



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 21, 2017 – 05:28 PM EST

PDB ID : 5OBM
Title : Crystal structure of Gentamicin bound to the yeast 80S ribosome
Authors : Prokhorova, I.; Djumagulov, M.; Urzhumtsev, A.; Yusupov, M.; Yusupova, G.
Deposited on : 2017-06-28
Resolution : 3.40 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

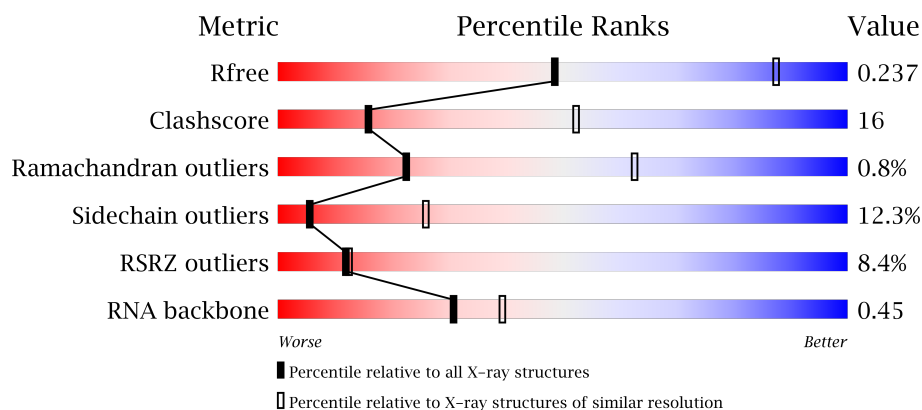
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




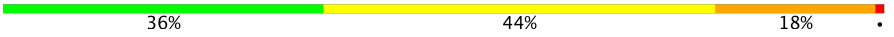


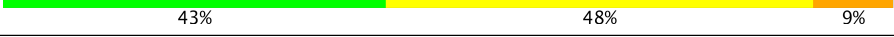

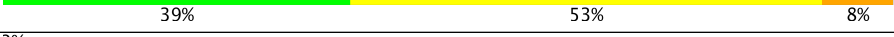

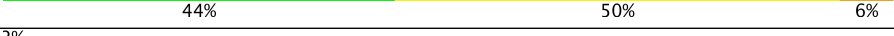

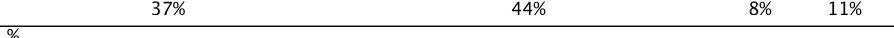
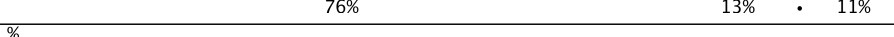

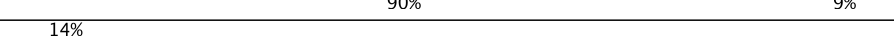


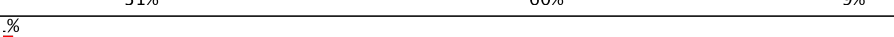

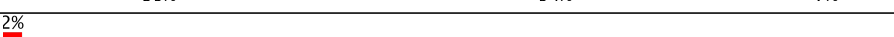




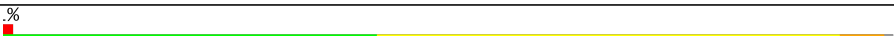

| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 100719 | 1679 (3.50-3.30) |
| Clashscore | 112137 | 1832 (3.50-3.30) |
| Ramachandran outliers | 110173 | 1789 (3.50-3.30) |
| Sidechain outliers | 110143 | 1789 (3.50-3.30) |
| RSRZ outliers | 101464 | 1709 (3.50-3.30) |
| RNA backbone | 2435 | 1009 (3.96-2.84) |

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>37%</div> <div>38%</div> <div>13%</div> <div>9%</div> </div> |
| 1 | 5 | 3396 | <div> <div>34%</div> <div>41%</div> <div>15%</div> <div>8%</div> </div> |
| 2 | 3 | 121 | <div> <div>41%</div> <div>49%</div> <div>9%</div> </div> |
| 2 | 7 | 121 | <div> <div>34%</div> <div>50%</div> <div>12%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 3 | 4 | 158 |  |
| 3 | 8 | 158 |  |
| 4 | L2 | 252 |  |
| 4 | l2 | 252 |  |
| 5 | L3 | 386 |  |
| 5 | l3 | 386 |  |
| 6 | L4 | 361 |  |
| 6 | l4 | 361 |  |
| 7 | L5 | 296 |  |
| 7 | l5 | 296 |  |
| 8 | L6 | 176 |  |
| 8 | l6 | 176 |  |
| 9 | L7 | 223 |  |
| 9 | l7 | 223 |  |
| 10 | L8 | 233 |  |
| 10 | l8 | 233 |  |
| 11 | L9 | 191 |  |
| 11 | l9 | 191 |  |
| 12 | M0 | 221 |  |
| 12 | m0 | 221 |  |
| 13 | M1 | 169 |  |
| 13 | m1 | 169 |  |
| 14 | M3 | 194 |  |
| 14 | m3 | 194 |  |
| 15 | M4 | 137 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15 | m4 | 137 | |
| 16 | M5 | 203 | |
| 16 | m5 | 203 | |
| 17 | M6 | 197 | |
| 17 | m6 | 197 | |
| 18 | M7 | 184 | |
| 18 | m7 | 184 | |
| 19 | M8 | 185 | |
| 19 | m8 | 185 | |
| 20 | M9 | 188 | |
| 20 | m9 | 188 | |
| 21 | N0 | 172 | |
| 21 | n0 | 172 | |
| 22 | N1 | 159 | |
| 22 | n1 | 159 | |
| 23 | N2 | 100 | |
| 23 | n2 | 100 | |
| 24 | N3 | 136 | |
| 24 | n3 | 136 | |
| 25 | N4 | 155 | |
| 26 | N5 | 121 | |
| 26 | n5 | 121 | |
| 27 | N6 | 126 | |
| 27 | n6 | 126 | |
| 28 | N7 | 135 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 28 | n7 | 135 | |
| 29 | N8 | 148 | |
| 29 | n8 | 148 | |
| 30 | N9 | 58 | |
| 30 | n9 | 58 | |
| 31 | O0 | 100 | |
| 31 | o0 | 100 | |
| 32 | O1 | 109 | |
| 32 | o1 | 109 | |
| 33 | O2 | 127 | |
| 33 | o2 | 127 | |
| 34 | O3 | 106 | |
| 34 | o3 | 106 | |
| 35 | O4 | 112 | |
| 35 | o4 | 112 | |
| 36 | O5 | 119 | |
| 36 | o5 | 119 | |
| 37 | O6 | 99 | |
| 37 | o6 | 99 | |
| 38 | O7 | 87 | |
| 38 | o7 | 87 | |
| 39 | O8 | 77 | |
| 39 | o8 | 77 | |
| 40 | O9 | 50 | |
| 40 | o9 | 50 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 41 | Q0 | 52 | |
| 41 | q0 | 52 | |
| 42 | Q1 | 25 | |
| 42 | q1 | 25 | |
| 43 | Q2 | 105 | |
| 43 | q2 | 105 | |
| 44 | Q3 | 91 | |
| 44 | q3 | 91 | |
| 45 | 2 | 1800 | |
| 45 | 6 | 1800 | |
| 46 | S0 | 206 | |
| 46 | s0 | 206 | |
| 47 | S1 | 216 | |
| 47 | s1 | 216 | |
| 48 | S2 | 217 | |
| 48 | s2 | 217 | |
| 49 | S3 | 223 | |
| 49 | s3 | 223 | |
| 50 | S4 | 260 | |
| 50 | s4 | 260 | |
| 51 | S5 | 206 | |
| 51 | s5 | 206 | |
| 52 | S6 | 236 | |
| 52 | s6 | 236 | |
| 53 | S7 | 186 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 53 | s7 | 186 | |
| 54 | S8 | 200 | |
| 54 | s8 | 200 | |
| 55 | S9 | 185 | |
| 55 | s9 | 185 | |
| 56 | C0 | 105 | |
| 56 | c0 | 105 | |
| 57 | C1 | 156 | |
| 57 | c1 | 156 | |
| 58 | C2 | 143 | |
| 58 | c2 | 143 | |
| 59 | C3 | 150 | |
| 59 | c3 | 150 | |
| 60 | C4 | 128 | |
| 60 | c4 | 128 | |
| 61 | C5 | 141 | |
| 61 | c5 | 141 | |
| 62 | C6 | 142 | |
| 62 | c6 | 142 | |
| 63 | C7 | 136 | |
| 63 | c7 | 136 | |
| 64 | C8 | 145 | |
| 64 | c8 | 145 | |
| 65 | C9 | 143 | |
| 65 | c9 | 143 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 66 | D0 | 110 | |
| 66 | d0 | 110 | |
| 67 | D1 | 87 | |
| 67 | d1 | 87 | |
| 68 | D2 | 129 | |
| 68 | d2 | 129 | |
| 69 | D3 | 144 | |
| 69 | d3 | 144 | |
| 70 | D4 | 134 | |
| 70 | d4 | 134 | |
| 71 | D5 | 70 | |
| 71 | d5 | 70 | |
| 72 | D6 | 97 | |
| 72 | d6 | 97 | |
| 73 | D7 | 81 | |
| 73 | d7 | 81 | |
| 74 | D8 | 63 | |
| 74 | d8 | 63 | |
| 75 | D9 | 53 | |
| 75 | d9 | 53 | |
| 76 | E0 | 62 | |
| 76 | e0 | 62 | |
| 77 | E1 | 72 | |
| 77 | e1 | 72 | |
| 78 | SR | 318 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 78 | sR | 318 | |
| 79 | SM | 272 | |
| 79 | sM | 272 | |
| 80 | m2 | 165 | |
| 81 | n4 | 135 | |
| 82 | p0 | 312 | |
| 83 | p1 | 47 | |

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 | MG | 1 | 3401 | - | - | - | X |
| 84 | MG | 1 | 3403 | - | - | - | X |
| 84 | MG | 1 | 3405 | - | - | - | X |
| 84 | MG | 1 | 3407 | - | - | - | X |
| 84 | MG | 1 | 3408 | - | - | - | X |
| 84 | MG | 1 | 3412 | - | - | - | X |
| 84 | MG | 1 | 3417 | - | - | - | X |
| 84 | MG | 1 | 3423 | - | - | - | X |
| 84 | MG | 1 | 3430 | - | - | - | X |
| 84 | MG | 1 | 3432 | - | - | - | X |
| 84 | MG | 1 | 3433 | - | - | - | X |
| 84 | MG | 1 | 3436 | - | - | - | X |
| 84 | MG | 1 | 3438 | - | - | - | X |
| 84 | MG | 1 | 3441 | - | - | - | X |
| 84 | MG | 1 | 3446 | - | - | - | X |
| 84 | MG | 1 | 3449 | - | - | - | X |
| 84 | MG | 1 | 3465 | - | - | - | X |
| 84 | MG | 1 | 3473 | - | - | - | X |
| 84 | MG | 1 | 3474 | - | - | - | X |
| 84 | MG | 1 | 3484 | - | - | - | X |
| 84 | MG | 1 | 3499 | - | - | - | X |
| 84 | MG | 1 | 3502 | - | - | - | X |
| 84 | MG | 1 | 3508 | - | - | - | X |
| 84 | MG | 1 | 3509 | - | - | - | X |
| 84 | MG | 1 | 3516 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 84 | MG | 1 | 3517 | - | - | - | X |
| 84 | MG | 1 | 3518 | - | - | - | X |
| 84 | MG | 1 | 3521 | - | - | - | X |
| 84 | MG | 1 | 3522 | - | - | - | X |
| 84 | MG | 1 | 3526 | - | - | - | X |
| 84 | MG | 1 | 3529 | - | - | - | X |
| 84 | MG | 1 | 3531 | - | - | - | X |
| 84 | MG | 1 | 3532 | - | - | - | X |
| 84 | MG | 1 | 3535 | - | - | - | X |
| 84 | MG | 1 | 3536 | - | - | - | X |
| 84 | MG | 1 | 3537 | - | - | - | X |
| 84 | MG | 1 | 3540 | - | - | - | X |
| 84 | MG | 1 | 3544 | - | - | - | X |
| 84 | MG | 1 | 3545 | - | - | - | X |
| 84 | MG | 1 | 3548 | - | - | - | X |
| 84 | MG | 1 | 3549 | - | - | - | X |
| 84 | MG | 1 | 3559 | - | - | - | X |
| 84 | MG | 1 | 3586 | - | - | - | X |
| 84 | MG | 1 | 3587 | - | - | - | X |
| 84 | MG | 1 | 3588 | - | - | - | X |
| 84 | MG | 1 | 3590 | - | - | - | X |
| 84 | MG | 1 | 3596 | - | - | - | X |
| 84 | MG | 1 | 3599 | - | - | - | X |
| 84 | MG | 1 | 3601 | - | - | - | X |
| 84 | MG | 1 | 3604 | - | - | - | X |
| 84 | MG | 1 | 3605 | - | - | - | X |
| 84 | MG | 1 | 3606 | - | - | - | X |
| 84 | MG | 1 | 3611 | - | - | - | X |
| 84 | MG | 1 | 3612 | - | - | - | X |
| 84 | MG | 1 | 3619 | - | - | - | X |
| 84 | MG | 1 | 3634 | - | - | - | X |
| 84 | MG | 1 | 3644 | - | - | - | X |
| 84 | MG | 1 | 3674 | - | - | - | X |
| 84 | MG | 1 | 3678 | - | - | - | X |
| 84 | MG | 1 | 3680 | - | - | - | X |
| 84 | MG | 1 | 3686 | - | - | - | X |
| 84 | MG | 1 | 3687 | - | - | - | X |
| 84 | MG | 1 | 3688 | - | - | - | X |
| 84 | MG | 1 | 3690 | - | - | - | X |
| 84 | MG | 1 | 3695 | - | - | - | X |
| 84 | MG | 1 | 3701 | - | - | - | X |
| 84 | MG | 1 | 3737 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 84 | MG | 1 | 3739 | - | - | - | X |
| 84 | MG | 1 | 3756 | - | - | - | X |
| 84 | MG | 1 | 3760 | - | - | - | X |
| 84 | MG | 1 | 3766 | - | - | - | X |
| 84 | MG | 1 | 3767 | - | - | - | X |
| 84 | MG | 1 | 3770 | - | - | - | X |
| 84 | MG | 1 | 3795 | - | - | - | X |
| 84 | MG | 1 | 3820 | - | - | - | X |
| 84 | MG | 1 | 3824 | - | - | - | X |
| 84 | MG | 1 | 3826 | - | - | - | X |
| 84 | MG | 1 | 3827 | - | - | - | X |
| 84 | MG | 1 | 3831 | - | - | - | X |
| 84 | MG | 1 | 3833 | - | - | - | X |
| 84 | MG | 1 | 3838 | - | - | - | X |
| 84 | MG | 1 | 3839 | - | - | - | X |
| 84 | MG | 1 | 3856 | - | - | - | X |
| 84 | MG | 1 | 3875 | - | - | - | X |
| 84 | MG | 1 | 3894 | - | - | - | X |
| 84 | MG | 1 | 3914 | - | - | - | X |
| 84 | MG | 1 | 3917 | - | - | - | X |
| 84 | MG | 1 | 3924 | - | - | - | X |
| 84 | MG | 1 | 3925 | - | - | - | X |
| 84 | MG | 1 | 3929 | - | - | - | X |
| 84 | MG | 1 | 3930 | - | - | - | X |
| 84 | MG | 1 | 3931 | - | - | - | X |
| 84 | MG | 1 | 3937 | - | - | - | X |
| 84 | MG | 1 | 3962 | - | - | - | X |
| 84 | MG | 1 | 3967 | - | - | - | X |
| 84 | MG | 1 | 3977 | - | - | - | X |
| 84 | MG | 2 | 1908 | - | - | - | X |
| 84 | MG | 2 | 1923 | - | - | - | X |
| 84 | MG | 2 | 1925 | - | - | - | X |
| 84 | MG | 2 | 1926 | - | - | - | X |
| 84 | MG | 2 | 1927 | - | - | - | X |
| 84 | MG | 2 | 1931 | - | - | - | X |
| 84 | MG | 2 | 1932 | - | - | - | X |
| 84 | MG | 2 | 1943 | - | - | - | X |
| 84 | MG | 2 | 1971 | - | - | - | X |
| 84 | MG | 2 | 1975 | - | - | - | X |
| 84 | MG | 2 | 1980 | - | - | - | X |
| 84 | MG | 2 | 1985 | - | - | - | X |
| 84 | MG | 2 | 1995 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 84 | MG | 4 | 219 | - | - | - | X |
| 84 | MG | 4 | 223 | - | - | - | X |
| 84 | MG | 5 | 3401 | - | - | - | X |
| 84 | MG | 5 | 3405 | - | - | - | X |
| 84 | MG | 5 | 3407 | - | - | - | X |
| 84 | MG | 5 | 3411 | - | - | - | X |
| 84 | MG | 5 | 3412 | - | - | - | X |
| 84 | MG | 5 | 3413 | - | - | - | X |
| 84 | MG | 5 | 3416 | - | - | - | X |
| 84 | MG | 5 | 3417 | - | - | - | X |
| 84 | MG | 5 | 3418 | - | - | - | X |
| 84 | MG | 5 | 3420 | - | - | - | X |
| 84 | MG | 5 | 3427 | - | - | - | X |
| 84 | MG | 5 | 3429 | - | - | - | X |
| 84 | MG | 5 | 3435 | - | - | - | X |
| 84 | MG | 5 | 3437 | - | - | - | X |
| 84 | MG | 5 | 3446 | - | - | - | X |
| 84 | MG | 5 | 3448 | - | - | - | X |
| 84 | MG | 5 | 3449 | - | - | - | X |
| 84 | MG | 5 | 3454 | - | - | - | X |
| 84 | MG | 5 | 3465 | - | - | - | X |
| 84 | MG | 5 | 3466 | - | - | - | X |
| 84 | MG | 5 | 3478 | - | - | - | X |
| 84 | MG | 5 | 3483 | - | - | - | X |
| 84 | MG | 5 | 3485 | - | - | - | X |
| 84 | MG | 5 | 3503 | - | - | - | X |
| 84 | MG | 5 | 3530 | - | - | - | X |
| 84 | MG | 5 | 3531 | - | - | - | X |
| 84 | MG | 5 | 3535 | - | - | - | X |
| 84 | MG | 5 | 3546 | - | - | - | X |
| 84 | MG | 5 | 3551 | - | - | - | X |
| 84 | MG | 5 | 3560 | - | - | - | X |
| 84 | MG | 5 | 3561 | - | - | - | X |
| 84 | MG | 5 | 3569 | - | - | - | X |
| 84 | MG | 5 | 3577 | - | - | - | X |
| 84 | MG | 5 | 3585 | - | - | - | X |
| 84 | MG | 5 | 3587 | - | - | - | X |
| 84 | MG | 5 | 3589 | - | - | - | X |
| 84 | MG | 5 | 3592 | - | - | - | X |
| 84 | MG | 5 | 3602 | - | - | - | X |
| 84 | MG | 5 | 3610 | - | - | - | X |
| 84 | MG | 5 | 3611 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 84 | MG | 5 | 3613 | - | - | - | X |
| 84 | MG | 5 | 3618 | - | - | - | X |
| 84 | MG | 5 | 3634 | - | - | - | X |
| 84 | MG | 5 | 3639 | - | - | - | X |
| 84 | MG | 5 | 3643 | - | - | - | X |
| 84 | MG | 5 | 3663 | - | - | - | X |
| 84 | MG | 5 | 3667 | - | - | - | X |
| 84 | MG | 5 | 3668 | - | - | - | X |
| 84 | MG | 5 | 3673 | - | - | - | X |
| 84 | MG | 5 | 3690 | - | - | - | X |
| 84 | MG | 5 | 3693 | - | - | - | X |
| 84 | MG | 5 | 3694 | - | - | - | X |
| 84 | MG | 5 | 3700 | - | - | - | X |
| 84 | MG | 5 | 3737 | - | - | - | X |
| 84 | MG | 5 | 3738 | - | - | - | X |
| 84 | MG | 5 | 3740 | - | - | - | X |
| 84 | MG | 5 | 3743 | - | - | - | X |
| 84 | MG | 5 | 3745 | - | - | - | X |
| 84 | MG | 5 | 3764 | - | - | - | X |
| 84 | MG | 5 | 3768 | - | - | - | X |
| 84 | MG | 5 | 3811 | - | - | - | X |
| 84 | MG | 5 | 3817 | - | - | - | X |
| 84 | MG | 5 | 3832 | - | - | - | X |
| 84 | MG | 5 | 3835 | - | - | - | X |
| 84 | MG | 5 | 3845 | - | - | - | X |
| 84 | MG | 5 | 3848 | - | - | - | X |
| 84 | MG | 5 | 3852 | - | - | - | X |
| 84 | MG | 5 | 3868 | - | - | - | X |
| 84 | MG | 5 | 3871 | - | - | - | X |
| 84 | MG | 5 | 3881 | - | - | - | X |
| 84 | MG | 5 | 3895 | - | - | - | X |
| 84 | MG | 5 | 3904 | - | - | - | X |
| 84 | MG | 5 | 3905 | - | - | - | X |
| 84 | MG | 5 | 3939 | - | - | - | X |
| 84 | MG | 5 | 3949 | - | - | - | X |
| 84 | MG | 5 | 3954 | - | - | - | X |
| 84 | MG | 5 | 3955 | - | - | - | X |
| 84 | MG | 5 | 3956 | - | - | - | X |
| 84 | MG | 5 | 3957 | - | - | - | X |
| 84 | MG | 5 | 3959 | - | - | - | X |
| 84 | MG | 5 | 3964 | - | - | - | X |
| 84 | MG | 5 | 3968 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 84 | MG | 5 | 3981 | - | - | - | X |
| 84 | MG | 5 | 3986 | - | - | - | X |
| 84 | MG | 5 | 3987 | - | - | - | X |
| 84 | MG | 5 | 3993 | - | - | - | X |
| 84 | MG | 5 | 4009 | - | - | - | X |
| 84 | MG | 5 | 4012 | - | - | - | X |
| 84 | MG | 5 | 4029 | - | - | - | X |
| 84 | MG | 5 | 4042 | - | - | - | X |
| 84 | MG | 5 | 4045 | - | - | - | X |
| 84 | MG | 5 | 4047 | - | - | - | X |
| 84 | MG | 5 | 4048 | - | - | - | X |
| 84 | MG | 5 | 4052 | - | - | - | X |
| 84 | MG | 5 | 4055 | - | - | - | X |
| 84 | MG | 5 | 4059 | - | - | - | X |
| 84 | MG | 5 | 4064 | - | - | - | X |
| 84 | MG | 5 | 4098 | - | - | - | X |
| 84 | MG | 5 | 4123 | - | - | - | X |
| 84 | MG | 6 | 1904 | - | - | - | X |
| 84 | MG | 6 | 1906 | - | - | - | X |
| 84 | MG | 6 | 1917 | - | - | - | X |
| 84 | MG | 6 | 1921 | - | - | - | X |
| 84 | MG | 6 | 1925 | - | - | - | X |
| 84 | MG | 6 | 1928 | - | - | - | X |
| 84 | MG | 6 | 1929 | - | - | - | X |
| 84 | MG | 6 | 1935 | - | - | - | X |
| 84 | MG | 6 | 1943 | - | - | - | X |
| 84 | MG | 6 | 1948 | - | - | - | X |
| 84 | MG | 6 | 1950 | - | - | - | X |
| 84 | MG | 6 | 1999 | - | - | - | X |
| 84 | MG | 6 | 2022 | - | - | - | X |
| 84 | MG | 6 | 2026 | - | - | - | X |
| 84 | MG | 6 | 2029 | - | - | - | X |
| 84 | MG | 6 | 2034 | - | - | - | X |
| 84 | MG | 6 | 2038 | - | - | - | X |
| 84 | MG | 6 | 2043 | - | - | - | X |
| 84 | MG | 6 | 2057 | - | - | - | X |
| 84 | MG | 6 | 2077 | - | - | - | X |
| 84 | MG | 6 | 2079 | - | - | - | X |
| 84 | MG | 6 | 2080 | - | - | - | X |
| 84 | MG | 6 | 2084 | - | - | - | X |
| 84 | MG | 6 | 2095 | - | - | - | X |
| 84 | MG | 6 | 2096 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 84 | MG | 6 | 2098 | - | - | - | X |
| 84 | MG | 6 | 2099 | - | - | - | X |
| 84 | MG | 6 | 2127 | - | - | - | X |
| 84 | MG | 6 | 2158 | - | - | - | X |
| 84 | MG | 8 | 207 | - | - | - | X |
| 84 | MG | 8 | 214 | - | - | - | X |
| 84 | MG | D3 | 203 | - | - | - | X |
| 84 | MG | L2 | 305 | - | - | - | X |
| 84 | MG | M5 | 305 | - | - | - | X |
| 84 | MG | N3 | 202 | - | - | - | X |
| 84 | MG | N3 | 204 | - | - | - | X |
| 84 | MG | O3 | 201 | - | - | - | X |
| 84 | MG | Q2 | 505 | - | - | - | X |
| 84 | MG | l3 | 401 | - | - | - | X |
| 84 | MG | l3 | 405 | - | - | - | X |
| 84 | MG | l3 | 408 | - | - | - | X |
| 84 | MG | m4 | 204 | - | - | - | X |
| 84 | MG | m5 | 301 | - | - | - | X |
| 84 | MG | m6 | 204 | - | - | - | X |
| 84 | MG | m8 | 202 | - | - | - | X |
| 84 | MG | n3 | 201 | - | - | - | X |
| 84 | MG | n8 | 201 | - | - | - | X |
| 84 | MG | o2 | 201 | - | - | - | X |
| 84 | MG | o4 | 502 | - | - | - | X |
| 85 | LLL | 1 | 3994 | - | - | - | X |
| 85 | LLL | 1 | 3995 | - | - | - | X |
| 85 | LLL | 1 | 3997 | - | - | - | X |
| 85 | LLL | 1 | 3998 | - | - | - | X |
| 85 | LLL | 1 | 4000 | - | - | - | X |
| 85 | LLL | 2 | 2044 | - | - | - | X |
| 85 | LLL | 2 | 2045 | - | - | - | X |
| 85 | LLL | 3 | 220 | - | - | - | X |
| 85 | LLL | 5 | 4151 | - | - | - | X |
| 85 | LLL | 5 | 4152 | - | - | - | X |
| 85 | LLL | 5 | 4153 | - | - | - | X |
| 85 | LLL | 5 | 4156 | - | - | - | X |
| 85 | LLL | 5 | 4161 | - | - | - | X |
| 85 | LLL | 5 | 4166 | - | - | - | X |
| 85 | LLL | 5 | 4169 | - | - | - | X |
| 85 | LLL | 5 | 4173 | - | - | - | X |
| 85 | LLL | 5 | 4174 | - | - | - | X |
| 85 | LLL | 5 | 4175 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 85 | LLL | 5 | 4176 | - | - | - | X |
| 85 | LLL | 5 | 4177 | - | - | - | X |
| 85 | LLL | 5 | 4178 | - | - | - | X |
| 85 | LLL | 6 | 2167 | - | - | - | X |
| 85 | LLL | 6 | 2172 | - | - | - | X |
| 85 | LLL | 6 | 2173 | - | - | - | X |
| 85 | LLL | 6 | 2174 | - | - | - | X |
| 85 | LLL | 6 | 2175 | - | - | - | X |
| 85 | LLL | 7 | 232 | - | - | - | X |

