 | 0.15 | - | 42,42,42,42 | 0 |
| 85 | MG | A | 2124 | 1/1 | 0.80 | 0.74 | - | 57,57,57,57 | 0 |
| 85 | MG | AR | 3913 | 1/1 | 0.89 | 0.35 | - | 20,20,20,20 | 0 |
| 85 | MG | DD | 101 | 1/1 | 0.88 | 0.23 | - | 32,32,32,32 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | OHX | AR | 3724 | 7/7 | 0.91 | 0.34 | - | 203,204,205,205 | 0 |
| 84 | OHX | AR | 3544 | 7/7 | 0.97 | 0.11 | - | 177,178,179,179 | 0 |
| 84 | OHX | 6 | 2054 | 7/7 | 0.85 | 0.24 | - | 253,254,256,256 | 0 |
| 85 | MG | AT | 226 | 1/1 | 0.82 | 0.34 | - | 44,44,44,44 | 0 |
| 85 | MG | 1 | 4176 | 1/1 | 0.93 | 0.19 | - | 27,27,27,27 | 0 |
| 85 | MG | 1 | 4023 | 1/1 | 0.89 | 0.72 | - | 44,44,44,44 | 0 |
| 85 | MG | 6 | 2085 | 1/1 | 0.83 | 0.42 | - | 40,40,40,40 | 0 |
| 85 | MG | 6 | 2110 | 1/1 | 0.81 | 0.33 | - | 40,40,40,40 | 0 |
| 85 | MG | 1 | 3964 | 1/1 | 0.83 | 0.33 | - | 51,51,51,51 | 0 |
| 85 | MG | 3 | 220 | 1/1 | 0.95 | 0.34 | - | 31,31,31,31 | 0 |
| 85 | MG | AR | 3822 | 1/1 | 0.88 | 0.14 | - | 52,52,52,52 | 0 |
| 84 | OHX | 1 | 3614 | 7/7 | 0.95 | 0.18 | - | 199,200,201,203 | 0 |
| 84 | OHX | AR | 3632 | 7/7 | 0.90 | 0.14 | - | 227,227,228,228 | 0 |
| 85 | MG | AR | 4045 | 1/1 | 0.96 | 0.12 | - | 33,33,33,33 | 0 |
| 85 | MG | t | 201 | 1/1 | 0.85 | 0.25 | - | 37,37,37,37 | 0 |
| 85 | MG | 1 | 3871 | 1/1 | 0.87 | 0.28 | - | 27,27,27,27 | 0 |
| 85 | MG | AT | 201 | 1/1 | 0.94 | 0.29 | - | 31,31,31,31 | 0 |
| 85 | MG | 1 | 3774 | 1/1 | 0.89 | 0.21 | - | 84,84,84,84 | 0 |
| 85 | MG | 1 | 4076 | 1/1 | 0.73 | 0.27 | - | 71,71,71,71 | 0 |
| 85 | MG | 1 | 3754 | 1/1 | 0.92 | 0.32 | - | 38,38,38,38 | 0 |
| 85 | MG | 9 | 201 | 1/1 | 0.89 | 0.19 | - | 33,33,33,33 | 0 |
| 85 | MG | 1 | 3958 | 1/1 | 0.93 | 0.20 | - | 54,54,54,54 | 0 |
| 85 | MG | 1 | 3888 | 1/1 | 0.95 | 0.26 | - | 21,21,21,21 | 0 |
| 85 | MG | AR | 4118 | 1/1 | 0.98 | 0.28 | - | 29,29,29,29 | 0 |
| 85 | MG | AR | 3805 | 1/1 | 0.90 | 0.18 | - | 39,39,39,39 | 0 |
| 85 | MG | 1 | 4120 | 1/1 | 0.92 | 0.18 | - | 46,46,46,46 | 0 |
| 85 | MG | AR | 3848 | 1/1 | 0.95 | 0.25 | - | 15,15,15,15 | 0 |
| 85 | MG | AR | 4096 | 1/1 | 0.89 | 0.27 | - | 53,53,53,53 | 0 |
| 84 | OHX | 6 | 2010 | 7/7 | 0.90 | 0.24 | - | 213,214,215,216 | 0 |
| 85 | MG | l | 403 | 1/1 | 0.95 | 0.26 | - | 20,20,20,20 | 0 |
| 85 | MG | AR | 3894 | 1/1 | 0.97 | 0.50 | - | 24,24,24,24 | 0 |
| 85 | MG | AR | 3923 | 1/1 | 0.80 | 0.66 | - | 32,32,32,32 | 0 |
| 85 | MG | AT | 229 | 1/1 | 0.96 | 0.33 | - | 30,30,30,30 | 0 |
| 85 | MG | 1 | 3779 | 1/1 | 0.88 | 0.31 | - | 29,29,29,29 | 0 |
| 85 | MG | AR | 3747 | 1/1 | 0.90 | 0.22 | - | 23,23,23,23 | 0 |
| 85 | MG | 1 | 3844 | 1/1 | 0.96 | 0.44 | - | 9,9,9,9 | 0 |
| 85 | MG | 1 | 3792 | 1/1 | 0.97 | 0.26 | - | 16,16,16,16 | 0 |
| 85 | MG | AR | 4168 | 1/1 | 0.96 | 0.32 | - | 45,45,45,45 | 0 |
| 85 | MG | AS | 217 | 1/1 | 0.98 | 0.16 | - | 18,18,18,18 | 0 |
| 85 | MG | AR | 3945 | 1/1 | 0.95 | 0.43 | - | 22,22,22,22 | 0 |
| 85 | MG | AR | 4142 | 1/1 | 0.90 | 0.42 | - | 55,55,55,55 | 0 |
| 85 | MG | 6 | 2136 | 1/1 | 0.97 | 0.25 | - | 29,29,29,29 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 85 | MG | AR | 4049 | 1/1 | 0.95 | 0.09 | - | 74,74,74,74 | 0 |
| 85 | MG | AR | 3999 | 1/1 | 0.97 | 0.37 | - | 28,28,28,28 | 0 |
| 85 | MG | w | 201 | 1/1 | 0.95 | 0.17 | - | 33,33,33,33 | 0 |
| 84 | OHX | A | 1934 | 7/7 | 0.94 | 0.14 | - | 176,177,179,179 | 0 |
| 85 | MG | 6 | 2067 | 1/1 | 0.97 | 0.34 | - | 41,41,41,41 | 0 |
| 85 | MG | 1 | 4092 | 1/1 | 0.70 | 0.16 | - | 53,53,53,53 | 0 |
| 85 | MG | 1 | 3957 | 1/1 | 0.93 | 0.42 | - | 29,29,29,29 | 0 |
| 84 | OHX | AR | 3679 | 7/7 | 0.94 | 0.24 | - | 218,220,221,221 | 0 |
| 84 | OHX | 1 | 3720 | 7/7 | 0.90 | 0.23 | - | 197,197,199,199 | 0 |
| 85 | MG | 1 | 4096 | 1/1 | 0.86 | 0.57 | - | 53,53,53,53 | 0 |
| 84 | OHX | AR | 3708 | 7/7 | 0.91 | 0.30 | - | 228,228,229,229 | 0 |
| 84 | OHX | AR | 3561 | 7/7 | 0.96 | 0.19 | - | 171,171,172,172 | 0 |
| 85 | MG | AR | 4066 | 1/1 | 0.97 | 0.17 | - | 35,35,35,35 | 0 |
| 85 | MG | AR | 4121 | 1/1 | 0.93 | 0.37 | - | 42,42,42,42 | 0 |
| 84 | OHX | 1 | 3477 | 7/7 | 0.97 | 0.13 | - | 118,119,120,120 | 0 |
| 85 | MG | 1 | 3841 | 1/1 | 0.96 | 0.30 | - | 19,19,19,19 | 0 |
| 84 | OHX | CO | 201 | 7/7 | 0.83 | 0.33 | - | 281,282,283,284 | 0 |