2 Entry composition [i](#)

There are 87 unique types of molecules in this entry. The entry contains 404238 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 | 3100 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 66304 | 29617 | 11950 | 21637 | 3100 | | | |
| 1 | 5 | 3134 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 67039 | 29943 | 12089 | 21873 | 3134 | | | |

- 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 | 7 | 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 | 156 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 3313 | 1482 | 582 | 1093 | 156 | | | |
| 3 | 8 | 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 | L2 | 252 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1914 | 1191 | 388 | 334 | 1 | | | |
| 4 | 12 | 252 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1912 | 1190 | 388 | 333 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5 | L3 | 386 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3081 | 1956 | 584 | 533 | 8 | | | |
| 5 | l3 | 386 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3081 | 1956 | 584 | 533 | 8 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 6 | L4 | 361 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2749 | 1730 | 522 | 494 | 3 | | | |
| 6 | l4 | 361 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2749 | 1730 | 522 | 494 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 7 | L5 | 296 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2375 | 1501 | 414 | 458 | 2 | | | |
| 7 | l5 | 294 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2359 | 1489 | 412 | 456 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | L6 | 156 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1239 | 800 | 222 | 216 | 1 | | | |
| 8 | l6 | 157 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1248 | 806 | 224 | 217 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 9 | L7 | 222 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1784 | 1151 | 324 | 308 | 1 | | | |
| 9 | l7 | 223 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1791 | 1155 | 325 | 310 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 10 | L8 | 233 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1817 | 1159 | 326 | 329 | 3 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 10 | l8 | 231 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1763 | 1130 | 316 | 314 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | L9 | 191 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1518 | 963 | 274 | 277 | 4 | | | |
| 11 | l9 | 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 | M0 | 212 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1707 | 1084 | 323 | 295 | 5 | | | |
| 12 | m0 | 211 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1716 | 1090 | 324 | 296 | 6 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | M1 | 169 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1353 | 847 | 253 | 249 | 4 | | | |
| 13 | m1 | 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 | M3 | 193 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1543 | 962 | 315 | 266 | | | |
| 14 | m3 | 194 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1548 | 965 | 316 | 267 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 15 | M4 | 136 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1053 | 675 | 199 | 177 | | | |
| 15 | m4 | 137 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1059 | 678 | 200 | 179 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 16 | M5 | 203 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1720 | 1077 | 361 | 281 | 1 | | | |
| 16 | m5 | 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 | M6 | 197 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1555 | 1003 | 289 | 262 | 1 | | | |
| 17 | m6 | 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 | M7 | 183 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1415 | 877 | 281 | 257 | | | | |
| 18 | m7 | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1227 | 764 | 238 | 225 | | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | M8 | 185 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1441 | 908 | 290 | 241 | 2 | | | |
| 19 | m8 | 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 | M9 | 182 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1474 | 905 | 319 | 250 | | | | |
| 20 | m9 | 188 | Total | C | N | O | S | 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 | N0 | 172 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1445 | 930 | 267 | 244 | 4 | | | |
| 21 | n0 | 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 | N1 | 159 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1276 | 805 | 246 | 221 | 4 | | | |
| 22 | n1 | 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 | N2 | 100 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 796 | 516 | 131 | 149 | | | | |
| 23 | n2 | 98 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 778 | 505 | 127 | 146 | | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24 | N3 | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1003 | 628 | 189 | 179 | 7 | | | |
| 24 | n3 | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1003 | 628 | 189 | 179 | 7 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 25 | N4 | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 699 | 443 | 137 | 118 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26 | N5 | 121 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 964 | 620 | 169 | 173 | 2 | | | |
| 26 | n5 | 120 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 959 | 617 | 168 | 172 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 27 | N6 | 126 | Total | C | N | O | 0 | 0 | 0 |
| | | | 993 | 625 | 192 | 176 | | | |
| 27 | n6 | 126 | Total | C | N | O | 0 | 0 | 0 |
| | | | 993 | 625 | 192 | 176 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 28 | N7 | 135 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1092 | 710 | 202 | 180 | | | |
| 28 | n7 | 135 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1092 | 710 | 202 | 180 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 29 | N8 | 148 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1173 | 749 | 231 | 190 | 3 | | | |
| 29 | n8 | 148 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1173 | 749 | 231 | 190 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 30 | N9 | 58 | Total | C | N | O | 0 | 0 | 0 |
| | | | 462 | 289 | 100 | 73 | | | |
| 30 | n9 | 58 | Total | C | N | O | 0 | 0 | 0 |
| | | | 462 | 289 | 100 | 73 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31 | O0 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 743 | 479 | 124 | 139 | 1 | | | |
| 31 | o0 | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 767 | 492 | 128 | 146 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32 | O1 | 109 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 890 | 565 | 168 | 156 | 1 | | | |
| 32 | o1 | 109 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 890 | 565 | 168 | 156 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33 | O2 | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1020 | 647 | 205 | 167 | 1 | | | |
| 33 | o2 | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1020 | 647 | 205 | 167 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34 | O3 | 106 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 850 | 540 | 165 | 144 | 1 | | | |
| 34 | o3 | 106 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 850 | 540 | 165 | 144 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35 | O4 | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 881 | 546 | 179 | 152 | 4 | | | |
| 35 | o4 | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 881 | 546 | 179 | 152 | 4 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36 | O5 | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 969 | 615 | 186 | 167 | 1 | | | |
| 36 | o5 | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 969 | 615 | 186 | 167 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37 | O6 | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 771 | 481 | 156 | 132 | 2 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37 | o6 | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 771 | 481 | 156 | 132 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38 | O7 | 87 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 681 | 414 | 148 | 114 | 5 | | | |
| 38 | o7 | 87 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 681 | 414 | 148 | 114 | 5 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39 | O8 | 77 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 612 | 391 | 115 | 106 | | | | |
| 39 | o8 | 77 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 612 | 391 | 115 | 106 | | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 40 | O9 | 50 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 436 | 272 | 97 | 65 | 2 | | | |
| 40 | o9 | 50 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 436 | 272 | 97 | 65 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 41 | Q0 | 52 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 417 | 259 | 86 | 67 | 5 | | | |
| 41 | q0 | 52 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 417 | 259 | 86 | 67 | 5 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 42 | Q1 | 25 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 233 | 142 | 63 | 27 | 1 | | | |
| 42 | q1 | 25 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 233 | 142 | 63 | 27 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43 | Q2 | 105 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 847 | 534 | 170 | 138 | 5 | | | |
| 43 | q2 | 105 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 847 | 534 | 170 | 138 | 5 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44 | Q3 | 91 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 694 | 429 | 138 | 121 | 6 | | | |
| 44 | q3 | 91 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 694 | 429 | 138 | 121 | 6 | | | |

- Molecule 45 is a RNA chain called 18S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 45 | 2 | 1712 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 36488 | 16313 | 6466 | 11997 | 1712 | | | |
| 45 | 6 | 1739 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 37060 | 16570 | 6568 | 12183 | 1739 | | | |

- Molecule 46 is a protein called 40S ribosomal protein S0-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 46 | S0 | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1612 | 1034 | 285 | 291 | 2 | | | |
| 46 | s0 | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1612 | 1034 | 285 | 291 | 2 | | | |

- Molecule 47 is a protein called 40S ribosomal protein S1-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 47 | S1 | 214 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1709 | 1084 | 310 | 311 | 4 | | | |
| 47 | s1 | 216 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1722 | 1091 | 312 | 315 | 4 | | | |

- Molecule 48 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 48 | S2 | 217 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1635 | 1047 | 289 | 297 | 2 | | | |
| 48 | s2 | 217 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1635 | 1047 | 289 | 297 | 2 | | | |

- Molecule 49 is a protein called 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 49 | S3 | 223 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1734 | 1101 | 313 | 314 | 6 | | | |
| 49 | s3 | 223 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1728 | 1098 | 310 | 314 | 6 | | | |

- Molecule 50 is a protein called 40S ribosomal protein S4-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 50 | S4 | 260 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2068 | 1316 | 389 | 360 | 3 | | | |
| 50 | s4 | 260 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2068 | 1316 | 389 | 360 | 3 | | | |

- Molecule 51 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 51 | S5 | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1609 | 1007 | 300 | 299 | 3 | | | |
| 51 | s5 | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1609 | 1007 | 300 | 299 | 3 | | | |

- Molecule 52 is a protein called 40S ribosomal protein S6-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 52 | S6 | 226 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1813 | 1137 | 350 | 323 | 3 | | | |
| 52 | s6 | 218 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1755 | 1102 | 337 | 313 | 3 | | | |

- Molecule 53 is a protein called 40S ribosomal protein S7-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 53 | S7 | 184 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1481 | 951 | 265 | 265 | | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 53 | s7 | 186 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1491 | 957 | 267 | 267 | | | |

- Molecule 54 is a protein called 40S ribosomal protein S8-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 54 | S8 | 188 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1489 | 925 | 298 | 264 | 2 | | | |
| 54 | s8 | 186 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1471 | 913 | 294 | 262 | 2 | | | |

- Molecule 55 is a protein called 40S ribosomal protein S9-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 55 | S9 | 185 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1494 | 943 | 289 | 261 | 1 | | | |
| 55 | s9 | 185 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1494 | 943 | 289 | 261 | 1 | | | |

- Molecule 56 is a protein called 40S ribosomal protein S10-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 56 | C0 | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 772 | 499 | 126 | 145 | 2 | | | |
| 56 | c0 | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 761 | 490 | 125 | 144 | 2 | | | |

- Molecule 57 is a protein called 40S ribosomal protein S11-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 57 | C1 | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1213 | 774 | 230 | 206 | 3 | | | |
| 57 | c1 | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1138 | 729 | 217 | 189 | 3 | | | |

- Molecule 58 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 58 | C2 | 124 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 890 | 560 | 156 | 172 | 2 | | | |
| 58 | c2 | 124 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 890 | 560 | 156 | 172 | 2 | | | |

- Molecule 59 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 59 | C3 | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1192 | 759 | 224 | 207 | 2 | | | |
| 59 | c3 | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1192 | 759 | 224 | 207 | 2 | | | |

- Molecule 60 is a protein called 40S ribosomal protein S14-B.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 60 | C4 | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 891 | 545 | 182 | 163 | 1 | | | |
| 60 | c4 | 128 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 949 | 582 | 188 | 176 | 3 | | | |

- Molecule 61 is a protein called 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 61 | C5 | 124 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 977 | 622 | 182 | 166 | 7 | | | |
| 61 | c5 | 135 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1039 | 658 | 196 | 178 | 7 | | | |

- Molecule 62 is a protein called 40S ribosomal protein S16-A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 62 | C6 | 141 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1105 | 708 | 203 | 194 | | | |
| 62 | c6 | 142 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1111 | 711 | 204 | 196 | | | |

- Molecule 63 is a protein called 40S ribosomal protein S17-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 63 | C7 | 120 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 965 | 603 | 183 | 177 | 2 | | | |
| 63 | c7 | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 917 | 569 | 175 | 171 | 2 | | | |

- Molecule 64 is a protein called 40S ribosomal protein S18-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 64 | C8 | 145 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1192 | 743 | 237 | 210 | 2 | | | |
| 64 | c8 | 145 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1192 | 743 | 237 | 210 | 2 | | | |

- Molecule 65 is a protein called 40S ribosomal protein S19-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 65 | C9 | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1112 | 694 | 208 | 208 | 2 | | | |
| 65 | c9 | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1112 | 694 | 208 | 208 | 2 | | | |

- Molecule 66 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 66 | D0 | 107 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 855 | 539 | 156 | 159 | 1 | | | |
| 66 | d0 | 110 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 882 | 554 | 161 | 166 | 1 | | | |

- Molecule 67 is a protein called 40S ribosomal protein S21-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 67 | D1 | 87 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 684 | 420 | 125 | 137 | 2 | | | |
| 67 | d1 | 87 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 684 | 420 | 125 | 137 | 2 | | | |

- Molecule 68 is a protein called 40S ribosomal protein S22-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 68 | D2 | 129 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1021 | 650 | 188 | 180 | 3 | | | |
| 68 | d2 | 129 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1021 | 650 | 188 | 180 | 3 | | | |

- Molecule 69 is a protein called 40S ribosomal protein S23-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 69 | D3 | 144 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1121 | 708 | 220 | 191 | 2 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 69 | d3 | 144 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1121 | 708 | 220 | 191 | 2 | | | |

- Molecule 70 is a protein called 40S ribosomal protein S24-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 70 | D4 | 134 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 1073 | 676 | 208 | 189 | | | | |
| 70 | d4 | 133 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 1065 | 672 | 207 | 186 | | | | |

- Molecule 71 is a protein called 40S ribosomal protein S25-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|--|---------|---------|-------|
| 71 | D5 | 70 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 563 | 360 | 104 | 99 | | | | |
| 71 | d5 | 69 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 558 | 357 | 103 | 98 | | | | |

- Molecule 72 is a protein called 40S ribosomal protein S26-B.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 72 | D6 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 769 | 475 | 160 | 129 | 5 | | | |
| 72 | d6 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 769 | 475 | 160 | 129 | 5 | | | |

- Molecule 73 is a protein called 40S ribosomal protein S27-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 73 | D7 | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 610 | 382 | 110 | 113 | 5 | | | |
| 73 | d7 | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 610 | 382 | 110 | 113 | 5 | | | |

- Molecule 74 is a protein called 40S ribosomal protein S28-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 74 | D8 | 63 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 497 | 306 | 99 | 91 | 1 | | | |
| 74 | d8 | 63 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 497 | 306 | 99 | 91 | 1 | | | |

- Molecule 75 is a protein called 40S ribosomal protein S29-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 75 | D9 | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 443 | 275 | 92 | 72 | 4 | | | |
| 75 | d9 | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 443 | 275 | 92 | 72 | 4 | | | |

- Molecule 76 is a protein called 40S ribosomal protein S30-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 76 | E0 | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 475 | 299 | 98 | 77 | 1 | | | |
| 76 | e0 | 62 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 491 | 309 | 101 | 80 | 1 | | | |

- Molecule 77 is a protein called Ubiquitin-40S ribosomal protein S31.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 77 | E1 | 71 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 566 | 362 | 106 | 94 | 4 | | | |
| 77 | e1 | 72 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 575 | 368 | 108 | 95 | 4 | | | |

- Molecule 78 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 78 | SR | 318 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2441 | 1543 | 418 | 472 | 8 | | | |
| 78 | sR | 318 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2441 | 1543 | 418 | 472 | 8 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| SR | 161 | ALA | LYS | conflict | UNP P38011 |
| sR | 161 | ALA | LYS | conflict | UNP P38011 |

- Molecule 79 is a protein called Suppressor protein STM1.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 79 | SM | 159 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1104 | 652 | 221 | 231 | | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 79 | sM | 129 | Total | C | N | O | 0 | 0 | 0 |
| | | | 923 | 546 | 184 | 193 | | | |

- Molecule 80 is a protein called 60S ribosomal protein L12.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 80 | m2 | 150 | Total | C | N | O | 0 | 0 | 0 |
| | | | 750 | 450 | 150 | 150 | | | |

- Molecule 81 is a protein called 60S ribosomal protein L24-A.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 81 | n4 | 135 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1044 | 654 | 209 | 180 | 1 | | | |

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

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

- Molecule 83 is a protein called Ribosomal protein P1 alpha.

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

- Molecule 84 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 84 | s0 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 84 | n8 | 3 | Total | Mg | 0 | 0 |
| | | | 3 | 3 | | |
| 84 | N0 | 4 | Total | Mg | 0 | 0 |
| | | | 4 | 4 | | |
| 84 | S3 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 84 | N5 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 84 | d2 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 84 | s3 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 84 | n5 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 84 | q0 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 84 | c1 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 84 | o1 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 84 | L5 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 84 | O2 | 4 | Total 4 | Mg 4 | 0 | 0 |
| 84 | m9 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 84 | M3 | 5 | Total 5 | Mg 5 | 0 | 0 |
| 84 | S4 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 84 | l5 | 6 | Total 6 | Mg 6 | 0 | 0 |
| 84 | o2 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 84 | d5 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 84 | d9 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 84 | m3 | 4 | Total 4 | Mg 4 | 0 | 0 |
| 84 | 2 | 142 | Total 142 | Mg 142 | 0 | 0 |
| 84 | M6 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 84 | l6 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 84 | m6 | 8 | Total 8 | Mg 8 | 0 | 0 |
| 84 | n9 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 84 | M5 | 5 | Total 5 | Mg 5 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 84 | S2 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 84 | m5 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 84 | s4 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 84 | s2 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 84 | M8 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 84 | q3 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 84 | N3 | 4 | Total 4 | Mg 4 | 0 | 0 |
| 84 | 4 | 23 | Total 23 | Mg 23 | 0 | 0 |
| 84 | L2 | 5 | Total 5 | Mg 5 | 0 | 0 |
| 84 | m8 | 4 | Total 4 | Mg 4 | 0 | 0 |
| 84 | n3 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 84 | l2 | 5 | Total 5 | Mg 5 | 0 | 0 |
| 84 | c3 | 6 | Total 6 | Mg 6 | 0 | 0 |
| 84 | L7 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 84 | D3 | 5 | Total 5 | Mg 5 | 0 | 0 |
| 84 | 6 | 263 | Total 263 | Mg 263 | 0 | 0 |
| 84 | d7 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 84 | O4 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 84 | C1 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 84 | n0 | 7 | Total 7 | Mg 7 | 0 | 0 |
| 84 | l7 | 3 | Total 3 | Mg 3 | 0 | 0 |

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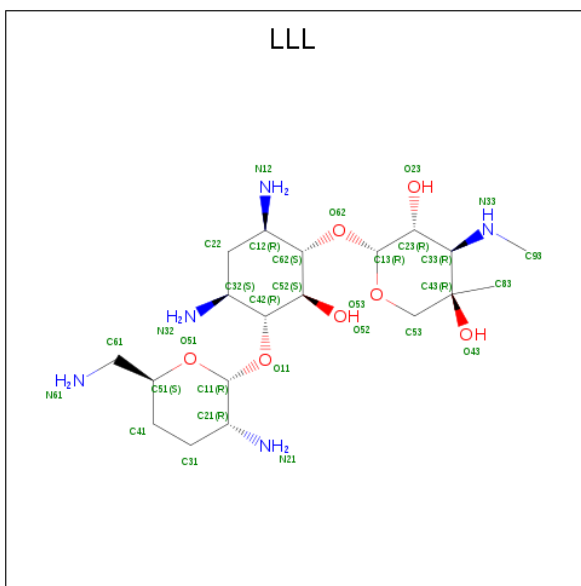
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 84 | L8 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 84 | o4 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 84 | O7 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 84 | s6 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 84 | 1 | 588 | Total 588 | Mg 588 | 0 | 0 |
| 84 | S1 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 84 | c4 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 84 | l8 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 84 | Q2 | 4 | Total 4 | Mg 4 | 0 | 0 |
| 84 | m4 | 6 | Total 6 | Mg 6 | 0 | 0 |
| 84 | d6 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 84 | q2 | 7 | Total 7 | Mg 7 | 0 | 0 |
| 84 | N4 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 84 | Q1 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 84 | L3 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 84 | 8 | 20 | Total 20 | Mg 20 | 0 | 0 |
| 84 | 3 | 19 | Total 19 | Mg 19 | 0 | 0 |
| 84 | d1 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 84 | q1 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 84 | l3 | 11 | Total 11 | Mg 11 | 0 | 0 |
| 84 | N1 | 2 | Total 2 | Mg 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 84 | C8 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 84 | O3 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 84 | L4 | 6 | Total 6 | Mg 6 | 0 | 0 |
| 84 | M0 | 4 | Total 4 | Mg 4 | 0 | 0 |
| 84 | 5 | 750 | Total 750 | Mg 750 | 0 | 0 |
| 84 | n1 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 84 | c8 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 84 | l4 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 84 | L9 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 84 | d3 | 5 | Total 5 | Mg 5 | 0 | 0 |
| 84 | o3 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 84 | m0 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 84 | O6 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 84 | s5 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 84 | C3 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 84 | M7 | 5 | Total 5 | Mg 5 | 0 | 0 |
| 84 | N8 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 84 | l9 | 8 | Total 8 | Mg 8 | 0 | 0 |
| 84 | sR | 1 | Total 1 | Mg 1 | 0 | 0 |
| 84 | 7 | 30 | Total 30 | Mg 30 | 0 | 0 |
| 84 | m7 | 7 | Total 7 | Mg 7 | 0 | 0 |

- Molecule 85 is (2R,3R,4R,5R)-2-((1S,2S,3R,4S,6R)-4,6-DIAMINO-3-((2R,3R,6S)-3-AMINO-6-(AMINOMETHYL)-TETRAHYDRO-2H-PYRAN-2-YLOXY)-2-HYDROXYCYCLOHEXYLOXY)-5-METHYL-4-(METHYLAMINO)-TETRAHYDRO-2H-PYRAN-3,5-DIOL (three-letter code: LLL) (formula: C₁₉H₃₉N₅O₇).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 85 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 85 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 1 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 3 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 4 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | L3 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 2 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 2 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 2 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 85 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 5 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 7 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 7 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 7 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 85 | 8 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 8 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | l3 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 6 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 6 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 6 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 6 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 6 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 6 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 6 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 6 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 6 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 6 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 85 | 6 | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |

- Molecule 86 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 86 | o4 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 86 | O7 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 86 | q3 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 86 | q0 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 86 | Q2 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 86 | e1 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 86 | Q3 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 86 | D9 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 86 | E1 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 86 | Q0 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 86 | d7 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 86 | O4 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 86 | d9 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 86 | D7 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 86 | d6 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 86 | o7 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 86 | D6 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 86 | q2 | 1 | Total 1 | Zn 1 | 0 | 0 |

- Molecule 87 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 87 | 1 | 473 | Total 473 | O 473 | 0 | 0 |
| 87 | 3 | 15 | Total 15 | O 15 | 0 | 0 |
| 87 | 4 | 5 | Total 5 | O 5 | 0 | 0 |
| 87 | L2 | 1 | Total 1 | O 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 87 | L3 | 7 | Total 7 | O 7 | 0 | 0 |
| 87 | L4 | 2 | Total 2 | O 2 | 0 | 0 |
| 87 | L5 | 2 | Total 2 | O 2 | 0 | 0 |
| 87 | M0 | 1 | Total 1 | O 1 | 0 | 0 |
| 87 | M3 | 2 | Total 2 | O 2 | 0 | 0 |
| 87 | M5 | 3 | Total 3 | O 3 | 0 | 0 |
| 87 | M6 | 6 | Total 6 | O 6 | 0 | 0 |
| 87 | M7 | 5 | Total 5 | O 5 | 0 | 0 |
| 87 | N0 | 4 | Total 4 | O 4 | 0 | 0 |
| 87 | N1 | 3 | Total 3 | O 3 | 0 | 0 |
| 87 | N3 | 5 | Total 5 | O 5 | 0 | 0 |
| 87 | N4 | 2 | Total 2 | O 2 | 0 | 0 |
| 87 | N5 | 2 | Total 2 | O 2 | 0 | 0 |
| 87 | N8 | 3 | Total 3 | O 3 | 0 | 0 |
| 87 | N9 | 2 | Total 2 | O 2 | 0 | 0 |
| 87 | O2 | 2 | Total 2 | O 2 | 0 | 0 |
| 87 | O4 | 1 | Total 1 | O 1 | 0 | 0 |
| 87 | O7 | 1 | Total 1 | O 1 | 0 | 0 |
| 87 | Q1 | 1 | Total 1 | O 1 | 0 | 0 |
| 87 | Q2 | 1 | Total 1 | O 1 | 0 | 0 |
| 87 | 2 | 111 | Total 111 | O 111 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 87 | S1 | 1 | Total 1 | O 1 | 0 | 0 |
| 87 | S3 | 3 | Total 3 | O 3 | 0 | 0 |
| 87 | S4 | 1 | Total 1 | O 1 | 0 | 0 |
| 87 | S8 | 1 | Total 1 | O 1 | 0 | 0 |
| 87 | C9 | 2 | Total 2 | O 2 | 0 | 0 |
| 87 | D0 | 1 | Total 1 | O 1 | 0 | 0 |
| 87 | D3 | 1 | Total 1 | O 1 | 0 | 0 |
| 87 | SR | 2 | Total 2 | O 2 | 0 | 0 |
| 87 | 5 | 514 | Total 514 | O 514 | 0 | 0 |
| 87 | 7 | 33 | Total 33 | O 33 | 0 | 0 |
| 87 | 8 | 11 | Total 11 | O 11 | 0 | 0 |
| 87 | 12 | 7 | Total 7 | O 7 | 0 | 0 |
| 87 | 13 | 6 | Total 6 | O 6 | 0 | 0 |
| 87 | 15 | 5 | Total 5 | O 5 | 0 | 0 |
| 87 | 19 | 3 | Total 3 | O 3 | 0 | 0 |
| 87 | m0 | 1 | Total 1 | O 1 | 0 | 0 |
| 87 | m4 | 1 | Total 1 | O 1 | 0 | 0 |
| 87 | m5 | 2 | Total 2 | O 2 | 0 | 0 |
| 87 | m6 | 8 | Total 8 | O 8 | 0 | 0 |
| 87 | m7 | 4 | Total 4 | O 4 | 0 | 0 |
| 87 | m9 | 3 | Total 3 | O 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 87 | n0 | 4 | Total 4 | O 4 | 0 | 0 |
| 87 | n1 | 2 | Total 2 | O 2 | 0 | 0 |
| 87 | n3 | 2 | Total 2 | O 2 | 0 | 0 |
| 87 | n4 | 1 | Total 1 | O 1 | 0 | 0 |
| 87 | n5 | 2 | Total 2 | O 2 | 0 | 0 |
| 87 | n6 | 1 | Total 1 | O 1 | 0 | 0 |
| 87 | n8 | 4 | Total 4 | O 4 | 0 | 0 |
| 87 | n9 | 1 | Total 1 | O 1 | 0 | 0 |
| 87 | o0 | 1 | Total 1 | O 1 | 0 | 0 |
| 87 | o1 | 2 | Total 2 | O 2 | 0 | 0 |
| 87 | o2 | 4 | Total 4 | O 4 | 0 | 0 |
| 87 | o4 | 2 | Total 2 | O 2 | 0 | 0 |
| 87 | q0 | 1 | Total 1 | O 1 | 0 | 0 |
| 87 | q2 | 2 | Total 2 | O 2 | 0 | 0 |
| 87 | q3 | 3 | Total 3 | O 3 | 0 | 0 |
| 87 | 6 | 224 | Total 224 | O 224 | 0 | 0 |
| 87 | s4 | 1 | Total 1 | O 1 | 0 | 0 |
| 87 | s5 | 1 | Total 1 | O 1 | 0 | 0 |
| 87 | s7 | 1 | Total 1 | O 1 | 0 | 0 |
| 87 | c3 | 5 | Total 5 | O 5 | 0 | 0 |
| 87 | c6 | 1 | Total 1 | O 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 87 | c8 | 3 | Total 3 | O 3 | 0 | 0 |
| 87 | c9 | 5 | Total 5 | O 5 | 0 | 0 |
| 87 | d3 | 5 | Total 5 | O 5 | 0 | 0 |
| 87 | d5 | 3 | Total 3 | O 3 | 0 | 0 |
| 87 | d6 | 3 | Total 3 | O 3 | 0 | 0 |
| 87 | d9 | 2 | Total 2 | O 2 | 0 | 0 |
| 87 | e1 | 1 | Total 1 | O 1 | 0 | 0 |
| 87 | sR | 1 | Total 1 | O 1 | 0 | 0 |

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 ($\text{RSRZ} > 2$). 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.

Chain 1: ■ 37% ■ 38% ■ 13% ■ 9%

The visualization displays a chain of 1000 nodes, labeled G809 through G875. The nodes are arranged in a grid-like pattern, with each node having a unique color. The colors are categorized into four groups: red (37%), orange (38%), yellow (13%), and grey (9%). The nodes are connected by lines, forming a complex network structure. The connections between nodes are represented by thin lines, some of which are thicker, indicating stronger or more frequent connections. The overall layout is a dense, interconnected web of nodes and edges, with the nodes themselves being small squares with text labels.

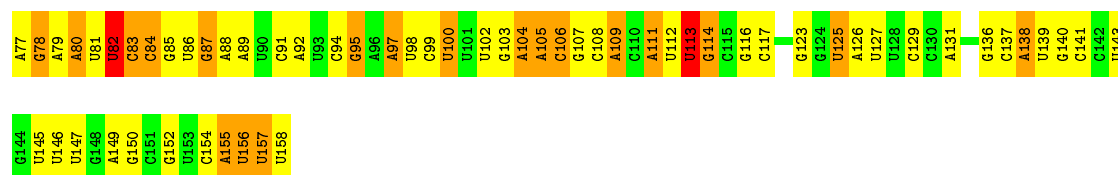
WORLDWIDE
PDB
PROTEIN DATA BANK

| | | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|---|-------|-------|-------|-------|---|
| U3131 | U3042 | U2962 | U2875 | U2804 | A2727 | C2658 | G2585 | U2521 | A | C2378 | U2298 | C2227 | U2154 | U |
| C3132 | C3043 | C2963 | C2876 | G2805 | G2728 | G2659 | G2586 | U2521 | G | U2379 | A2299 | A2228 | G2155 | C |
| G3133 | G3044 | C2964 | U2729 | G2806 | U2729 | G2660 | U2587 | G2522 | A | G2385 | G2300 | A2229 | C2156 | G |
| A3134 | G3045 | U2965 | U2880 | A2808 | G2730 | G2661 | U2881 | A2523 | A | A2386 | A2303 | C2230 | G2157 | C |
| U3135 | A3046 | C2966 | C2881 | C2809 | A2733 | G2662 | G2592 | G2524 | U | U2387 | A2304 | C2231 | A2158 | U |
| G3136 | U3047 | U2967 | U2882 | C2810 | A2734 | G2663 | A2593 | G2525 | A | U2388 | C2304 | A2232 | U2159 | U |
| C3137 | A3048 | C2968 | U2883 | A2811 | U2734 | C2664 | C2594 | C2526 | A | U2389 | G2305 | A2233 | C | |
| U3138 | U3049 | A2969 | C2884 | C2812 | U2735 | U2665 | C2594 | G2527 | G | A2390 | G2306 | G2234 | G | |
| G3053 | G3054 | C2970 | C2885 | A2813 | U2736 | C2666 | G2602 | G2528 | U | G2391 | G2307 | C2235 | C | |
| U3054 | U3055 | A2971 | U2886 | G2814 | G2737 | U2667 | G2602 | A2529 | G | G2392 | C2308 | C2235 | U | |
| A3142 | U3056 | A2972 | A2887 | G2815 | A2738 | U2668 | G2605 | U2532 | G | G2393 | A2309 | U2241 | A | |
| C3143 | G2973 | G2973 | G2816 | G2817 | C2741 | G2672 | G2606 | U2533 | G | G2394 | U2310 | U2242 | C | |
| G3147 | U3058 | U2978 | C2817 | U2818 | U2744 | A2673 | G2607 | G2533 | A | G2395 | U2311 | A2243 | C | |
| U3151 | G3059 | U2979 | A2819 | A2820 | G2744 | A2674 | G2608 | A2535 | G | G2396 | U2170 | A2244 | A | |
| U3152 | A2980 | U2980 | A2821 | C2821 | G2745 | C2675 | G2609 | A2536 | C | A2397 | A2312 | C2245 | U | |
| U3153 | C3063 | C2983 | U2888 | G2824 | A2747 | G2676 | U2612 | U2537 | U | G2400 | U2314 | U2246 | U | |
| C3154 | U3064 | C2984 | C2889 | G2825 | A2748 | U2677 | U2613 | U2538 | C | G2401 | G2315 | G2174 | A | |
| U3155 | C3076 | C2985 | U2890 | U2826 | G2749 | U2678 | G2614 | A2540 | G | A2402 | U2316 | U2175 | C2093 | |
| U3156 | A3077 | U2986 | U2891 | G2827 | U2752 | U2679 | G2615 | U2541 | C | G2403 | U2317 | G2176 | C2094 | |
| U3157 | U3078 | A2987 | U2892 | U2828 | U2753 | U2680 | C2616 | U2542 | C | A2404 | U2318 | A2178 | G2095 | |
| G3158 | U3079 | C2988 | U2893 | G2829 | G2753 | U2683 | U2617 | U2543 | G | C2405 | U2320 | G2179 | A2100 | |
| C3159 | G3080 | U2989 | G2912 | U2829 | U2754 | U2684 | G2618 | U2544 | C | C2406 | U2321 | G2180 | U2101 | |
| G3160 | C3081 | G2990 | C2913 | U2830 | C2756 | C2684 | G2619 | U2545 | C | C2407 | U2322 | U2181 | U2102 | |
| C3161 | C3082 | A2991 | G2914 | G2831 | U2757 | U2685 | G2620 | C2546 | A | U2408 | U2323 | G2182 | A2107 | |
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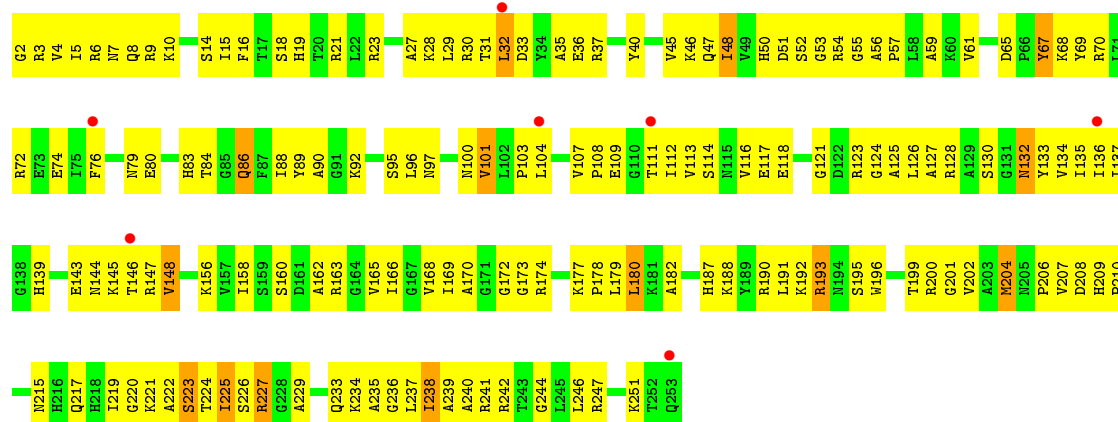