| 84 | OHX | AR | 3719 | 7/7 | 0.89 | 0.25 | - | 220,220,221,221 | 0 |
| 85 | MG | 6 | 2190 | 1/1 | 0.67 | 0.41 | - | 84,84,84,84 | 0 |
| 85 | MG | AR | 4213 | 1/1 | 0.94 | 0.21 | - | 34,34,34,34 | 0 |
| 85 | MG | AR | 4147 | 1/1 | 0.73 | 0.21 | - | 62,62,62,62 | 0 |
| 85 | MG | A | 2065 | 1/1 | 0.86 | 0.34 | - | 31,31,31,31 | 0 |
| 85 | MG | 1 | 4078 | 1/1 | 0.73 | 0.21 | - | 44,44,44,44 | 0 |
| 85 | MG | 1 | 4136 | 1/1 | 0.74 | 0.38 | - | 49,49,49,49 | 0 |
| 84 | OHX | AR | 3573 | 7/7 | 0.94 | 0.19 | - | 178,178,179,180 | 0 |
| 85 | MG | 1 | 3865 | 1/1 | 0.98 | 0.47 | - | 13,13,13,13 | 0 |
| 85 | MG | A | 2093 | 1/1 | 0.88 | 0.19 | - | 93,93,93,93 | 0 |
| 84 | OHX | 1 | 3707 | 7/7 | 0.83 | 0.25 | - | 237,237,239,239 | 0 |
| 85 | MG | DH | 202 | 1/1 | 0.94 | 0.16 | - | 30,30,30,30 | 0 |
| 85 | MG | AR | 4155 | 1/1 | 0.85 | 0.29 | - | 27,27,27,27 | 0 |
| 85 | MG | AR | 3874 | 1/1 | 0.97 | 0.31 | - | 18,18,18,18 | 0 |
| 84 | OHX | 1 | 3696 | 7/7 | 0.92 | 0.54 | - | 240,240,241,242 | 0 |
| 85 | MG | A | 2116 | 1/1 | 0.82 | 0.33 | - | 49,49,49,49 | 0 |
| 85 | MG | 1 | 3948 | 1/1 | 0.97 | 0.40 | - | 46,46,46,46 | 0 |
| 85 | MG | AR | 4158 | 1/1 | 0.92 | 0.30 | - | 21,21,21,21 | 0 |
| 85 | MG | A | 2137 | 1/1 | 0.79 | 0.34 | - | 40,40,40,40 | 0 |
| 85 | MG | 1 | 4115 | 1/1 | 0.98 | 0.17 | - | 97,97,97,97 | 0 |
| 84 | OHX | 1 | 3699 | 7/7 | 0.75 | 0.23 | - | 304,306,307,308 | 0 |
| 85 | MG | AR | 3881 | 1/1 | 0.98 | 0.41 | - | 12,12,12,12 | 0 |
| 85 | MG | A | 2104 | 1/1 | 0.82 | 0.27 | - | 131,131,131,131 | 0 |
| 85 | MG | 1 | 3909 | 1/1 | 0.97 | 0.18 | - | 24,24,24,24 | 0 |
| 85 | MG | A | 2060 | 1/1 | 0.98 | 0.41 | - | 20,20,20,20 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 85 | MG | AR | 4161 | 1/1 | 0.74 | 0.38 | - | 56,56,56,56 | 0 |
| 85 | MG | A | 2111 | 1/1 | 0.93 | 0.22 | - | 68,68,68,68 | 0 |
| 85 | MG | AR | 3812 | 1/1 | 0.62 | 0.41 | - | 46,46,46,46 | 0 |
| 85 | MG | 3 | 213 | 1/1 | 0.86 | 0.51 | - | 23,23,23,23 | 0 |
| 85 | MG | AR | 3748 | 1/1 | 0.93 | 0.24 | - | 41,41,41,41 | 0 |
| 85 | MG | d6 | 101 | 1/1 | 0.91 | 0.24 | - | 37,37,37,37 | 0 |
| 85 | MG | 1 | 4179 | 1/1 | 0.88 | 0.15 | - | 42,42,42,42 | 0 |
| 85 | MG | 4 | 215 | 1/1 | 0.93 | 0.49 | - | 23,23,23,23 | 0 |
| 85 | MG | 1 | 4111 | 1/1 | 0.86 | 0.65 | - | 62,62,62,62 | 0 |
| 85 | MG | 1 | 3830 | 1/1 | 0.78 | 0.57 | - | 60,60,60,60 | 0 |
| 85 | MG | 1 | 4126 | 1/1 | 0.98 | 0.33 | - | 30,30,30,30 | 0 |
| 85 | MG | 4 | 230 | 1/1 | 0.92 | 0.17 | - | 54,54,54,54 | 0 |
| 85 | MG | AR | 3752 | 1/1 | 0.94 | 0.53 | - | 16,16,16,16 | 0 |
| 84 | OHX | 6 | 2044 | 7/7 | 0.92 | 0.35 | - | 238,238,239,240 | 0 |
| 85 | MG | AR | 3880 | 1/1 | 0.77 | 0.43 | - | 20,20,20,20 | 0 |
| 85 | MG | AR | 4233 | 1/1 | 0.80 | 0.40 | - | 55,55,55,55 | 0 |
| 85 | MG | 1 | 4105 | 1/1 | 0.91 | 0.51 | - | 64,64,64,64 | 0 |
| 85 | MG | AR | 3750 | 1/1 | 0.94 | 0.39 | - | 19,19,19,19 | 0 |
| 85 | MG | 1 | 3788 | 1/1 | 0.94 | 0.33 | - | 34,34,34,34 | 0 |
| 85 | MG | AR | 4164 | 1/1 | 0.77 | 0.32 | - | 30,30,30,30 | 0 |
| 84 | OHX | A | 1943 | 7/7 | 0.91 | 0.25 | - | 161,163,164,165 | 0 |
| 85 | MG | 1 | 3947 | 1/1 | 0.81 | 0.42 | - | 34,34,34,34 | 0 |
| 84 | OHX | 1 | 3559 | 7/7 | 0.95 | 0.16 | - | 182,183,184,184 | 0 |
| 85 | MG | 1 | 4173 | 1/1 | 0.97 | 0.14 | - | 33,33,33,33 | 0 |
| 85 | MG | 1 | 3855 | 1/1 | 0.94 | 0.44 | - | 26,26,26,26 | 0 |
| 85 | MG | AR | 3826 | 1/1 | 0.70 | 0.61 | - | 42,42,42,42 | 0 |
| 85 | MG | 1 | 4130 | 1/1 | 0.94 | 0.27 | - | 68,68,68,68 | 0 |
| 85 | MG | 6 | 2185 | 1/1 | 0.50 | 0.59 | - | 60,60,60,60 | 0 |
| 85 | MG | 6 | 2195 | 1/1 | 0.74 | 0.37 | - | 64,64,64,64 | 0 |
| 85 | MG | 1 | 3821 | 1/1 | 0.86 | 0.56 | - | 37,37,37,37 | 0 |
| 85 | MG | AR | 4023 | 1/1 | 0.93 | 0.11 | - | 36,36,36,36 | 0 |
| 85 | MG | 1 | 3812 | 1/1 | 0.94 | 0.37 | - | 29,29,29,29 | 0 |
| 85 | MG | AR | 4019 | 1/1 | 0.95 | 0.14 | - | 29,29,29,29 | 0 |
| 84 | OHX | AR | 3585 | 7/7 | 0.96 | 0.16 | - | 165,166,167,167 | 0 |
| 85 | MG | AR | 4009 | 1/1 | 0.95 | 0.28 | - | 25,25,25,25 | 0 |
| 85 | MG | AR | 4181 | 1/1 | 0.90 | 0.20 | - | 37,37,37,37 | 0 |
| 85 | MG | 1 | 4022 | 1/1 | 0.96 | 0.18 | - | 24,24,24,24 | 0 |