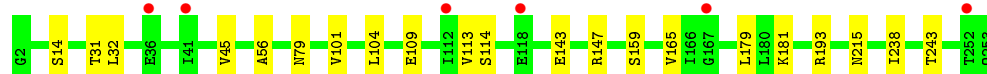
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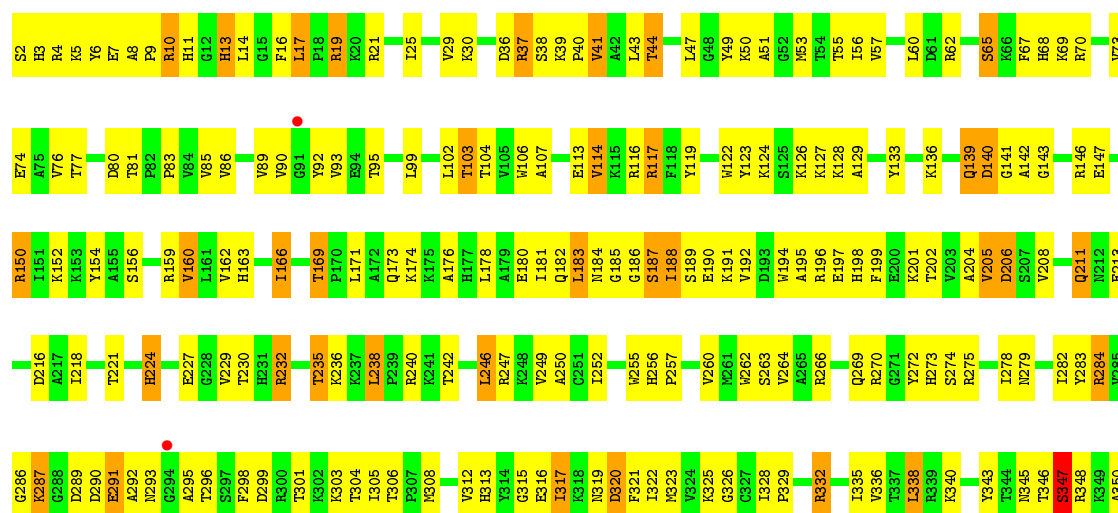
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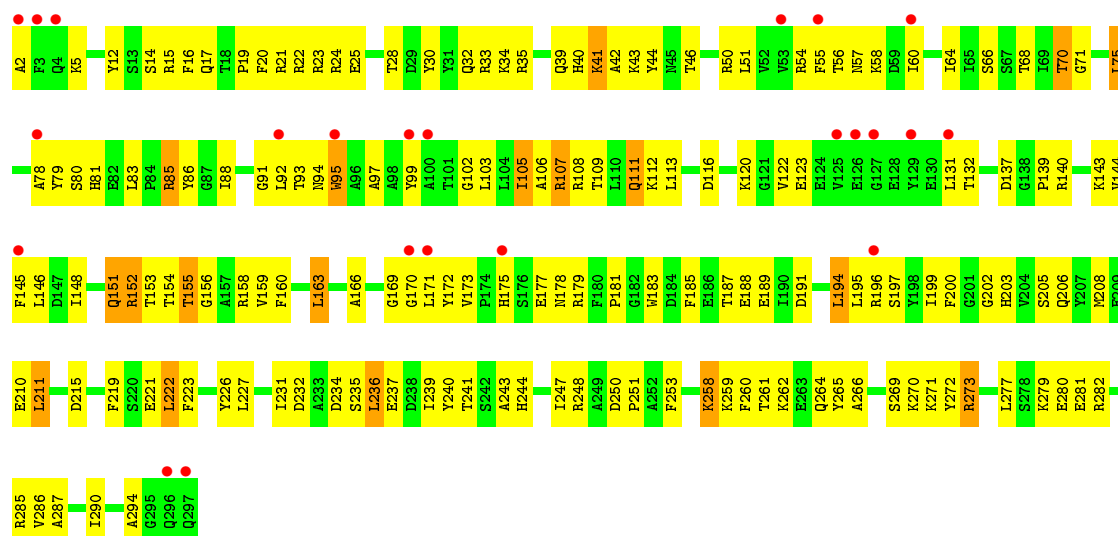


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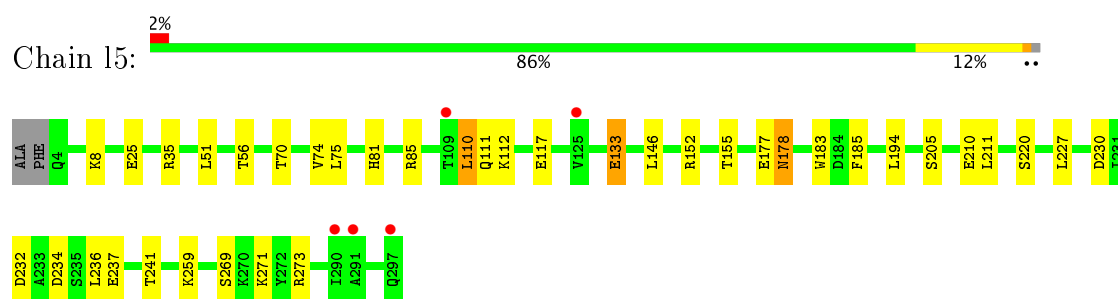


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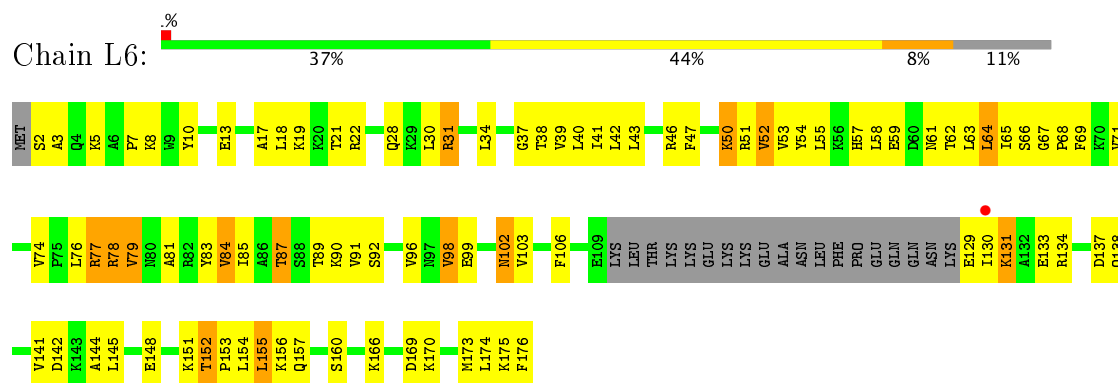




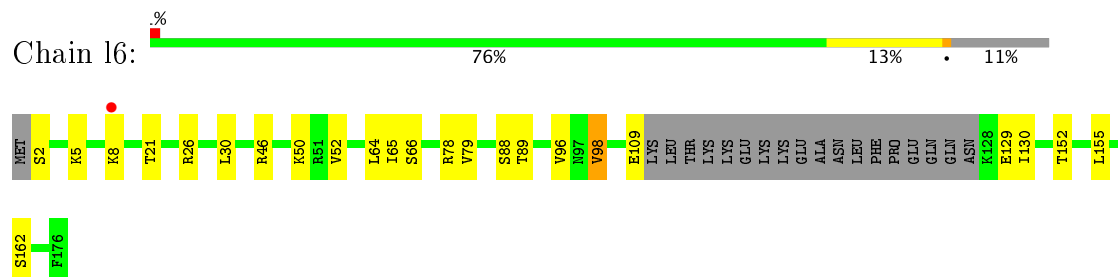
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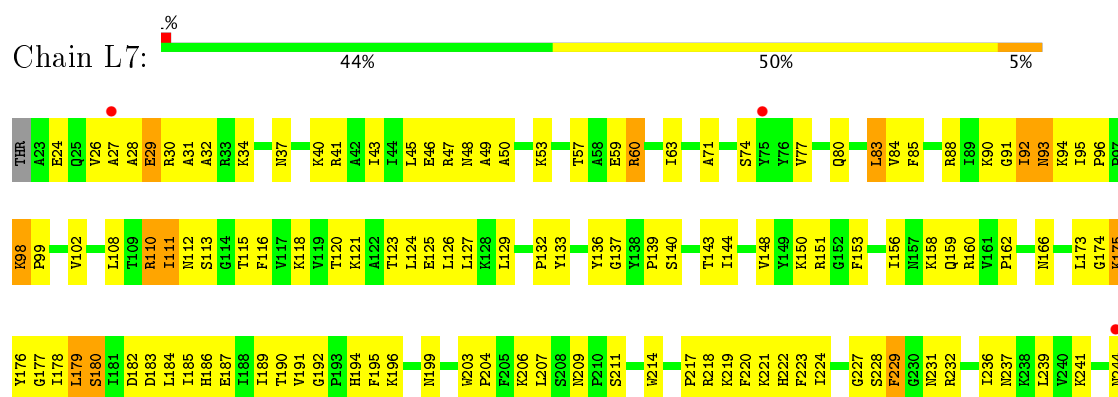
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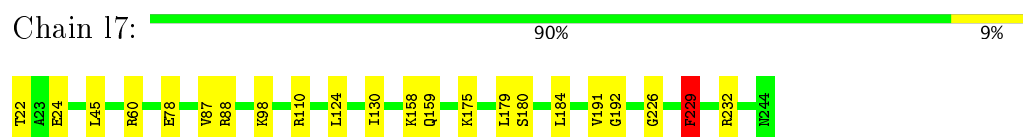
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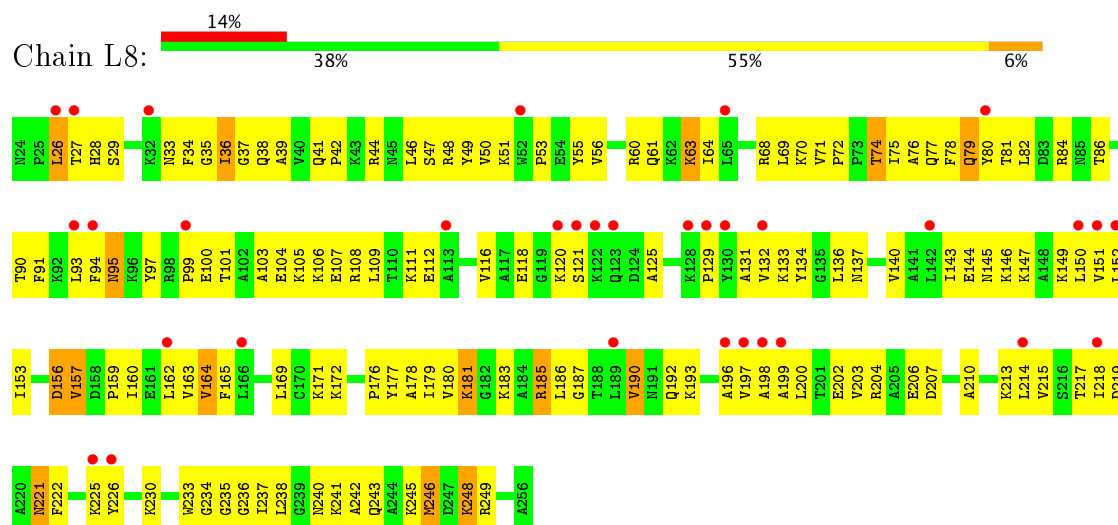
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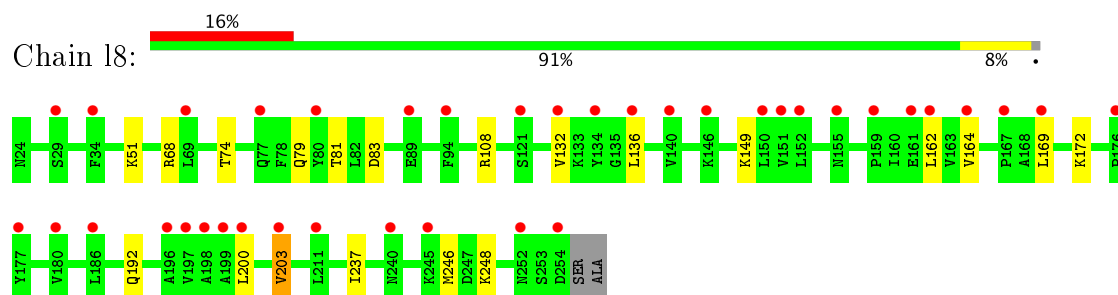
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• Molecule 10: 60S ribosomal protein L8-A

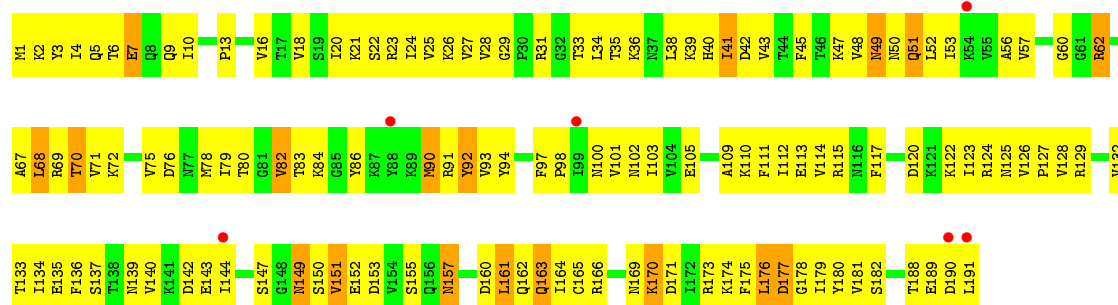


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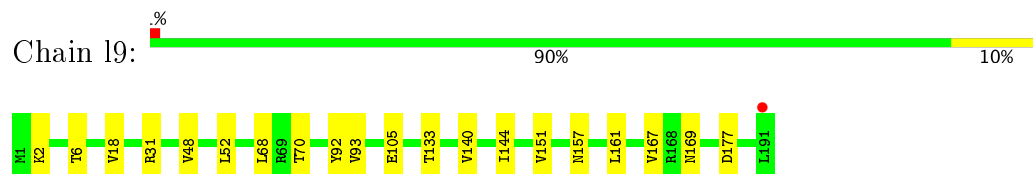


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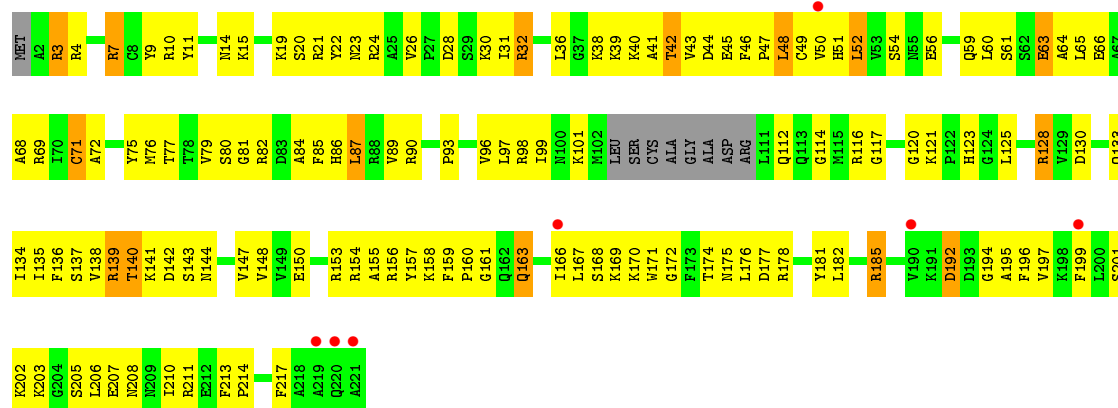




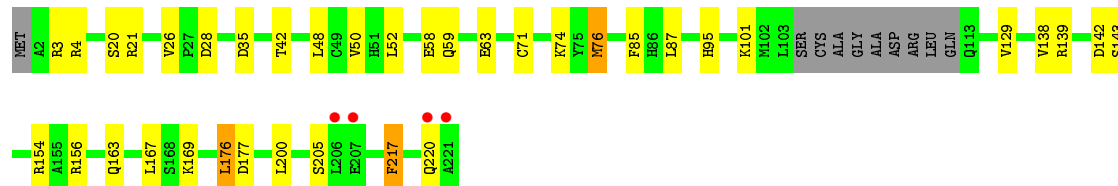
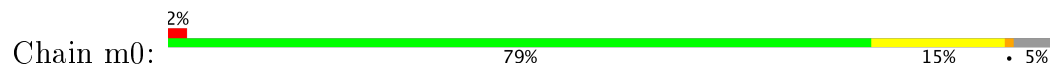
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• Molecule 12: 60S ribosomal protein L10

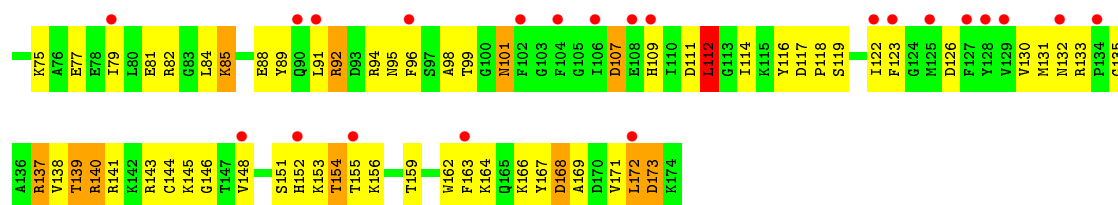


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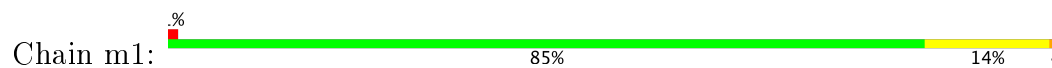


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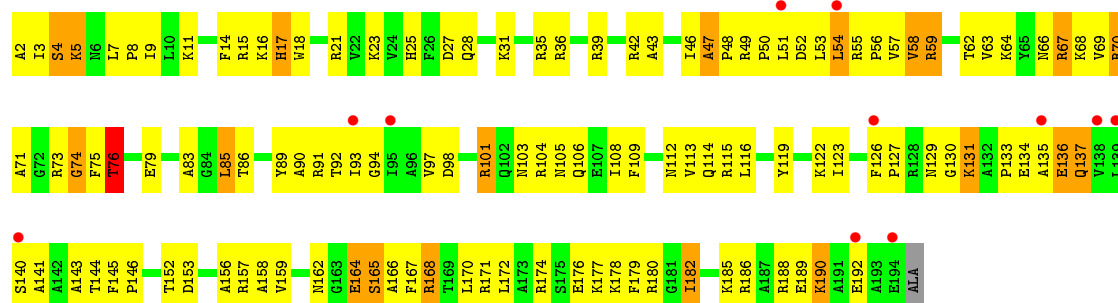




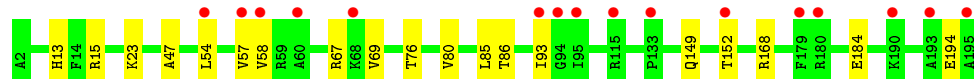
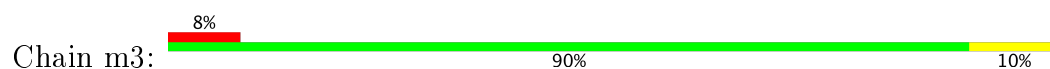
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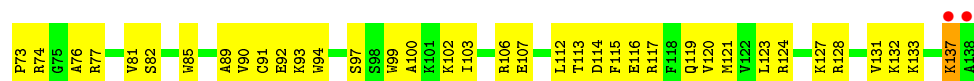
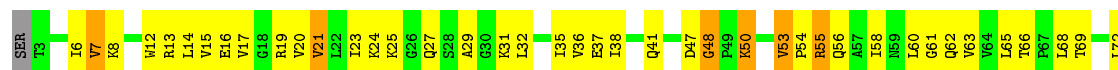
- Molecule 14: 60S ribosomal protein L13-A



- Molecule 14: 60S ribosomal protein L13-A



- Molecule 15: 60S ribosomal protein L14-A

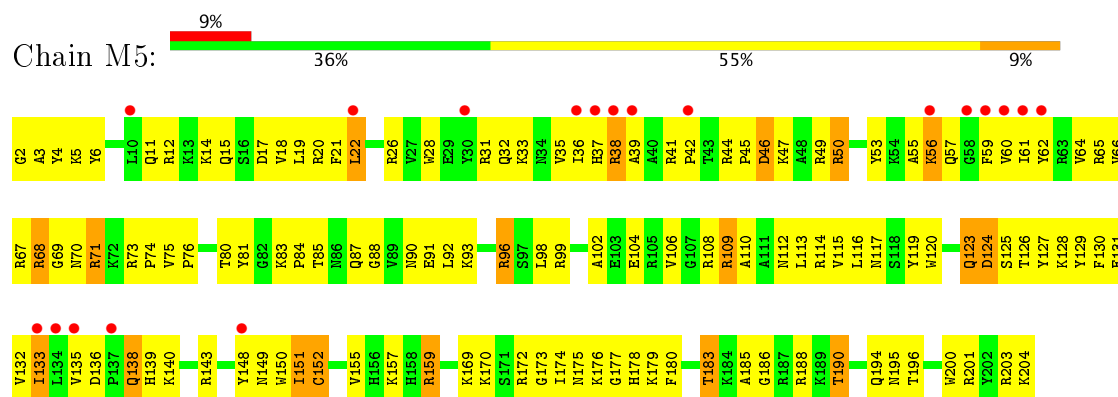


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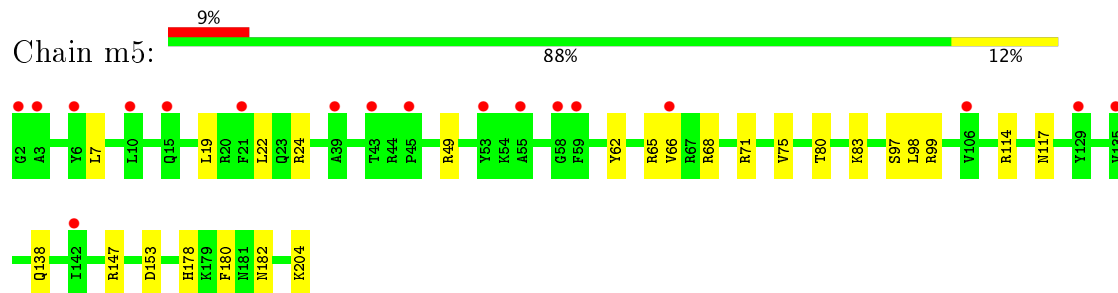




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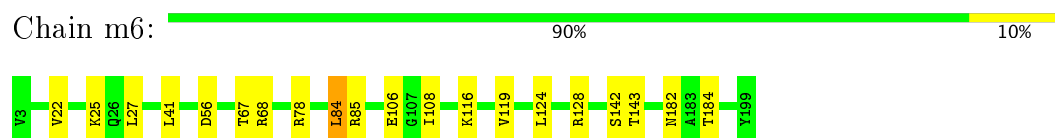
• Molecule 16: 60S ribosomal protein L15-A



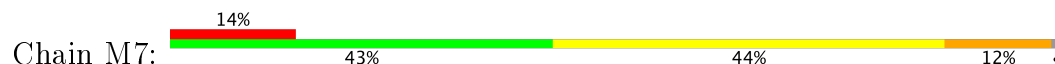
• Molecule 17: 60S ribosomal protein L16-A

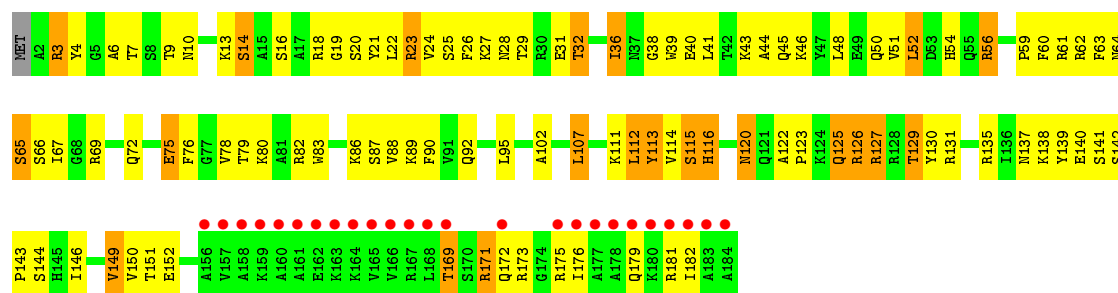


• Molecule 17: 60S ribosomal protein L16-A

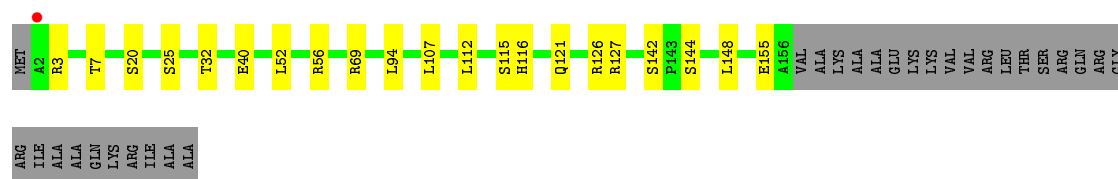
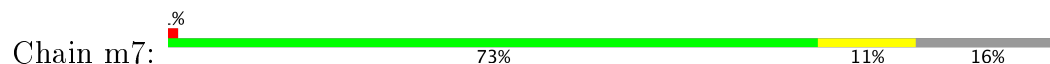


• Molecule 18: 60S ribosomal protein L17-A

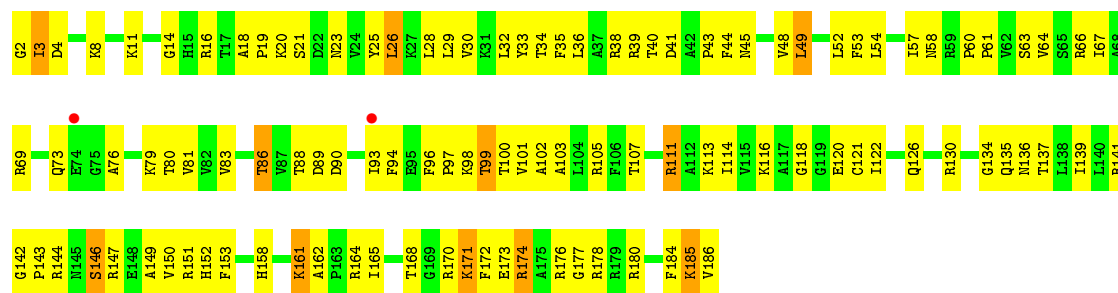
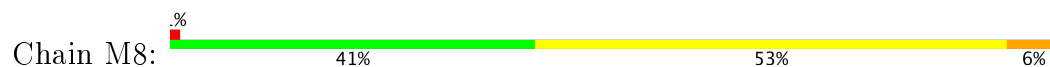




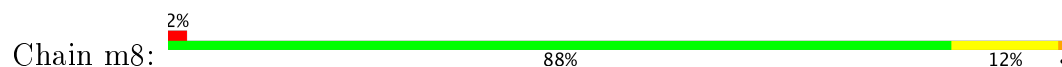
- Molecule 18: 60S ribosomal protein L17-A



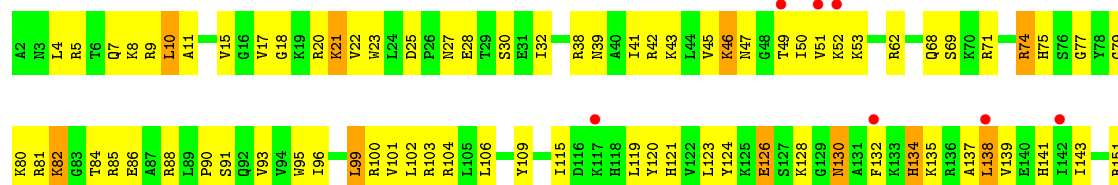
- Molecule 19: 60S ribosomal protein L18-A



- Molecule 19: 60S ribosomal protein L18-A



- Molecule 20: 60S ribosomal protein L19-A

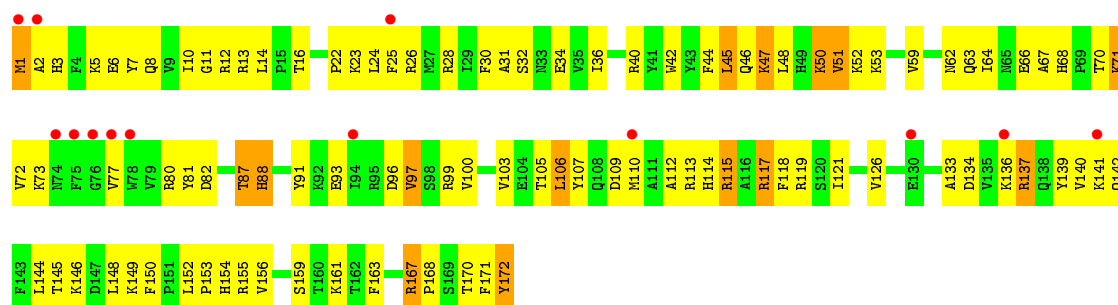
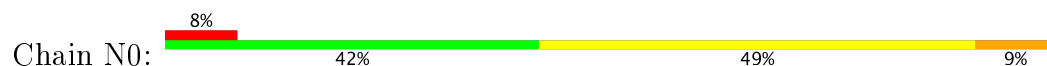




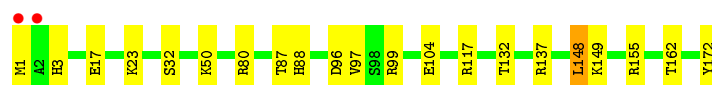
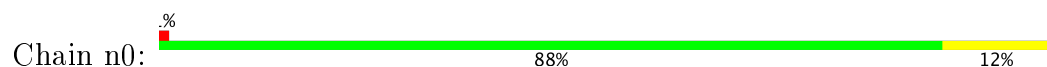
- Molecule 20: 60S ribosomal protein L19-A



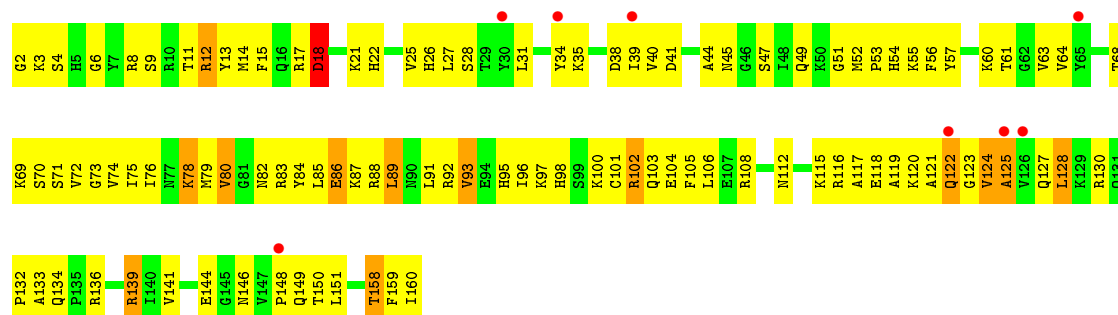
- Molecule 21: 60S ribosomal protein L20-A



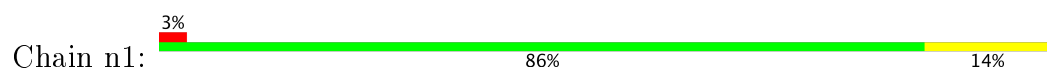
- Molecule 21: 60S ribosomal protein L20-A

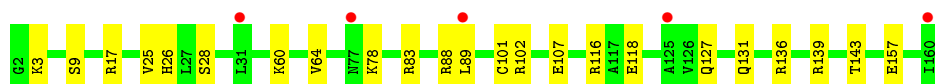


- Molecule 22: 60S ribosomal protein L21-A

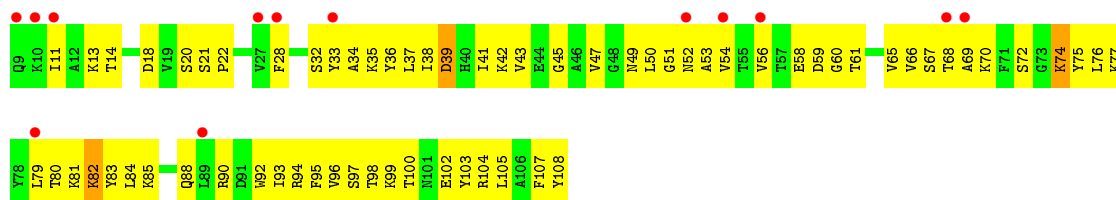


- Molecule 22: 60S ribosomal protein L21-A

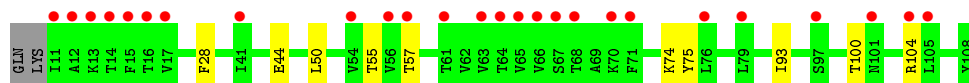
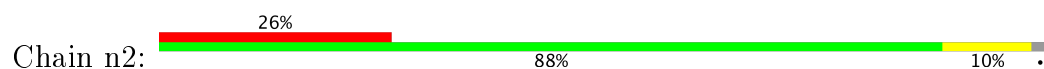




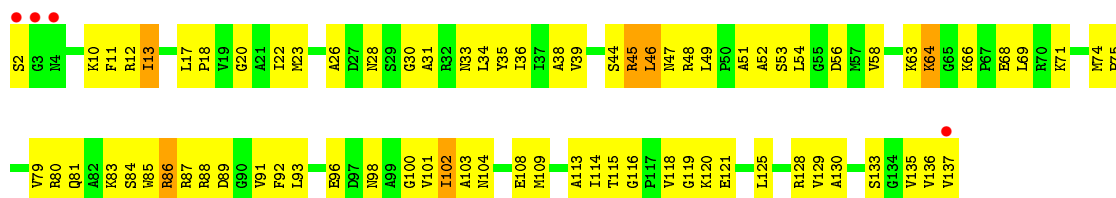
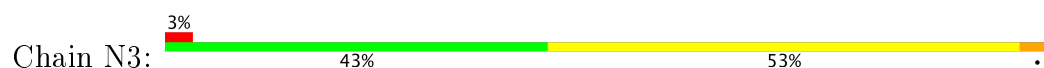
• Molecule 23: 60S ribosomal protein L22-A



• Molecule 23: 60S ribosomal protein L22-A



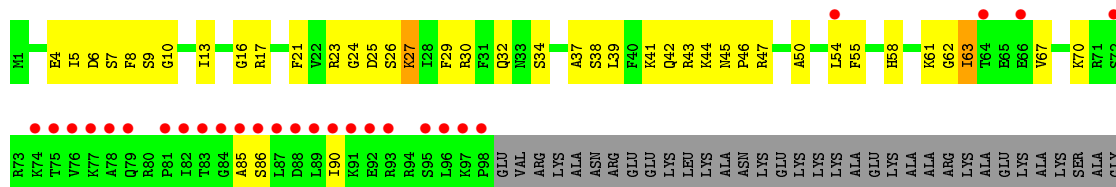
• Molecule 24: 60S ribosomal protein L23-A



• Molecule 24: 60S ribosomal protein L23-A

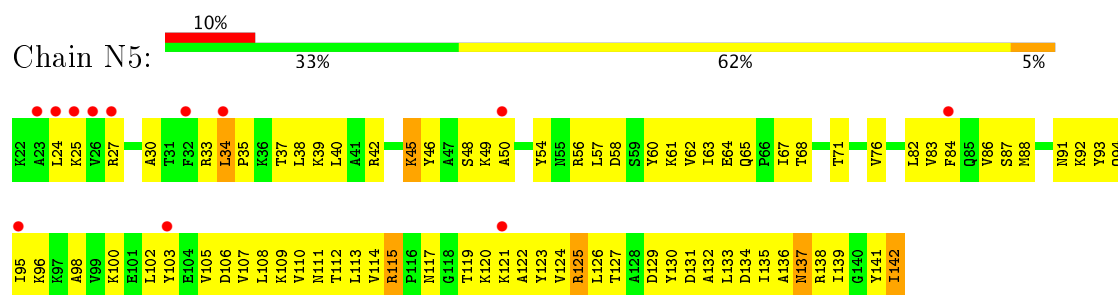


• Molecule 25: 60S ribosomal protein L24-A

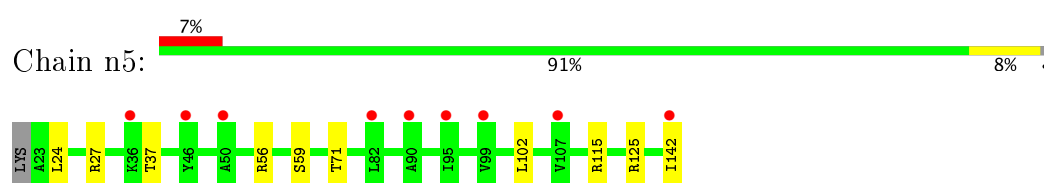


THR
GLN
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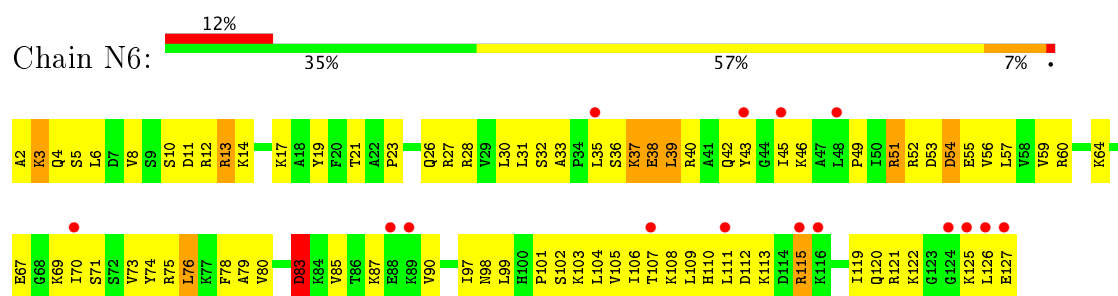
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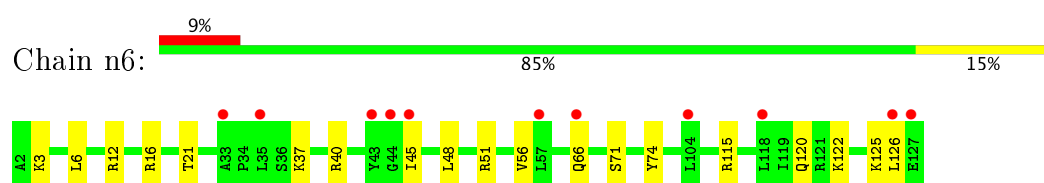
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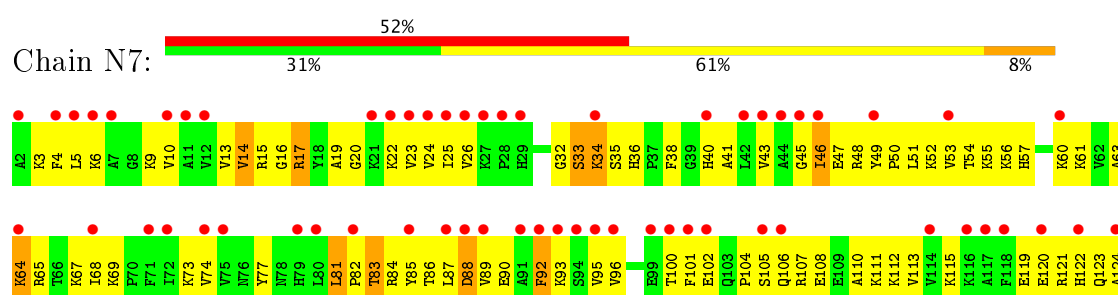
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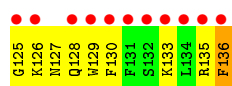