| 85 | MG | CQ | 202 | 1/1 | 0.89 | 0.19 | - | 26,26,26,26 | 0 |
| 85 | MG | 1 | 3807 | 1/1 | 0.89 | 0.31 | - | 37,37,37,37 | 0 |
| 85 | MG | 6 | 2182 | 1/1 | 0.81 | 0.28 | - | 53,53,53,53 | 0 |
| 85 | MG | 1 | 3963 | 1/1 | 0.83 | 0.16 | - | 69,69,69,69 | 0 |
| 85 | MG | AR | 3984 | 1/1 | 0.91 | 0.34 | - | 49,49,49,49 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 85 | MG | 1 | 4184 | 1/1 | 0.84 | 0.23 | - | 55,55,55,55 | 0 |
| 85 | MG | DR | 503 | 1/1 | 0.69 | 0.33 | - | 54,54,54,54 | 0 |
| 85 | MG | AR | 4227 | 1/1 | 0.97 | 0.53 | - | 18,18,18,18 | 0 |
| 85 | MG | 1 | 3846 | 1/1 | 0.98 | 0.38 | - | 16,16,16,16 | 0 |
| 85 | MG | AR | 3995 | 1/1 | 0.90 | 0.11 | - | 38,38,38,38 | 0 |
| 85 | MG | 1 | 4019 | 1/1 | 0.97 | 0.19 | - | 31,31,31,31 | 0 |
| 85 | MG | 1 | 4021 | 1/1 | 0.92 | 0.24 | - | 29,29,29,29 | 0 |
| 85 | MG | 1 | 3973 | 1/1 | 0.97 | 0.26 | - | 33,33,33,33 | 0 |
| 85 | MG | AR | 4078 | 1/1 | 0.98 | 0.31 | - | 23,23,23,23 | 0 |
| 85 | MG | 6 | 2196 | 1/1 | 0.91 | 0.38 | - | 46,46,46,46 | 0 |
| 84 | OHX | 6 | 2029 | 7/7 | 0.86 | 0.45 | - | 246,248,249,250 | 0 |
| 85 | MG | 1 | 4059 | 1/1 | 0.97 | 0.26 | - | 32,32,32,32 | 0 |
| 85 | MG | 6 | 2112 | 1/1 | 0.96 | 0.54 | - | 25,25,25,25 | 0 |
| 85 | MG | A | 2141 | 1/1 | 0.98 | 0.32 | - | 73,73,73,73 | 0 |
| 85 | MG | 1 | 4168 | 1/1 | 0.94 | 0.21 | - | 51,51,51,51 | 0 |
| 85 | MG | AR | 3899 | 1/1 | 0.86 | 0.35 | - | 46,46,46,46 | 0 |
| 85 | MG | 6 | 2071 | 1/1 | 0.79 | 0.20 | - | 73,73,73,73 | 0 |
| 85 | MG | x | 206 | 1/1 | 0.85 | 0.36 | - | 32,32,32,32 | 0 |
| 85 | MG | 6 | 2146 | 1/1 | 0.99 | 0.14 | - | 44,44,44,44 | 0 |
| 85 | MG | 1 | 3733 | 1/1 | 0.88 | 0.44 | - | 33,33,33,33 | 0 |
| 85 | MG | 1 | 3972 | 1/1 | 0.98 | 0.31 | - | 31,31,31,31 | 0 |
| 85 | MG | 4 | 213 | 1/1 | 0.84 | 0.48 | - | 34,34,34,34 | 0 |
| 85 | MG | 1 | 4182 | 1/1 | 0.89 | 0.36 | - | 49,49,49,49 | 0 |
| 85 | MG | AR | 3860 | 1/1 | 0.96 | 0.47 | - | 6,6,6,6 | 0 |
| 85 | MG | 1 | 4201 | 1/1 | 0.98 | 0.53 | - | 31,31,31,31 | 0 |
| 85 | MG | AR | 4176 | 1/1 | 0.90 | 0.20 | - | 52,52,52,52 | 0 |
| 85 | MG | AR | 3944 | 1/1 | 0.95 | 0.37 | - | 39,39,39,39 | 0 |
| 85 | MG | 1 | 4058 | 1/1 | 0.87 | 0.15 | - | 37,37,37,37 | 0 |
| 85 | MG | 1 | 3775 | 1/1 | 0.82 | 0.14 | - | 59,59,59,59 | 0 |
| 85 | MG | AT | 228 | 1/1 | 0.96 | 0.22 | - | 34,34,34,34 | 0 |
| 85 | MG | 1 | 4062 | 1/1 | 0.92 | 0.19 | - | 33,33,33,33 | 0 |
| 85 | MG | 1 | 3994 | 1/1 | 0.97 | 0.21 | - | 32,32,32,32 | 0 |
| 85 | MG | 6 | 2133 | 1/1 | 0.90 | 0.29 | - | 51,51,51,51 | 0 |
| 84 | OHX | 1 | 3631 | 7/7 | 0.92 | 0.18 | - | 198,199,199,199 | 0 |
| 85 | MG | 1 | 3758 | 1/1 | 0.77 | 0.46 | - | 31,31,31,31 | 0 |
| 85 | MG | 6 | 2118 | 1/1 | 0.97 | 0.25 | - | 54,54,54,54 | 0 |
| 84 | OHX | 6 | 2028 | 7/7 | 0.79 | 0.29 | - | 248,250,252,252 | 0 |
| 85 | MG | AS | 230 | 1/1 | 0.97 | 0.27 | - | 67,67,67,67 | 0 |
| 84 | OHX | 6 | 2012 | 7/7 | 0.94 | 0.11 | - | 188,189,190,191 | 0 |
| 85 | MG | AR | 4178 | 1/1 | 0.94 | 0.23 | - | 48,48,48,48 | 0 |
| 84 | OHX | AR | 3733 | 7/7 | 0.89 | 0.52 | - | 289,291,292,292 | 0 |
| 84 | OHX | CZ | 201 | 7/7 | 0.72 | 0.34 | - | 303,304,305,305 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 85 | MG | AR | 3892 | 1/1 | 0.96 | 0.44 | - | 19,19,19,19 | 0 |
| 84 | OHX | 1 | 3442 | 7/7 | 0.98 | 0.12 | - | 98,99,99,100 | 0 |
| 85 | MG | 1 | 4158 | 1/1 | 0.94 | 0.15 | - | 29,29,29,29 | 0 |
| 85 | MG | 1 | 3742 | 1/1 | 0.92 | 0.37 | - | 19,19,19,19 | 0 |
| 85 | MG | 1 | 4015 | 1/1 | 0.91 | 0.17 | - | 38,38,38,38 | 0 |
| 85 | MG | AR | 4235 | 1/1 | 0.98 | 0.40 | - | 15,15,15,15 | 0 |
| 85 | MG | A | 2084 | 1/1 | 0.73 | 0.16 | - | 53,53,53,53 | 0 |
| 85 | MG | 6 | 2069 | 1/1 | 0.92 | 0.59 | - | 26,26,26,26 | 0 |
| 85 | MG | s | 300 | 1/1 | 0.83 | 0.13 | - | 53,53,53,53 | 0 |
| 84 | OHX | 1 | 3639 | 7/7 | 0.97 | 0.29 | - | 201,203,203,204 | 0 |
| 85 | MG | AR | 4182 | 1/1 | 0.96 | 0.47 | - | 48,48,48,48 | 0 |
| 85 | MG | AR | 4055 | 1/1 | 0.82 | 0.39 | - | 47,47,47,47 | 0 |
| 85 | MG | AR | 3855 | 1/1 | 0.90 | 0.13 | - | 37,37,37,37 | 0 |
| 85 | MG | s2 | 301 | 1/1 | 0.94 | 0.61 | - | 46,46,46,46 | 0 |
| 84 | OHX | AR | 3627 | 7/7 | 0.97 | 0.20 | - | 173,173,174,174 | 0 |
| 85 | MG | AR | 4082 | 1/1 | 0.88 | 0.24 | - | 48,48,48,48 | 0 |