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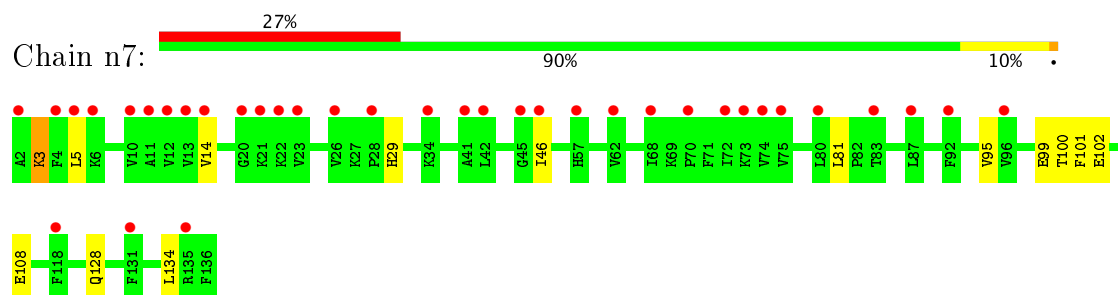


• Molecule 28: 60S ribosomal protein L27-A

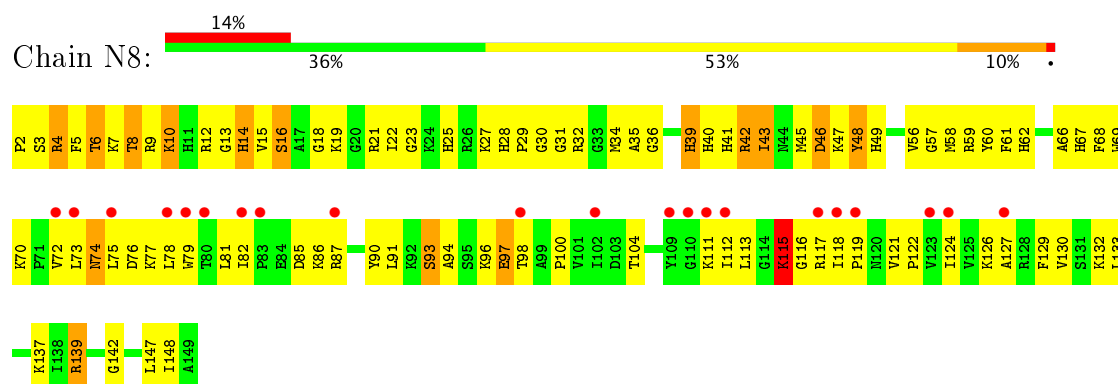




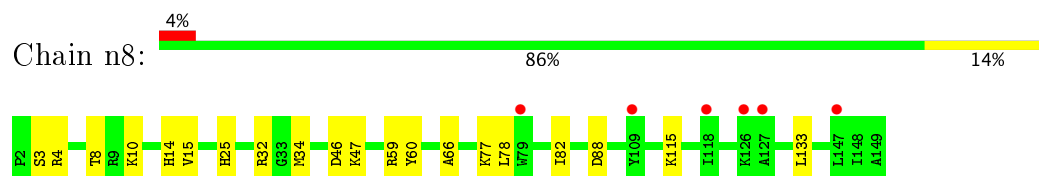
- Molecule 28: 60S ribosomal protein L27-A



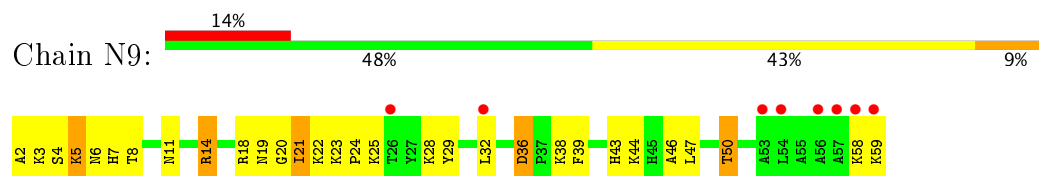
- Molecule 29: 60S ribosomal protein L28



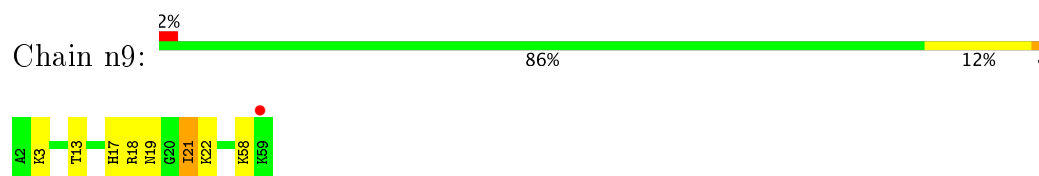
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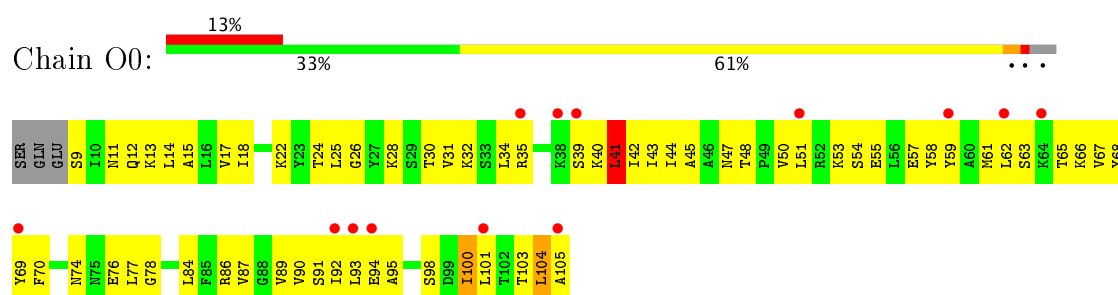
- Molecule 30: 60S ribosomal protein L29



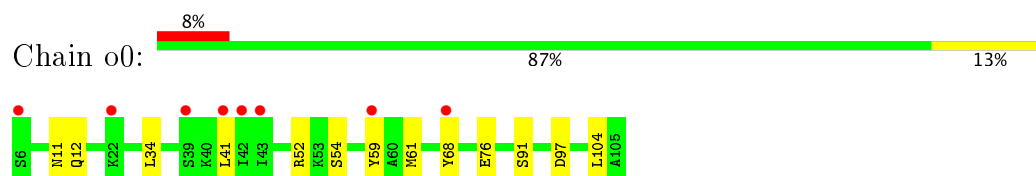
- Molecule 30: 60S ribosomal protein L29



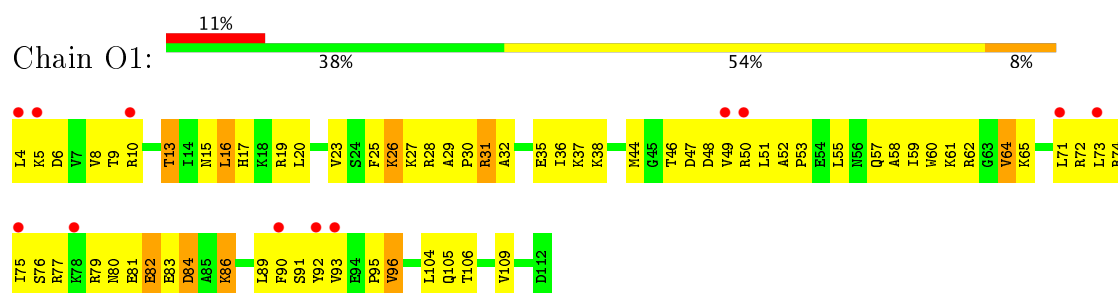
- Molecule 31: 60S ribosomal protein L30



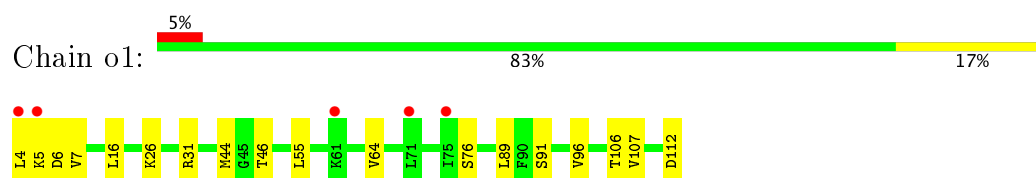
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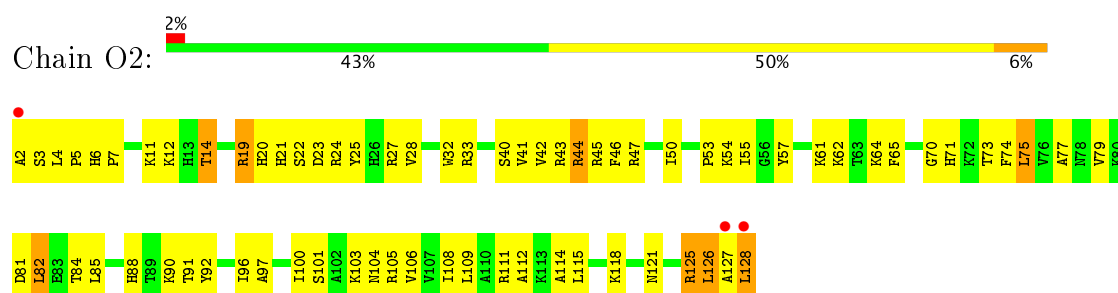
- Molecule 32: 60S ribosomal protein L31-A



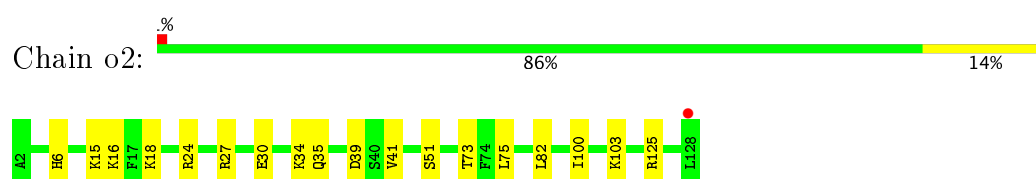
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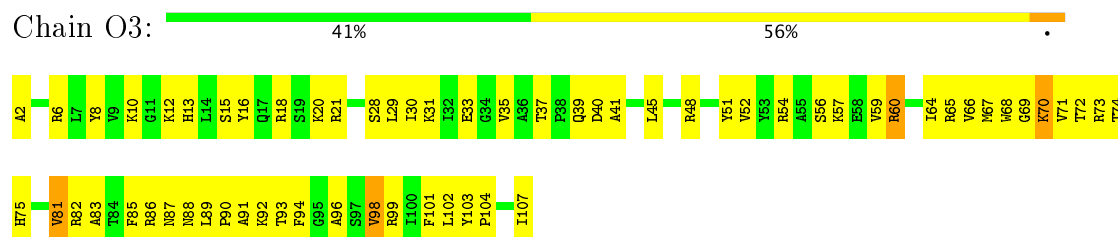
- Molecule 33: 60S ribosomal protein L32



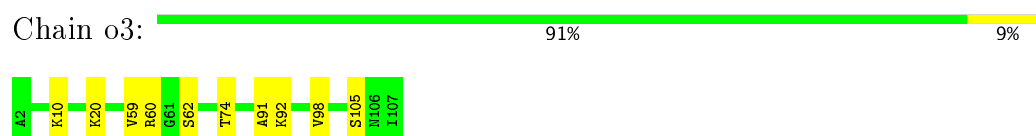
- Molecule 33: 60S ribosomal protein L32



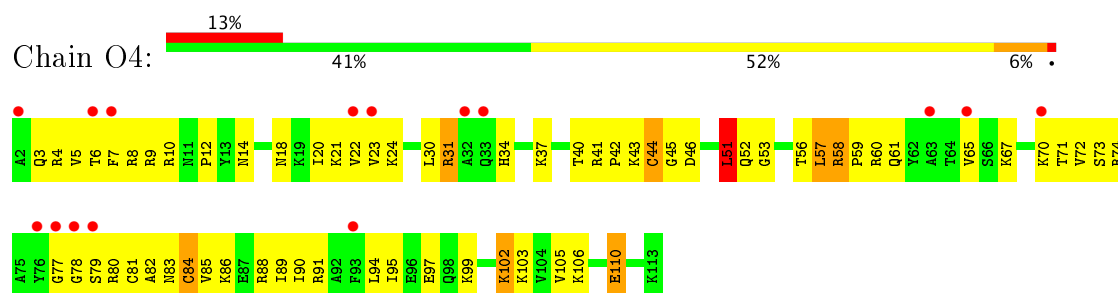
- Molecule 34: 60S ribosomal protein L33-A



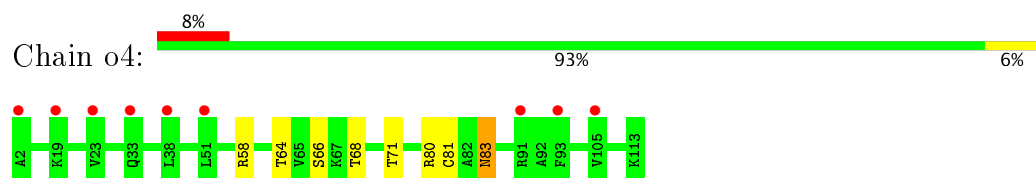
- Molecule 34: 60S ribosomal protein L33-A



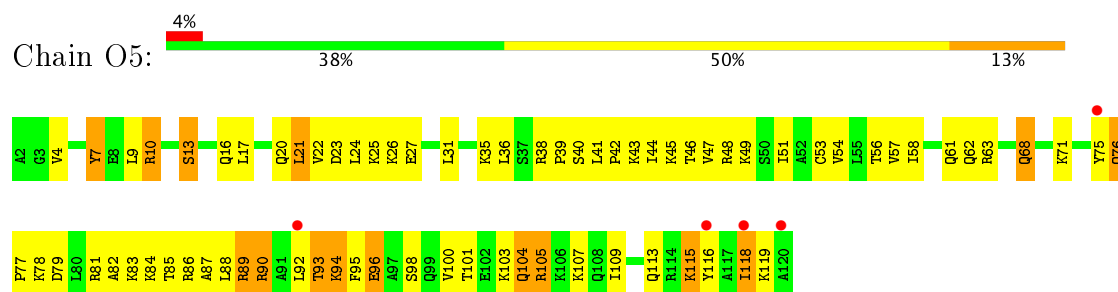
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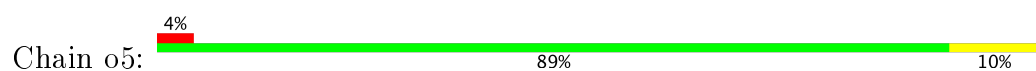
- Molecule 35: 60S ribosomal protein L34-A



- Molecule 36: 60S ribosomal protein L35-A

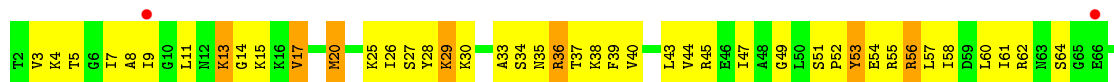


- Molecule 36: 60S ribosomal protein L35-A

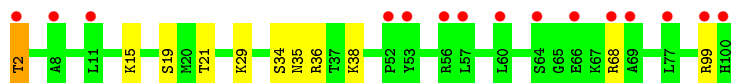
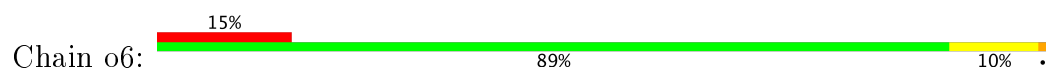




- Molecule 37: 60S ribosomal protein L36-A



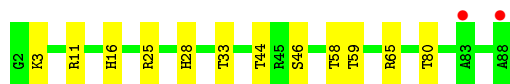
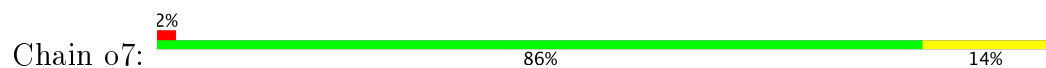
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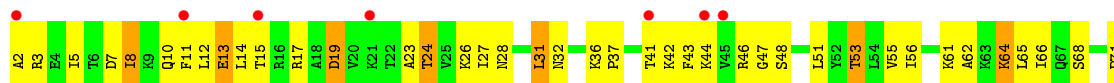
- Molecule 38: 60S ribosomal protein L37-A



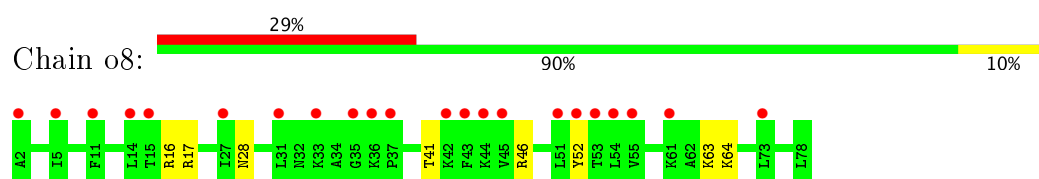
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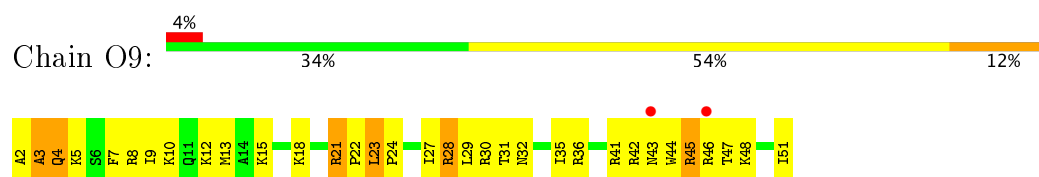
- Molecule 39: 60S ribosomal protein L38



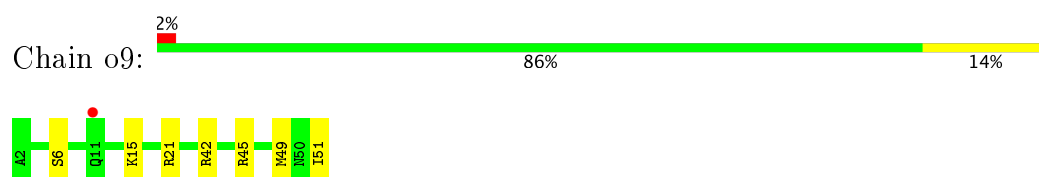
- Molecule 39: 60S ribosomal protein L38



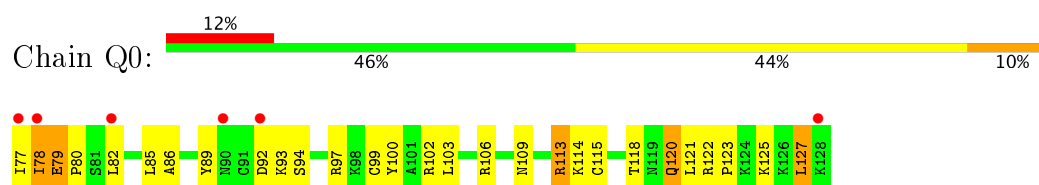
- Molecule 40: 60S ribosomal protein L39



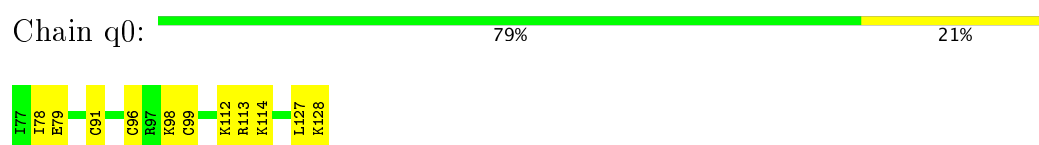
- Molecule 40: 60S ribosomal protein L39



- Molecule 41: Ubiquitin-60S ribosomal protein L40



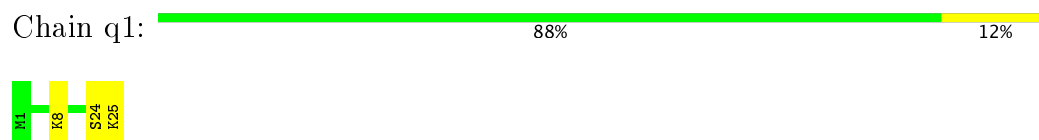
- Molecule 41: Ubiquitin-60S ribosomal protein L40



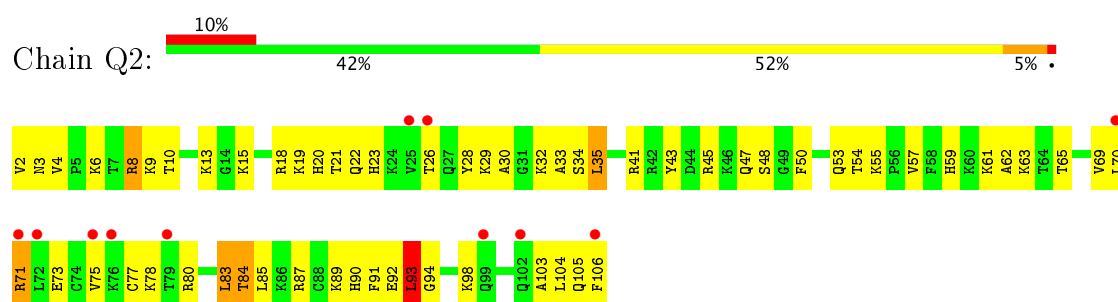
- Molecule 42: 60S ribosomal protein L41-A



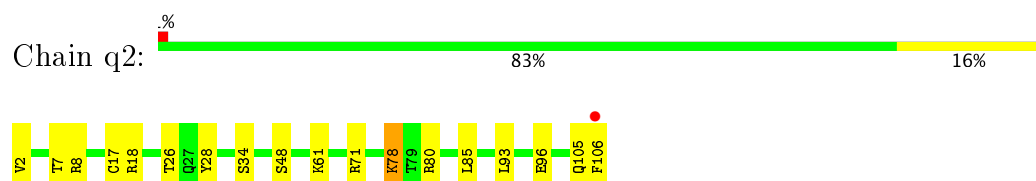
- Molecule 42: 60S ribosomal protein L41-A



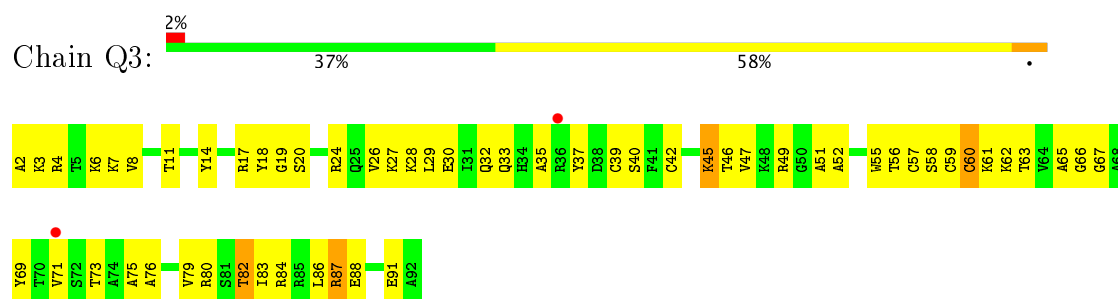
- Molecule 43: 60S ribosomal protein L42-A



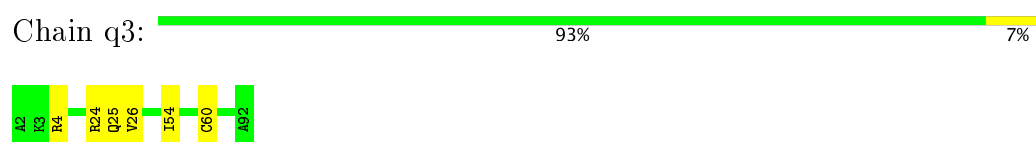
- Molecule 43: 60S ribosomal protein L42-A



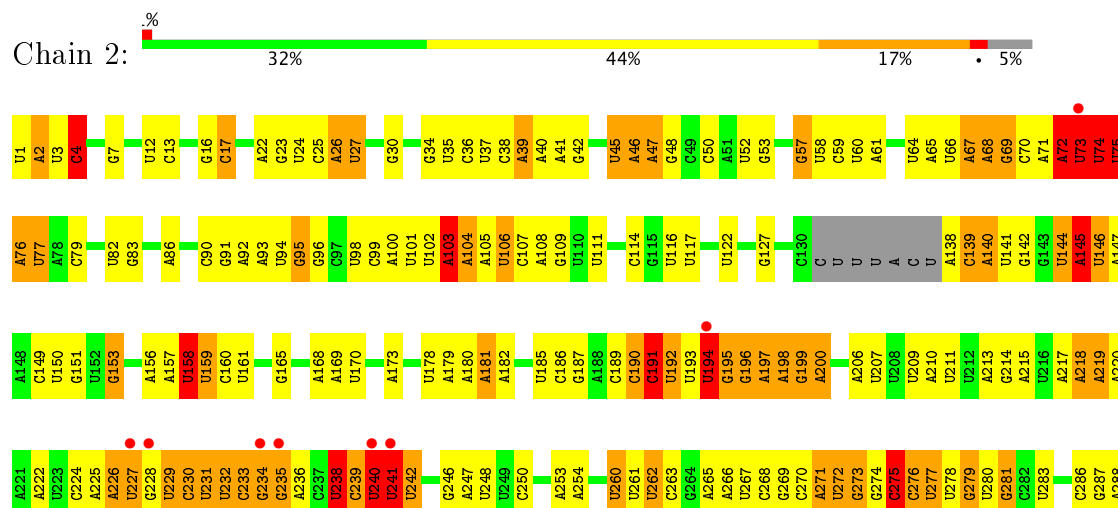
- Molecule 44: 60S ribosomal protein L43-A



- Molecule 44: 60S ribosomal protein L43-A



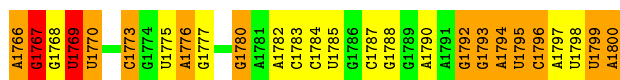
- Molecule 45: 18S ribosomal RNA



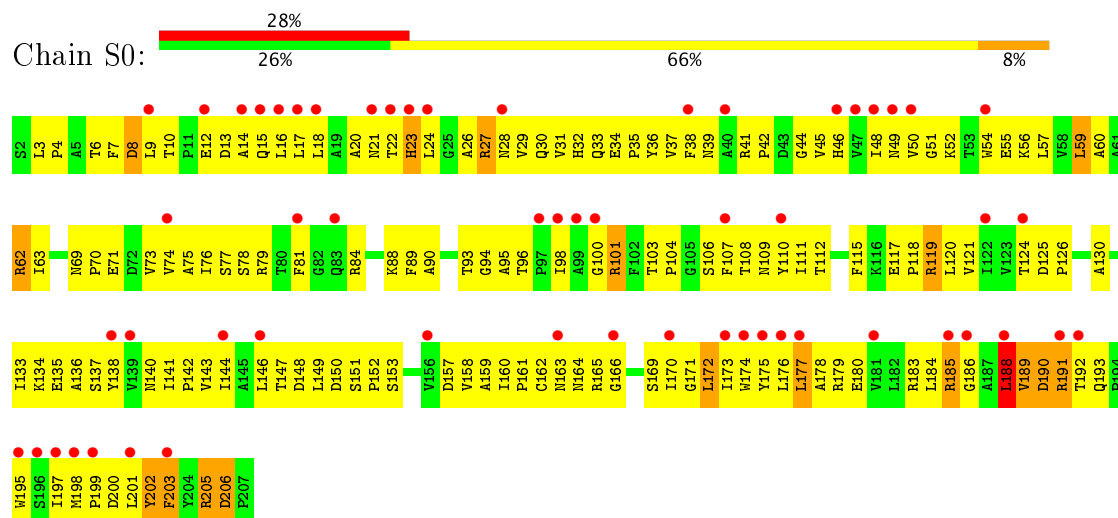
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| U1364 | U1365 | G1291 | A1217 | U1144 | C1075 | C1001 | C927 | U861 | A789 | C | U | G514 | C444 | A370 | G291 |
| U1366 | U1367 | G1292 | G1218 | U1145 | U1076 | A1002 | U928 | U862 | U790 | U | U | G515 | C448 | G371 | U292 |
| U1368 | U1369 | U1293 | G1219 | G1146 | C1077 | A1003 | A929 | U863 | A791 | C | U | A516 | C449 | U379 | U297 |
| U1370 | U1371 | G1294 | C1220 | A1147 | C1078 | U1004 | A930 | U864 | A792 | U | U | G517 | C450 | U380 | C298 |
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| U1376 | U1377 | U1297 | A1223 | A1151 | A1081 | G1011 | A933 | U867 | U795 | C | U | A520 | A453 | A301 | A301 |
| U1378 | U1379 | U1298 | G1224 | U1152 | C1082 | U1012 | U934 | U868 | A796 | C | U | A521 | U454 | A302 | U302 |
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| U1428 | U1429 | U1323 | U1258 | G1179 | G1111 | U1043 | C969 | U898 | U831 | U | U | C547 | C411 | U413 | A333 |
| U1430 | U1431 | U1324 | C1259 | C1180 | G1112 | U1044 | A970 | U899 | U832 | U | U | C548 | C412 | U414 | G337 |
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| U1434 | U1435 | U1326 | U1261 | U1182 | G1117 | G1046 | A972 | U901 | U834 | U | U | C550 | C414 | C414 | C339 |
| U1436 | U1437 | U1327 | C1262 | U1183 | G1118 | U1052 | A973 | U902 | G834 | U | U | C551 | C415 | C415 | U340 |
| U1438 | U1439 | U1328 | U1263 | U1184 | G1119 | G1053 | A974 | U903 | U835 | U | U | C552 | C416 | A417 | U341 |
| U1440 | U1441 | U1329 | G1264 | U1185 | U1120 | U1054 | U975 | U904 | U836 | U | U | C553 | C417 | G418 | A341 |
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| U1522 | U1523 | U1370 | G1230 | C1158 | U1088 | U1015 | C1015 | U945 | U878 | U | U | C594 | C458 | A457 | A385 |
| U1524 | U1525 | U1371 | A1231 | C1159 | U1089 | U1016 | C1016 | U946 | U879 | U | U | C595 | C459 | A458 | A386 |
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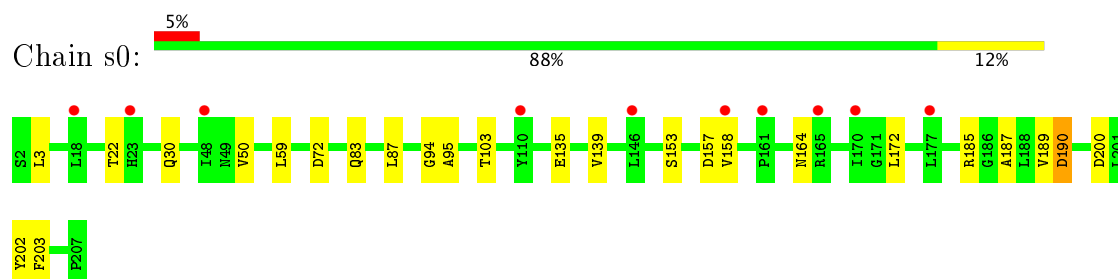




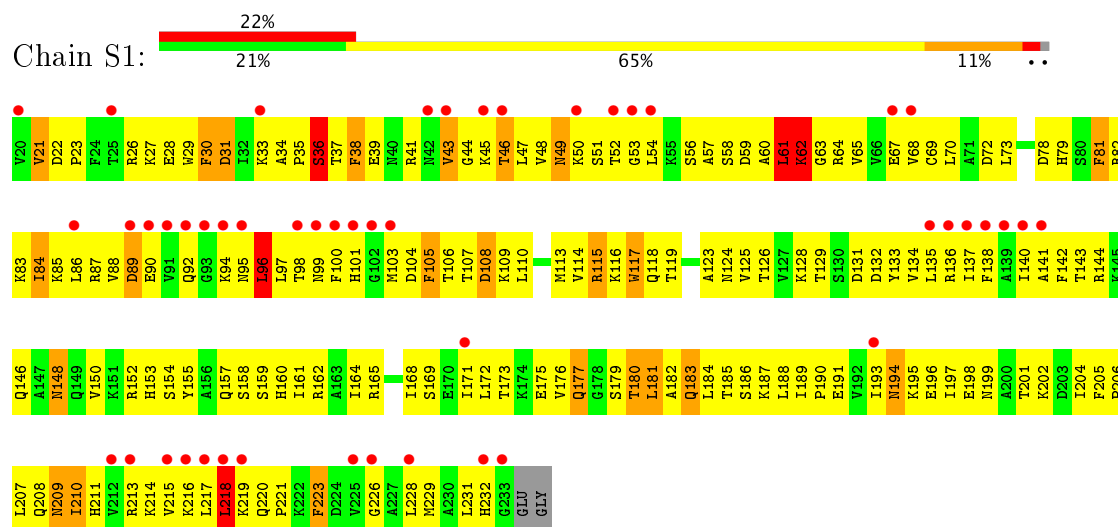
• Molecule 46: 40S ribosomal protein S0-A



• Molecule 46: 40S ribosomal protein S0-A

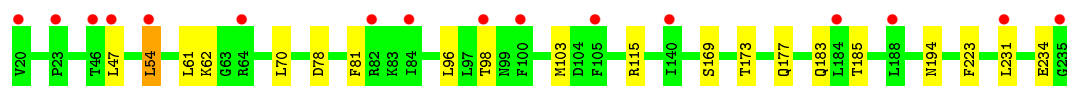


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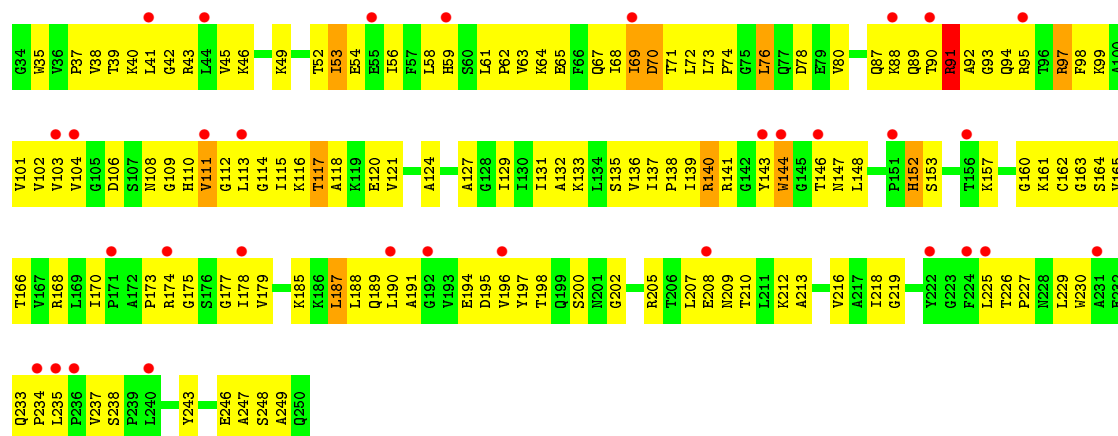