| 85 | MG | 1 | 3928 | 1/1 | 0.96 | 0.13 | - | 32,32,32,32 | 0 |
| 85 | MG | AR | 4022 | 1/1 | 0.95 | 0.21 | - | 41,41,41,41 | 0 |
| 85 | MG | AR | 3830 | 1/1 | 0.88 | 0.29 | - | 30,30,30,30 | 0 |
| 85 | MG | AR | 4071 | 1/1 | 0.82 | 0.36 | - | 32,32,32,32 | 0 |
| 85 | MG | AR | 4002 | 1/1 | 0.95 | 0.41 | - | 42,42,42,42 | 0 |
| 85 | MG | 1 | 4119 | 1/1 | 0.81 | 0.29 | - | 35,35,35,35 | 0 |
| 85 | MG | 6 | 2060 | 1/1 | 0.91 | 0.67 | - | 23,23,23,23 | 0 |
| 85 | MG | 1 | 4110 | 1/1 | 0.90 | 0.27 | - | 37,37,37,37 | 0 |
| 84 | OHX | A | 1989 | 7/7 | 0.91 | 0.28 | - | 253,254,256,256 | 0 |
| 85 | MG | 6 | 2180 | 1/1 | 0.97 | 0.16 | - | 94,94,94,94 | 0 |
| 85 | MG | AR | 3980 | 1/1 | 0.90 | 0.21 | - | 32,32,32,32 | 0 |
| 85 | MG | AR | 4159 | 1/1 | 0.82 | 0.22 | - | 64,64,64,64 | 0 |
| 84 | OHX | 1 | 3599 | 7/7 | 0.95 | 0.11 | - | 190,191,192,193 | 0 |
| 85 | MG | 1 | 4108 | 1/1 | 0.90 | 0.26 | - | 33,33,33,33 | 0 |
| 85 | MG | AR | 3954 | 1/1 | 0.97 | 0.34 | - | 36,36,36,36 | 0 |
| 85 | MG | AR | 3950 | 1/1 | 0.85 | 0.25 | - | 41,41,41,41 | 0 |
| 85 | MG | 4 | 229 | 1/1 | 0.93 | 0.26 | - | 57,57,57,57 | 0 |
| 85 | MG | 1 | 4180 | 1/1 | 0.86 | 0.45 | - | 55,55,55,55 | 0 |
| 85 | MG | AR | 3870 | 1/1 | 0.97 | 0.23 | - | 14,14,14,14 | 0 |
| 85 | MG | AR | 4218 | 1/1 | 0.85 | 0.26 | - | 31,31,31,31 | 0 |
| 84 | OHX | AR | 3513 | 7/7 | 0.98 | 0.11 | - | 152,153,154,154 | 0 |
| 85 | MG | 1 | 3906 | 1/1 | 0.95 | 0.23 | - | 29,29,29,29 | 0 |
| 85 | MG | Y | 201 | 1/1 | 0.80 | 0.47 | - | 51,51,51,51 | 0 |
| 84 | OHX | 1 | 3562 | 7/7 | 0.97 | 0.08 | - | 200,200,201,202 | 0 |
| 85 | MG | 1 | 4174 | 1/1 | 0.83 | 0.33 | - | 54,54,54,54 | 0 |
| 85 | MG | 1 | 4175 | 1/1 | 0.71 | 0.79 | - | 91,91,91,91 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 85 | MG | AR | 4106 | 1/1 | 0.95 | 0.19 | - | 55,55,55,55 | 0 |
| 85 | MG | 1 | 3776 | 1/1 | 0.95 | 0.28 | - | 29,29,29,29 | 0 |
| 84 | OHX | AR | 3726 | 7/7 | 0.87 | 0.42 | - | 220,220,221,221 | 0 |
| 85 | MG | 1 | 3845 | 1/1 | 0.99 | 0.36 | - | 14,14,14,14 | 0 |
| 85 | MG | 1 | 3780 | 1/1 | 0.90 | 0.27 | - | 26,26,26,26 | 0 |
| 84 | OHX | AR | 3550 | 7/7 | 0.96 | 0.17 | - | 164,164,165,165 | 0 |
| 85 | MG | 1 | 4141 | 1/1 | 0.84 | 0.33 | - | 36,36,36,36 | 0 |
| 85 | MG | 6 | 2123 | 1/1 | 0.85 | 0.30 | - | 60,60,60,60 | 0 |
| 84 | OHX | 6 | 1969 | 7/7 | 0.94 | 0.14 | - | 163,163,165,165 | 0 |
| 85 | MG | 6 | 2126 | 1/1 | 0.94 | 0.33 | - | 39,39,39,39 | 0 |
| 85 | MG | 6 | 2174 | 1/1 | 0.73 | 0.25 | - | 66,66,66,66 | 0 |
| 85 | MG | AR | 4057 | 1/1 | 0.96 | 0.17 | - | 46,46,46,46 | 0 |
| 85 | MG | 1 | 4051 | 1/1 | 0.91 | 0.37 | - | 63,63,63,63 | 0 |
| 85 | MG | 1 | 3769 | 1/1 | 0.88 | 0.45 | - | 61,61,61,61 | 0 |
| 85 | MG | 6 | 2107 | 1/1 | 0.96 | 0.41 | - | 24,24,24,24 | 0 |
| 85 | MG | 1 | 3869 | 1/1 | 0.98 | 0.34 | - | 33,33,33,33 | 0 |
| 85 | MG | 1 | 4090 | 1/1 | 0.93 | 0.10 | - | 54,54,54,54 | 0 |
| 85 | MG | AR | 4015 | 1/1 | 0.85 | 0.35 | - | 43,43,43,43 | 0 |
| 85 | MG | 1 | 4220 | 1/1 | 0.97 | 0.22 | - | 25,25,25,25 | 0 |
| 85 | MG | 1 | 4066 | 1/1 | 0.95 | 0.29 | - | 66,66,66,66 | 0 |
| 85 | MG | 6 | 2172 | 1/1 | 0.94 | 0.20 | - | 32,32,32,32 | 0 |
| 85 | MG | AR | 3902 | 1/1 | 0.95 | 0.69 | - | 24,24,24,24 | 0 |
| 85 | MG | 6 | 2176 | 1/1 | 0.97 | 0.16 | - | 73,73,73,73 | 0 |
| 85 | MG | 1 | 3853 | 1/1 | 0.86 | 0.52 | - | 61,61,61,61 | 0 |
| 85 | MG | A | 2074 | 1/1 | 0.95 | 0.55 | - | 38,38,38,38 | 0 |
| 85 | MG | AR | 4152 | 1/1 | 0.78 | 0.17 | - | 152,152,152,152 | 0 |
| 85 | MG | 1 | 4113 | 1/1 | 0.83 | 0.66 | - | 54,54,54,54 | 0 |
| 85 | MG | AR | 4063 | 1/1 | 0.89 | 0.17 | - | 39,39,39,39 | 0 |
| 85 | MG | AR | 3886 | 1/1 | 0.98 | 0.25 | - | 15,15,15,15 | 0 |
| 85 | MG | 4 | 232 | 1/1 | 0.89 | 0.29 | - | 43,43,43,43 | 0 |
| 85 | MG | AT | 231 | 1/1 | 0.83 | 0.56 | - | 46,46,46,46 | 0 |
| 85 | MG | 1 | 4104 | 1/1 | 0.97 | 0.22 | - | 32,32,32,32 | 0 |
| 85 | MG | 1 | 3986 | 1/1 | 0.91 | 0.13 | - | 30,30,30,30 | 0 |
| 84 | OHX | 3 | 205 | 7/7 | 0.93 | 0.13 | - | 169,171,171,173 | 0 |
| 85 | MG | AR | 3897 | 1/1 | 0.85 | 0.53 | - | 18,18,18,18 | 0 |
| 84 | OHX | 6 | 1975 | 7/7 | 0.97 | 0.16 | - | 160,161,162,162 | 0 |
| 85 | MG | AR | 4209 | 1/1 | 0.82 | 0.27 | - | 48,48,48,48 | 0 |
| 85 | MG | AR | 4128 | 1/1 | 0.78 | 0.17 | - | 54,54,54,54 | 0 |
| 84 | OHX | 4 | 207 | 7/7 | 0.97 | 0.10 | - | 174,175,175,176 | 0 |
| 85 | MG | 1 | 4032 | 1/1 | 0.86 | 0.29 | - | 49,49,49,49 | 0 |
| 85 | MG | DE | 201 | 1/1 | 0.85 | 0.15 | - | 55,55,55,55 | 0 |
| 85 | MG | A | 2075 | 1/1 | 0.68 | 0.37 | - | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 85 | MG | AS | 219 | 1/1 | 0.90 | 0.31 | - | 35,35,35,35 | 0 |
| 85 | MG | AR | 3994 | 1/1 | 0.87 | 0.41 | - | 44,44,44,44 | 0 |
| 85 | MG | 1 | 3784 | 1/1 | 0.97 | 0.30 | - | 30,30,30,30 | 0 |
| 84 | OHX | 1 | 3610 | 7/7 | 0.96 | 0.28 | - | 212,212,212,212 | 0 |
| 85 | MG | A | 2149 | 1/1 | 0.92 | 0.36 | - | 49,49,49,49 | 0 |
| 85 | MG | AR | 3876 | 1/1 | 0.92 | 0.43 | - | 30,30,30,30 | 0 |
| 85 | MG | DC | 201 | 1/1 | 0.96 | 0.36 | - | 16,16,16,16 | 0 |
| 85 | MG | AR | 4098 | 1/1 | 0.96 | 0.18 | - | 27,27,27,27 | 0 |
| 85 | MG | A | 2091 | 1/1 | 0.88 | 0.44 | - | 60,60,60,60 | 0 |
| 85 | MG | AR | 3758 | 1/1 | 0.95 | 0.35 | - | 81,81,81,81 | 0 |
| 85 | MG | AR | 3961 | 1/1 | 0.94 | 0.19 | - | 23,23,23,23 | 0 |
| 85 | MG | 6 | 2125 | 1/1 | 0.93 | 0.26 | - | 63,63,63,63 | 0 |
| 85 | MG | DP | 101 | 1/1 | 0.92 | 0.20 | - | 43,43,43,43 | 0 |
| 85 | MG | AR | 3924 | 1/1 | 0.97 | 0.47 | - | 13,13,13,13 | 0 |
| 85 | MG | 1 | 4026 | 1/1 | 0.95 | 0.54 | - | 44,44,44,44 | 0 |
| 85 | MG | 1 | 4008 | 1/1 | 0.73 | 1.07 | - | 76,76,76,76 | 0 |
| 85 | MG | 1 | 4095 | 1/1 | 0.78 | 0.37 | - | 53,53,53,53 | 0 |
| 85 | MG | 6 | 2153 | 1/1 | 0.89 | 0.24 | - | 39,39,39,39 | 0 |
| 85 | MG | 1 | 3740 | 1/1 | 0.95 | 0.41 | - | 7,7,7,7 | 0 |
| 85 | MG | AR | 3854 | 1/1 | 0.96 | 0.21 | - | 28,28,28,28 | 0 |
| 84 | OHX | 6 | 2031 | 7/7 | 0.91 | 0.27 | - | 210,211,213,213 | 0 |
| 85 | MG | AR | 4080 | 1/1 | 0.98 | 0.17 | - | 16,16,16,16 | 0 |
| 85 | MG | AR | 4073 | 1/1 | 0.96 | 0.15 | - | 33,33,33,33 | 0 |
| 84 | OHX | AR | 3569 | 7/7 | 0.96 | 0.10 | - | 182,182,183,183 | 0 |
| 85 | MG | 1 | 4106 | 1/1 | 0.81 | 0.38 | - | 30,30,30,30 | 0 |
| 85 | MG | 1 | 3951 | 1/1 | 0.88 | 0.33 | - | 43,43,43,43 | 0 |
| 84 | OHX | 1 | 3652 | 7/7 | 0.97 | 0.17 | - | 173,174,174,174 | 0 |
| 85 | MG | AR | 3814 | 1/1 | 0.97 | 0.33 | - | 27,27,27,27 | 0 |
| 85 | MG | 1 | 3743 | 1/1 | 0.94 | 0.39 | - | 23,23,23,23 | 0 |
| 84 | OHX | AR | 3702 | 7/7 | 0.86 | 0.41 | - | 218,219,220,220 | 0 |
| 84 | OHX | A | 2039 | 7/7 | 0.88 | 0.29 | - | 264,266,268,268 | 0 |
| 85 | MG | AR | 3786 | 1/1 | 0.97 | 0.19 | - | 16,16,16,16 | 0 |
| 85 | MG | 6 | 2193 | 1/1 | 0.20 | 0.90 | - | 76,76,76,76 | 0 |
| 85 | MG | 1 | 4129 | 1/1 | 0.69 | 0.38 | - | 51,51,51,51 | 0 |
| 85 | MG | AR | 4070 | 1/1 | 0.94 | 0.12 | - | 42,42,42,42 | 0 |
| 84 | OHX | 1 | 3641 | 7/7 | 0.94 | 0.23 | - | 195,196,197,197 | 0 |
| 85 | MG | A | 2043 | 1/1 | 0.96 | 0.26 | - | 47,47,47,47 | 0 |
| 84 | OHX | A | 1929 | 7/7 | 0.95 | 0.23 | - | 157,159,160,160 | 0 |
| 85 | MG | 1 | 4080 | 1/1 | 0.94 | 0.34 | - | 55,55,55,55 | 0 |
| 85 | MG | 1 | 3885 | 1/1 | 0.97 | 0.49 | - | 10,10,10,10 | 0 |
| 85 | MG | 1 | 3968 | 1/1 | 0.59 | 0.29 | - | 50,50,50,50 | 0 |
| 85 | MG | 6 | 2173 | 1/1 | 0.95 | 0.19 | - | 69,69,69,69 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 85 | MG | A | 2143 | 1/1 | 0.93 | 0.21 | - | 151,151,151,151 | 0 |
| 85 | MG | A | 2088 | 1/1 | 0.84 | 0.27 | - | 66,66,66,66 | 0 |
| 84 | OHX | AR | 3658 | 7/7 | 0.94 | 0.27 | - | 177,177,179,179 | 0 |
| 85 | MG | 1 | 4024 | 1/1 | 0.93 | 0.37 | - | 15,15,15,15 | 0 |
| 85 | MG | AR | 3919 | 1/1 | 0.95 | 0.56 | - | 11,11,11,11 | 0 |
| 85 | MG | AR | 4131 | 1/1 | 0.85 | 0.56 | - | 59,59,59,59 | 0 |
| 85 | MG | AR | 3831 | 1/1 | 0.91 | 0.32 | - | 45,45,45,45 | 0 |
| 85 | MG | AR | 3877 | 1/1 | 0.97 | 0.39 | - | 14,14,14,14 | 0 |
| 84 | OHX | 1 | 3676 | 7/7 | 0.84 | 0.42 | - | 223,223,225,225 | 0 |
| 85 | MG | 1 | 3752 | 1/1 | 0.99 | 0.28 | - | 27,27,27,27 | 0 |
| 85 | MG | AR | 4024 | 1/1 | 0.71 | 0.42 | - | 33,33,33,33 | 0 |
| 84 | OHX | AR | 3528 | 7/7 | 0.97 | 0.11 | - | 147,147,148,149 | 0 |
| 85 | MG | 1 | 3837 | 1/1 | 0.99 | 0.64 | - | 25,25,25,25 | 0 |
| 85 | MG | A | 2117 | 1/1 | 0.89 | 0.20 | - | 52,52,52,52 | 0 |
| 84 | OHX | 3 | 208 | 7/7 | 0.92 | 0.16 | - | 230,231,232,233 | 0 |
| 84 | OHX | 1 | 3615 | 7/7 | 0.92 | 0.39 | - | 185,186,186,187 | 0 |
| 85 | MG | 3 | 212 | 1/1 | 0.95 | 0.30 | - | 27,27,27,27 | 0 |
| 85 | MG | AR | 4206 | 1/1 | 0.86 | 0.40 | - | 31,31,31,31 | 0 |
| 85 | MG | 1 | 3985 | 1/1 | 0.88 | 0.34 | - | 22,22,22,22 | 0 |
| 85 | MG | 1 | 4171 | 1/1 | 0.91 | 0.14 | - | 26,26,26,26 | 0 |
| 85 | MG | AR | 3835 | 1/1 | 0.87 | 0.39 | - | 41,41,41,41 | 0 |
| 84 | OHX | AR | 3453 | 7/7 | 0.97 | 0.12 | - | 127,128,128,128 | 0 |
| 85 | MG | AR | 3815 | 1/1 | 0.86 | 0.19 | - | 75,75,75,75 | 0 |
| 84 | OHX | AR | 3687 | 7/7 | 0.78 | 0.36 | - | 244,245,246,247 | 0 |
| 84 | OHX | 1 | 3726 | 7/7 | 0.83 | 0.42 | - | 231,232,233,233 | 0 |
| 85 | MG | 1 | 4211 | 1/1 | 0.97 | 0.37 | - | 21,21,21,21 | 0 |
| 85 | MG | CO | 203 | 1/1 | 0.90 | 0.21 | - | 46,46,46,46 | 0 |
| 85 | MG | 6 | 2117 | 1/1 | 0.99 | 0.41 | - | 21,21,21,21 | 0 |
| 85 | MG | AS | 218 | 1/1 | 0.90 | 0.22 | - | 52,52,52,52 | 0 |
| 85 | MG | AR | 3988 | 1/1 | 0.83 | 0.31 | - | 32,32,32,32 | 0 |
| 85 | MG | 1 | 4056 | 1/1 | 0.89 | 0.39 | - | 82,82,82,82 | 0 |
| 85 | MG | AR | 4127 | 1/1 | 0.87 | 0.25 | - | 67,67,67,67 | 0 |
| 84 | OHX | AR | 3710 | 7/7 | 0.90 | 0.32 | - | 213,215,216,216 | 0 |
| 85 | MG | D | 301 | 1/1 | 0.82 | 0.58 | - | 42,42,42,42 | 0 |
| 85 | MG | A | 2131 | 1/1 | 0.91 | 0.13 | - | 88,88,88,88 | 0 |
| 85 | MG | AR | 3979 | 1/1 | 0.92 | 0.24 | - | 45,45,45,45 | 0 |
| 84 | OHX | 6 | 2014 | 7/7 | 0.94 | 0.23 | - | 219,220,221,221 | 0 |
| 85 | MG | 1 | 3798 | 1/1 | 0.94 | 0.19 | - | 29,29,29,29 | 0 |
| 84 | OHX | AR | 3634 | 7/7 | 0.92 | 0.18 | - | 213,214,215,216 | 0 |
| 84 | OHX | 1 | 3730 | 7/7 | 0.97 | 0.14 | - | 141,142,143,143 | 0 |
| 84 | OHX | 6 | 2047 | 7/7 | 0.89 | 0.32 | - | 237,239,240,241 | 0 |
| 85 | MG | AR | 4230 | 1/1 | 0.93 | 0.40 | - | 68,68,68,68 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 85 | MG | AR | 4166 | 1/1 | 0.98 | 0.11 | - | 58,58,58,58 | 0 |
| 85 | MG | 6 | 2097 | 1/1 | 0.75 | 0.30 | - | 79,79,79,79 | 0 |
| 85 | MG | AR | 3948 | 1/1 | 0.92 | 0.23 | - | 16,16,16,16 | 0 |
| 85 | MG | AR | 4199 | 1/1 | 0.93 | 0.28 | - | 64,64,64,64 | 0 |
| 85 | MG | A | 2107 | 1/1 | 0.76 | 0.24 | - | 69,69,69,69 | 0 |
| 85 | MG | 6 | 2081 | 1/1 | 0.80 | 0.31 | - | 94,94,94,94 | 0 |
| 85 | MG | CQ | 204 | 1/1 | 0.97 | 0.33 | - | 48,48,48,48 | 0 |
| 85 | MG | AR | 4195 | 1/1 | 0.97 | 0.17 | - | 21,21,21,21 | 0 |
| 84 | OHX | AR | 3508 | 7/7 | 0.96 | 0.21 | - | 139,139,140,140 | 0 |
| 84 | OHX | AR | 3519 | 7/7 | 0.98 | 0.12 | - | 135,135,136,136 | 0 |
| 85 | MG | AR | 3744 | 1/1 | 0.94 | 0.47 | - | 20,20,20,20 | 0 |
| 85 | MG | 1 | 3851 | 1/1 | 0.94 | 0.24 | - | 34,34,34,34 | 0 |
| 84 | OHX | 1 | 3552 | 7/7 | 0.96 | 0.20 | - | 173,174,175,175 | 0 |
| 85 | MG | 1 | 4101 | 1/1 | 0.85 | 0.22 | - | 37,37,37,37 | 0 |
| 85 | MG | 1 | 4146 | 1/1 | 0.92 | 0.16 | - | 39,39,39,39 | 0 |
| 84 | OHX | 6 | 2001 | 7/7 | 0.92 | 0.40 | - | 211,211,212,213 | 0 |
| 85 | MG | AR | 4179 | 1/1 | 0.90 | 0.21 | - | 58,58,58,58 | 0 |
| 85 | MG | 6 | 2074 | 1/1 | 0.91 | 0.31 | - | 37,37,37,37 | 0 |
| 85 | MG | 1 | 4094 | 1/1 | 0.99 | 0.13 | - | 43,43,43,43 | 0 |
| 84 | OHX | AR | 3535 | 7/7 | 0.96 | 0.14 | - | 157,157,158,158 | 0 |
| 85 | MG | AR | 4223 | 1/1 | 0.83 | 0.35 | - | 54,54,54,54 | 0 |
| 84 | OHX | 1 | 3659 | 7/7 | 0.93 | 0.14 | - | 208,210,211,211 | 0 |
| 85 | MG | AR | 3834 | 1/1 | 0.87 | 0.18 | - | 30,30,30,30 | 0 |
| 85 | MG | 1 | 3773 | 1/1 | 0.98 | 0.46 | - | 15,15,15,15 | 0 |
| 85 | MG | A | 2090 | 1/1 | 0.96 | 0.28 | - | 46,46,46,46 | 0 |
| 85 | MG | AR | 3767 | 1/1 | 1.00 | 0.11 | - | 34,34,34,34 | 0 |
| 85 | MG | 1 | 4206 | 1/1 | 0.77 | 0.46 | - | 28,28,28,28 | 0 |
| 85 | MG | A | 2059 | 1/1 | 0.95 | 0.40 | - | 25,25,25,25 | 0 |
| 85 | MG | AR | 3769 | 1/1 | 0.93 | 0.13 | - | 35,35,35,35 | 0 |
| 85 | MG | 1 | 4013 | 1/1 | 0.98 | 0.22 | - | 56,56,56,56 | 0 |
| 84 | OHX | AR | 3639 | 7/7 | 0.88 | 0.18 | - | 211,212,213,213 | 0 |
| 85 | MG | 1 | 4200 | 1/1 | 0.97 | 0.34 | - | 18,18,18,18 | 0 |
| 85 | MG | x | 203 | 1/1 | 0.79 | 0.26 | - | 64,64,64,64 | 0 |
| 85 | MG | 1 | 3891 | 1/1 | 0.87 | 0.66 | - | 16,16,16,16 | 0 |
| 85 | MG | AR | 4183 | 1/1 | 0.84 | 0.20 | - | 93,93,93,93 | 0 |
| 85 | MG | 1 | 4114 | 1/1 | 0.95 | 0.14 | - | 33,33,33,33 | 0 |
| 85 | MG | 6 | 2079 | 1/1 | 0.93 | 0.34 | - | 37,37,37,37 | 0 |
| 85 | MG | 1 | 3988 | 1/1 | 0.90 | 0.26 | - | 46,46,46,46 | 0 |
| 84 | OHX | 1 | 3634 | 7/7 | 0.93 | 0.21 | - | 206,207,207,209 | 0 |
| 84 | OHX | AR | 3445 | 7/7 | 0.98 | 0.13 | - | 94,94,94,95 | 0 |
| 85 | MG | A | 2099 | 1/1 | 0.94 | 0.76 | - | 64,64,64,64 | 0 |
| 85 | MG | 1 | 4163 | 1/1 | 0.86 | 0.40 | - | 68,68,68,68 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 85 | MG | 1 | 3834 | 1/1 | 0.92 | 0.42 | - | 18,18,18,18 | 0 |
| 84 | OHX | A | 1951 | 7/7 | 0.95 | 0.20 | - | 203,205,207,207 | 0 |
| 85 | MG | AR | 4053 | 1/1 | 0.95 | 0.27 | - | 50,50,50,50 | 0 |
| 84 | OHX | AR | 3571 | 7/7 | 0.95 | 0.18 | - | 194,194,195,195 | 0 |
| 85 | MG | 6 | 2099 | 1/1 | 0.94 | 0.22 | - | 19,19,19,19 | 0 |
| 85 | MG | 6 | 2063 | 1/1 | 0.98 | 0.28 | - | 31,31,31,31 | 0 |
| 85 | MG | AR | 3839 | 1/1 | 0.90 | 0.37 | - | 30,30,30,30 | 0 |
| 85 | MG | 6 | 2138 | 1/1 | 0.94 | 0.58 | - | 49,49,49,49 | 0 |
| 85 | MG | AR | 4014 | 1/1 | 0.98 | 0.35 | - | 32,32,32,32 | 0 |
| 85 | MG | 1 | 4077 | 1/1 | 0.96 | 0.15 | - | 42,42,42,42 | 0 |
| 84 | OHX | A | 1995 | 7/7 | 0.93 | 0.15 | - | 206,207,208,209 | 0 |
| 84 | OHX | 1 | 3691 | 7/7 | 0.94 | 0.30 | - | 206,207,208,208 | 0 |
| 85 | MG | 1 | 4085 | 1/1 | 0.84 | 0.28 | - | 43,43,43,43 | 0 |
| 85 | MG | AR | 4215 | 1/1 | 0.91 | 0.23 | - | 72,72,72,72 | 0 |
| 85 | MG | AR | 4056 | 1/1 | 0.83 | 0.29 | - | 44,44,44,44 | 0 |
| 84 | OHX | 1 | 3711 | 7/7 | 0.83 | 0.26 | - | 301,302,304,304 | 0 |
| 85 | MG | A | 2048 | 1/1 | 0.84 | 0.18 | - | 42,42,42,42 | 0 |
| 84 | OHX | 1 | 3704 | 7/7 | 0.90 | 0.40 | - | 277,278,278,278 | 0 |
| 85 | MG | d5 | 201 | 1/1 | 0.90 | 0.09 | - | 67,67,67,67 | 0 |
| 85 | MG | 6 | 2094 | 1/1 | 0.98 | 0.28 | - | 24,24,24,24 | 0 |
| 85 | MG | x | 204 | 1/1 | 0.95 | 0.15 | - | 18,18,18,18 | 0 |
| 85 | MG | 1 | 4017 | 1/1 | 0.85 | 0.21 | - | 59,59,59,59 | 0 |
| 85 | MG | AR | 4116 | 1/1 | 0.96 | 0.29 | - | 105,105,105,105 | 0 |
| 85 | MG | AR | 4074 | 1/1 | 0.84 | 0.30 | - | 44,44,44,44 | 0 |
| 85 | MG | 1 | 3793 | 1/1 | 0.98 | 0.46 | - | 12,12,12,12 | 0 |
| 84 | OHX | AR | 3711 | 7/7 | 0.88 | 0.20 | - | 227,227,228,228 | 0 |
| 84 | OHX | 1 | 3703 | 7/7 | 0.84 | 0.59 | - | 259,259,260,261 | 0 |
| 85 | MG | 1 | 3970 | 1/1 | 0.96 | 0.25 | - | 59,59,59,59 | 0 |
| 85 | MG | 6 | 2167 | 1/1 | 0.85 | 0.41 | - | 52,52,52,52 | 0 |
| 85 | MG | 1 | 4075 | 1/1 | 0.93 | 0.23 | - | 20,20,20,20 | 0 |
| 84 | OHX | AR | 3732 | 7/7 | 0.86 | 0.54 | - | 245,246,247,247 | 0 |
| 85 | MG | 6 | 2191 | 1/1 | 0.98 | 0.29 | - | 47,47,47,47 | 0 |
| 84 | OHX | AR | 3447 | 7/7 | 0.99 | 0.13 | - | 88,88,89,89 | 0 |
| 84 | OHX | AR | 3725 | 7/7 | 0.89 | 0.34 | - | 261,263,264,264 | 0 |
| 84 | OHX | AR | 3713 | 7/7 | 0.91 | 0.16 | - | 247,247,248,249 | 0 |
| 85 | MG | 1 | 4131 | 1/1 | 0.71 | 0.33 | - | 38,38,38,38 | 0 |
| 84 | OHX | c8 | 201 | 7/7 | 0.94 | 0.15 | - | 198,199,200,201 | 0 |
| 84 | OHX | 1 | 3499 | 7/7 | 0.99 | 0.10 | - | 124,125,126,126 | 0 |
| 85 | MG | 1 | 3860 | 1/1 | 0.95 | 0.47 | - | 19,19,19,19 | 0 |
| 84 | OHX | AR | 3456 | 7/7 | 0.98 | 0.12 | - | 109,110,110,111 | 0 |
| 85 | MG | AR | 3811 | 1/1 | 0.89 | 0.30 | - | 25,25,25,25 | 0 |
| 84 | OHX | 1 | 3497 | 7/7 | 0.97 | 0.12 | - | 140,141,142,142 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | OHX | AS | 208 | 7/7 | 0.82 | 0.30 | - | 226,226,228,228 | 0 |
| 85 | MG | 4 | 231 | 1/1 | 0.89 | 0.26 | - | 30,30,30,30 | 0 |
| 85 | MG | A | 2080 | 1/1 | 0.96 | 0.52 | - | 45,45,45,45 | 0 |
| 85 | MG | AR | 4038 | 1/1 | 0.95 | 0.26 | - | 30,30,30,30 | 0 |
| 85 | MG | AR | 4169 | 1/1 | 0.94 | 0.14 | - | 34,34,34,34 | 0 |
| 85 | MG | AR | 4097 | 1/1 | 0.93 | 0.33 | - | 26,26,26,26 | 0 |
| 85 | MG | AR | 3813 | 1/1 | 0.69 | 0.33 | - | 54,54,54,54 | 0 |
| 85 | MG | AR | 4163 | 1/1 | 0.96 | 0.12 | - | 30,30,30,30 | 0 |
| 85 | MG | AR | 4085 | 1/1 | 0.94 | 0.30 | - | 37,37,37,37 | 0 |
| 85 | MG | 1 | 4018 | 1/1 | 0.96 | 0.24 | - | 26,26,26,26 | 0 |
| 85 | MG | A | 2050 | 1/1 | 0.95 | 0.32 | - | 68,68,68,68 | 0 |
| 84 | OHX | 1 | 3619 | 7/7 | 0.92 | 0.39 | - | 190,191,192,193 | 0 |
| 84 | OHX | AR | 3680 | 7/7 | 0.93 | 0.40 | - | 220,222,222,223 | 0 |
| 85 | MG | 1 | 4138 | 1/1 | 0.89 | 0.37 | - | 37,37,37,37 | 0 |
| 85 | MG | 1 | 3946 | 1/1 | 0.95 | 0.17 | - | 68,68,68,68 | 0 |
| 85 | MG | 1 | 3783 | 1/1 | 0.94 | 0.29 | - | 27,27,27,27 | 0 |
| 85 | MG | 1 | 3936 | 1/1 | 0.97 | 0.13 | - | 48,48,48,48 | 0 |
| 85 | MG | 6 | 2189 | 1/1 | 0.89 | 0.29 | - | 67,67,67,67 | 0 |
| 84 | OHX | A | 1906 | 7/7 | 0.99 | 0.17 | - | 112,113,113,113 | 0 |
| 84 | OHX | A | 1983 | 7/7 | 0.96 | 0.20 | - | 188,190,192,192 | 0 |
| 85 | MG | 1 | 3826 | 1/1 | 0.95 | 0.26 | - | 44,44,44,44 | 0 |
| 85 | MG | CD | 302 | 1/1 | 0.89 | 0.75 | - | 39,39,39,39 | 0 |
| 85 | MG | 1 | 4164 | 1/1 | 0.96 | 0.16 | - | 48,48,48,48 | 0 |
| 85 | MG | 1 | 3894 | 1/1 | 0.96 | 0.42 | - | 26,26,26,26 | 0 |
| 85 | MG | AR | 3792 | 1/1 | 0.92 | 0.39 | - | 28,28,28,28 | 0 |
| 85 | MG | 6 | 2170 | 1/1 | 0.76 | 0.45 | - | 46,46,46,46 | 0 |
| 85 | MG | d3 | 203 | 1/1 | 0.88 | 0.23 | - | 29,29,29,29 | 0 |
| 85 | MG | AR | 4221 | 1/1 | 0.81 | 0.27 | - | 49,49,49,49 | 0 |
| 85 | MG | AR | 3967 | 1/1 | 0.88 | 0.34 | - | 64,64,64,64 | 0 |
| 85 | MG | 1 | 3892 | 1/1 | 0.98 | 0.52 | - | 14,14,14,14 | 0 |
| 84 | OHX | 1 | 3547 | 7/7 | 0.94 | 0.20 | - | 168,169,170,170 | 0 |
| 85 | MG | 1 | 3808 | 1/1 | 0.81 | 0.42 | - | 54,54,54,54 | 0 |
| 85 | MG | AR | 4021 | 1/1 | 0.83 | 0.33 | - | 36,36,36,36 | 0 |
| 85 | MG | A | 2118 | 1/1 | 0.52 | 0.95 | - | 75,75,75,75 | 0 |
| 85 | MG | AR | 4028 | 1/1 | 0.90 | 0.24 | - | 44,44,44,44 | 0 |
| 85 | MG | AR | 4146 | 1/1 | 0.88 | 0.40 | - | 37,37,37,37 | 0 |
| 85 | MG | 1 | 4197 | 1/1 | 0.97 | 0.13 | - | 48,48,48,48 | 0 |
| 85 | MG | 1 | 3842 | 1/1 | 0.93 | 0.58 | - | 27,27,27,27 | 0 |
| 85 | MG | 1 | 4140 | 1/1 | 0.69 | 0.48 | - | 49,49,49,49 | 0 |
| 85 | MG | 6 | 2164 | 1/1 | 0.93 | 0.19 | - | 63,63,63,63 | 0 |
| 84 | OHX | 6 | 1990 | 7/7 | 0.92 | 0.33 | - | 238,238,239,240 | 0 |
| 85 | MG | AR | 4197 | 1/1 | 0.98 | 0.24 | - | 29,29,29,29 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | OHX | AS | 204 | 7/7 | 0.98 | 0.12 | - | 140,141,141,141 | 0 |
| 84 | OHX | 1 | 3437 | 7/7 | 0.98 | 0.14 | - | 100,101,102,102 | 0 |
| 85 | MG | AR | 4212 | 1/1 | 0.93 | 0.12 | - | 48,48,48,48 | 0 |
| 85 | MG | DO | 202 | 1/1 | 0.86 | 0.27 | - | 46,46,46,46 | 0 |
| 85 | MG | 3 | 214 | 1/1 | 0.99 | 0.42 | - | 12,12,12,12 | 0 |
| 85 | MG | 1 | 3782 | 1/1 | 0.94 | 0.41 | - | 44,44,44,44 | 0 |
| 85 | MG | 1 | 3998 | 1/1 | 0.90 | 0.24 | - | 65,65,65,65 | 0 |
| 85 | MG | AR | 3807 | 1/1 | 0.91 | 0.24 | - | 27,27,27,27 | 0 |
| 85 | MG | AR | 4109 | 1/1 | 0.96 | 0.23 | - | 42,42,42,42 | 0 |
| 85 | MG | AR | 3782 | 1/1 | 0.89 | 0.27 | - | 30,30,30,30 | 0 |
| 85 | MG | AS | 211 | 1/1 | 0.96 | 0.29 | - | 22,22,22,22 | 0 |
| 85 | MG | AR | 3907 | 1/1 | 0.93 | 0.36 | - | 20,20,20,20 | 0 |
| 84 | OHX | AR | 3624 | 7/7 | 0.94 | 0.30 | - | 210,211,212,212 | 0 |
| 85 | MG | AS | 229 | 1/1 | 0.81 | 0.29 | - | 68,68,68,68 | 0 |
| 85 | MG | AR | 4244 | 1/1 | 0.92 | 0.34 | - | 44,44,44,44 | 0 |
| 85 | MG | AR | 3794 | 1/1 | 0.89 | 0.34 | - | 19,19,19,19 | 0 |
| 85 | MG | A | 2151 | 1/1 | 0.86 | 0.10 | - | 72,72,72,72 | 0 |
| 84 | OHX | A | 1969 | 7/7 | 0.92 | 0.20 | - | 220,222,223,223 | 0 |
| 85 | MG | 6 | 2130 | 1/1 | 0.91 | 0.26 | - | 42,42,42,42 | 0 |
| 85 | MG | AR | 4171 | 1/1 | 0.94 | 0.43 | - | 59,59,59,59 | 0 |
| 85 | MG | 1 | 3759 | 1/1 | 0.71 | 0.34 | - | 69,69,69,69 | 0 |
| 85 | MG | AR | 3969 | 1/1 | 0.94 | 0.25 | - | 38,38,38,38 | 0 |
| 84 | OHX | 4 | 204 | 7/7 | 0.96 | 0.28 | - | 160,160,161,161 | 0 |
| 85 | MG | AR | 4180 | 1/1 | 0.87 | 0.47 | - | 93,93,93,93 | 0 |
| 85 | MG | 1 | 4000 | 1/1 | 0.93 | 0.42 | - | 36,36,36,36 | 0 |
| 85 | MG | 3 | 216 | 1/1 | 0.94 | 0.21 | - | 35,35,35,35 | 0 |
| 84 | OHX | AR | 3666 | 7/7 | 0.91 | 0.20 | - | 217,218,218,219 | 0 |
| 84 | OHX | A | 1930 | 7/7 | 0.97 | 0.16 | - | 164,165,166,167 | 0 |
| 85 | MG | AR | 4088 | 1/1 | 0.94 | 0.15 | - | 50,50,50,50 | 0 |
| 85 | MG | AR | 4052 | 1/1 | 0.92 | 0.32 | - | 28,28,28,28 | 0 |
| 84 | OHX | 1 | 3508 | 7/7 | 0.98 | 0.12 | - | 140,142,143,144 | 0 |
| 85 | MG | 1 | 3744 | 1/1 | 0.96 | 0.73 | - | 43,43,43,43 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.