• Molecule 47: 40S ribosomal protein S1-A

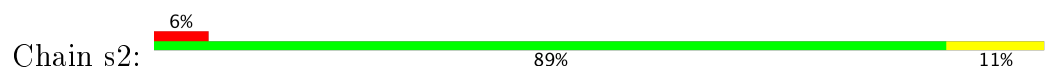




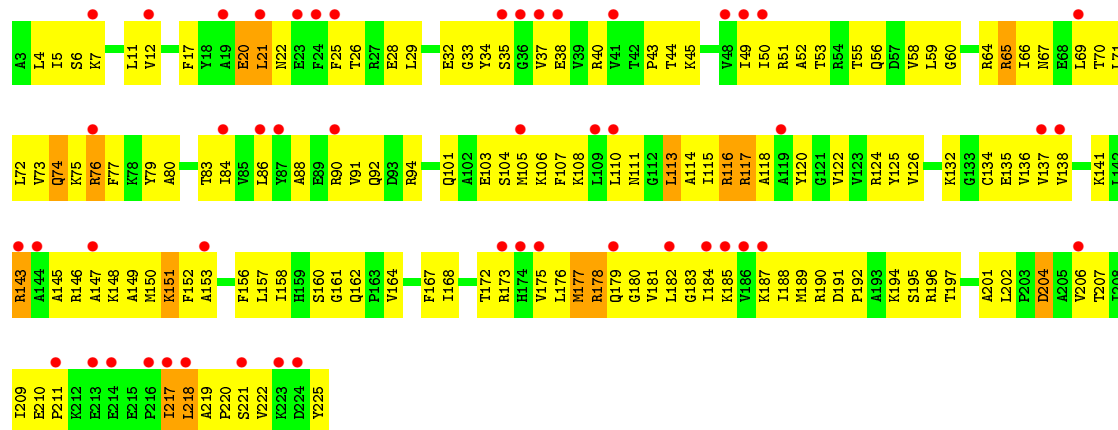
• Molecule 48: 40S ribosomal protein S2



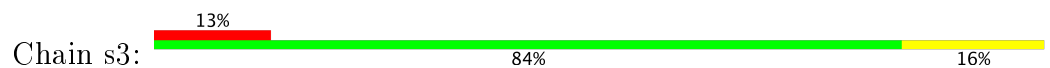
• Molecule 48: 40S ribosomal protein S2

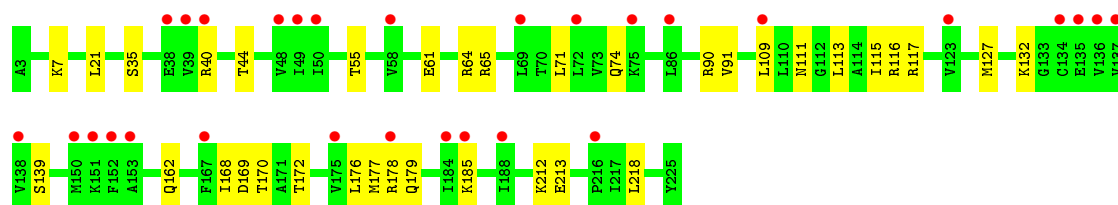


• Molecule 49: 40S ribosomal protein S3

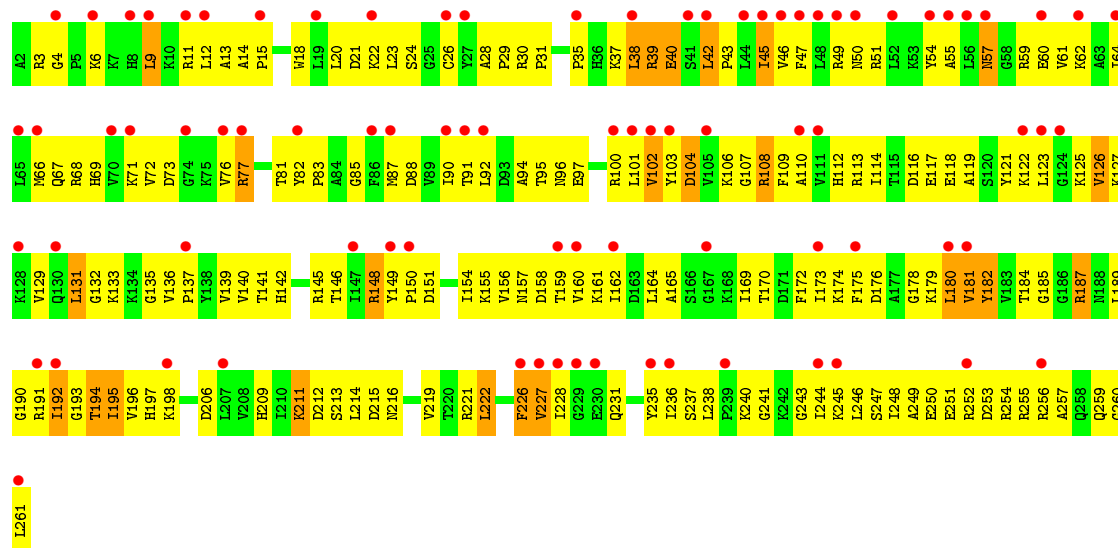


• Molecule 49: 40S ribosomal protein S3

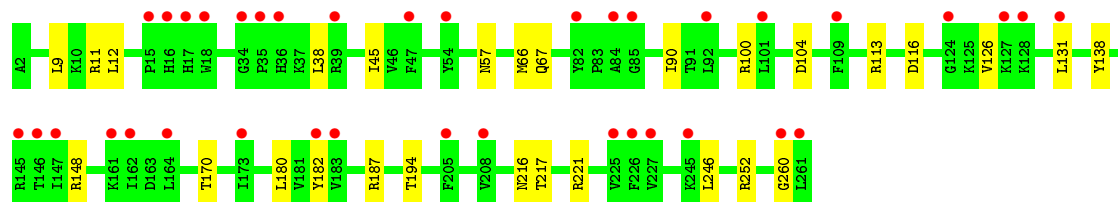
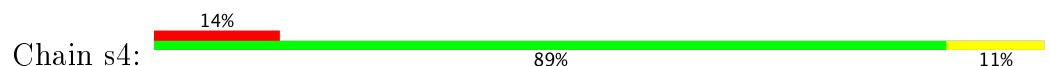




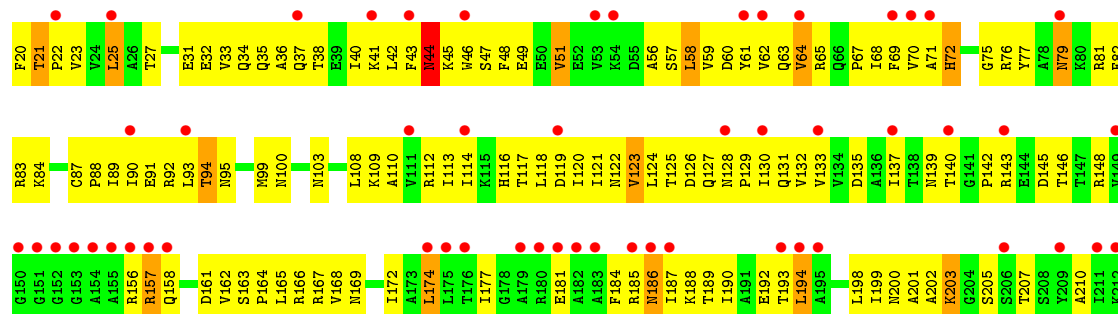
• Molecule 50: 40S ribosomal protein S4-A

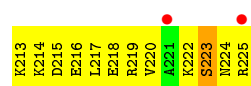


• Molecule 50: 40S ribosomal protein S4-A

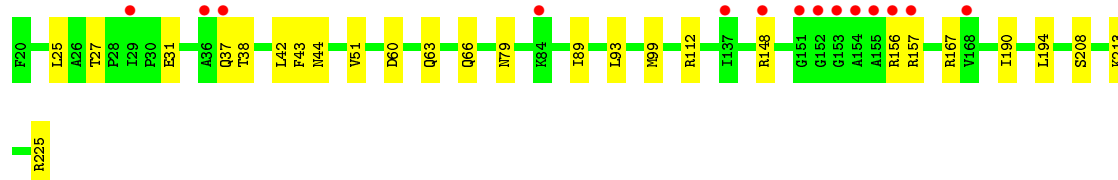
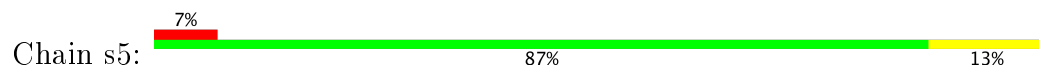


• Molecule 51: 40S ribosomal protein S5

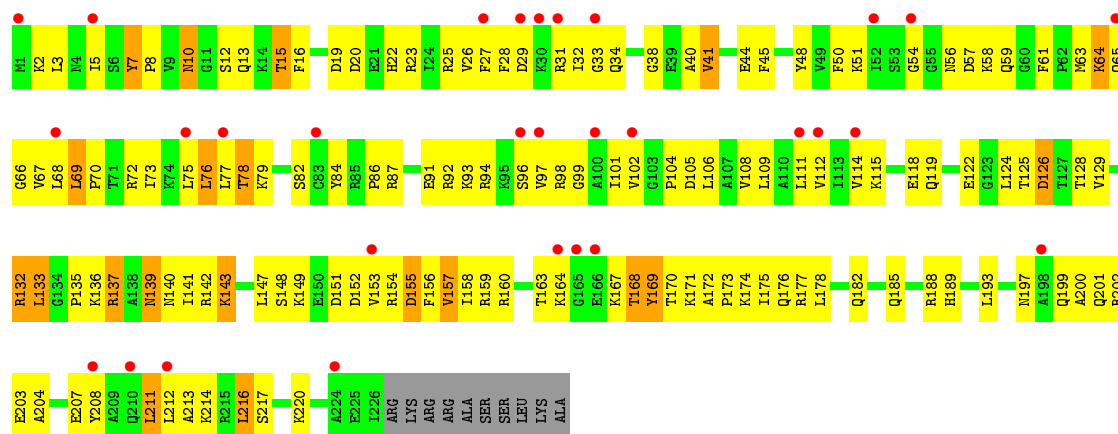




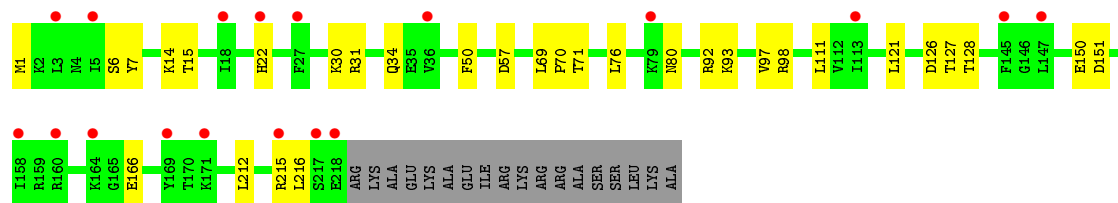
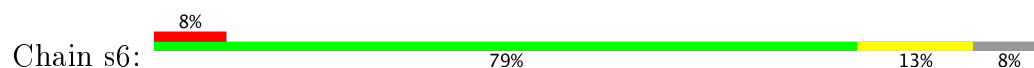
- Molecule 51: 40S ribosomal protein S5



- Molecule 52: 40S ribosomal protein S6-A

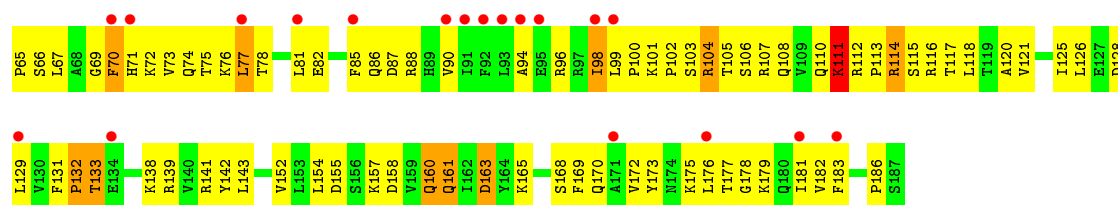


- Molecule 52: 40S ribosomal protein S6-A

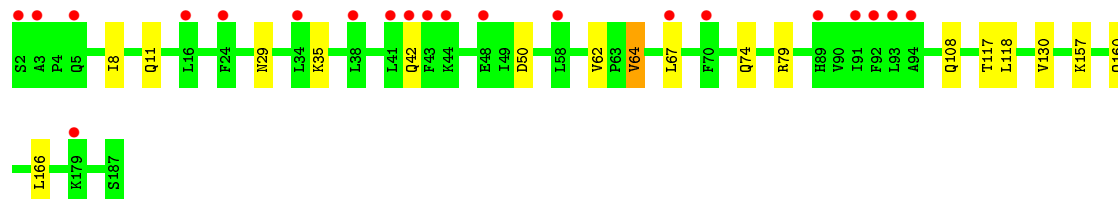
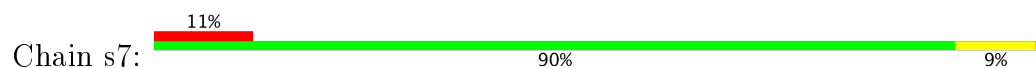


- Molecule 53: 40S ribosomal protein S7-A

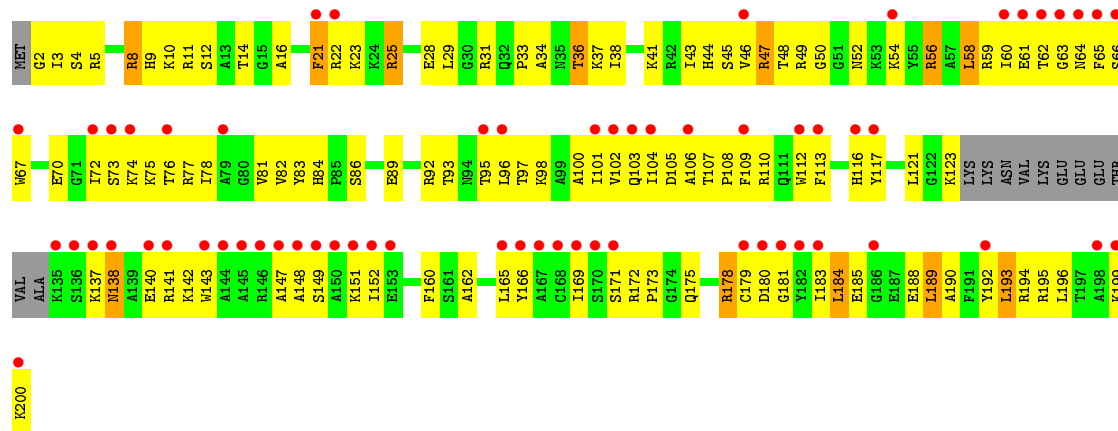




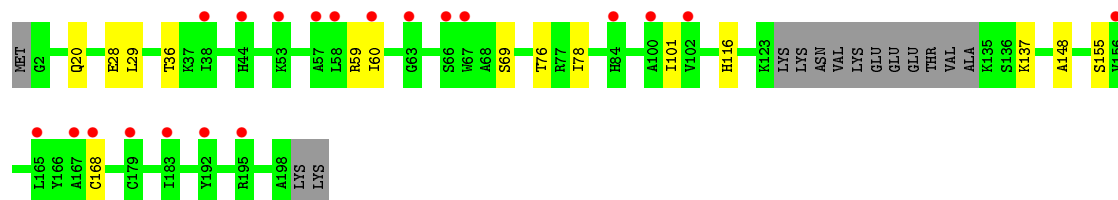
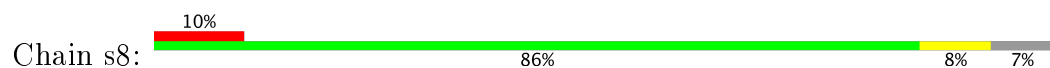
• Molecule 53: 40S ribosomal protein S7-A



• Molecule 54: 40S ribosomal protein S8-A

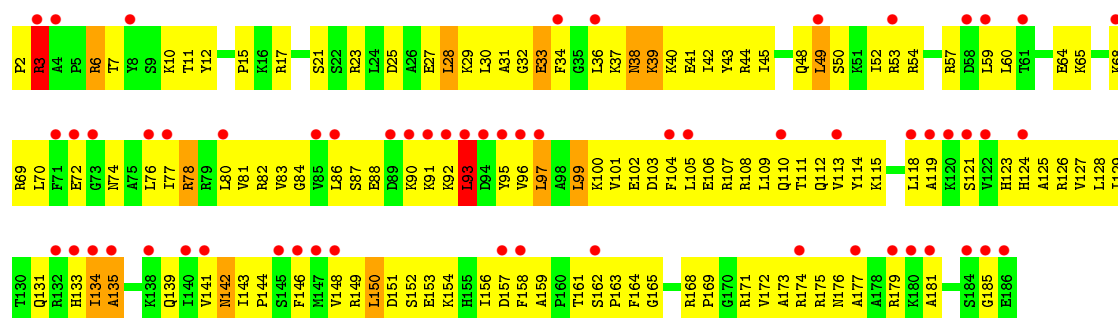


• Molecule 54: 40S ribosomal protein S8-A

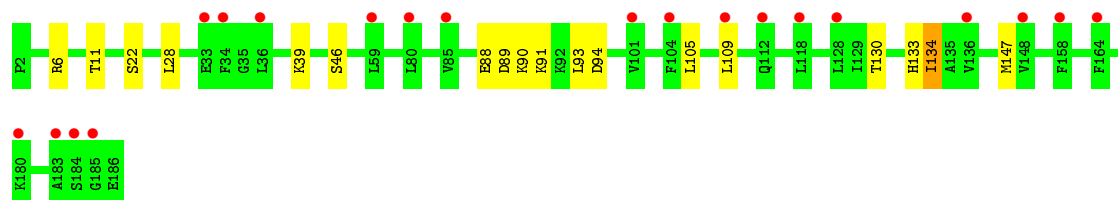
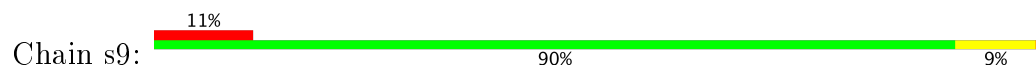


• Molecule 55: 40S ribosomal protein S9-A

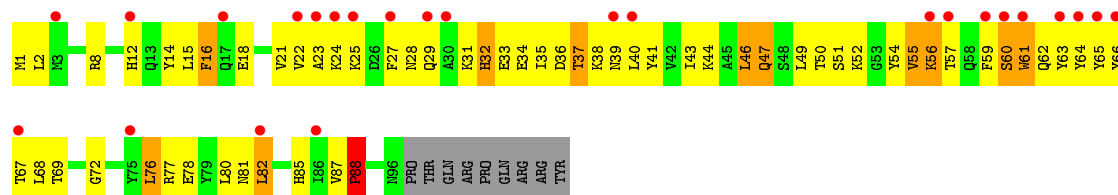




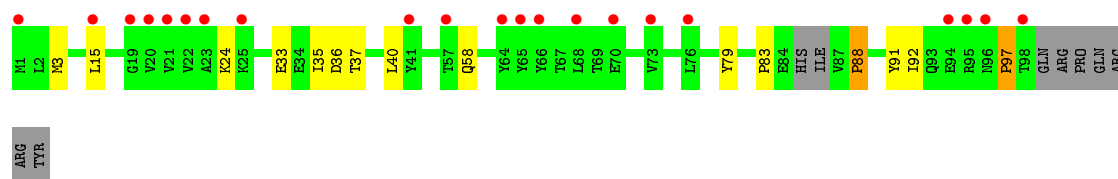
- Molecule 55: 40S ribosomal protein S9-A



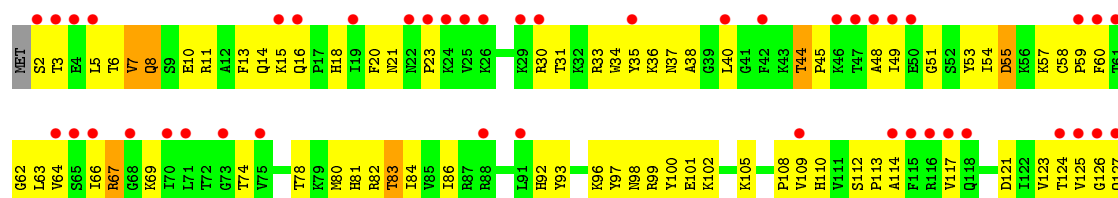
- Molecule 56: 40S ribosomal protein S10-A



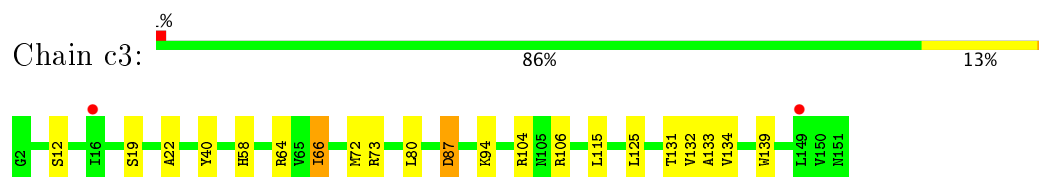
- Molecule 56: 40S ribosomal protein S10-A



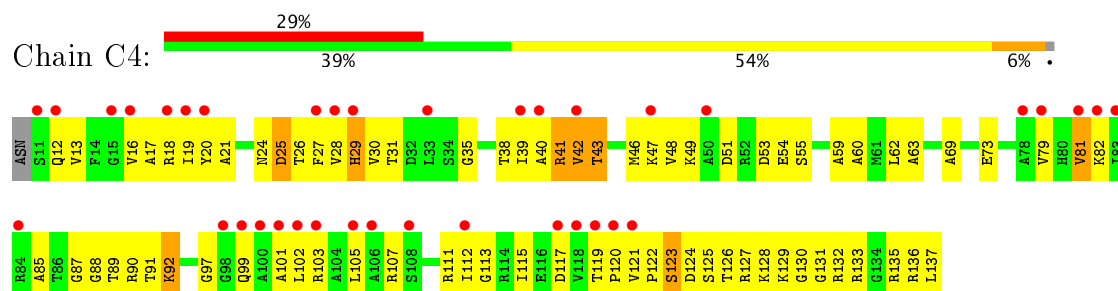
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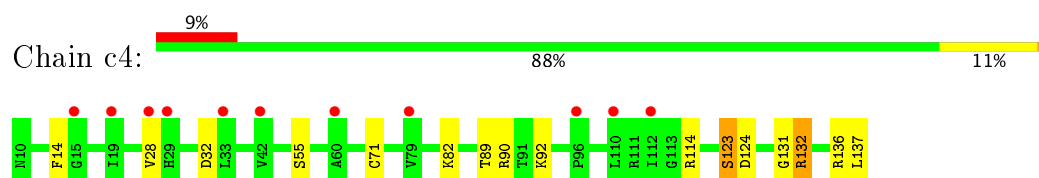
- Molecule 59: 40S ribosomal protein S13



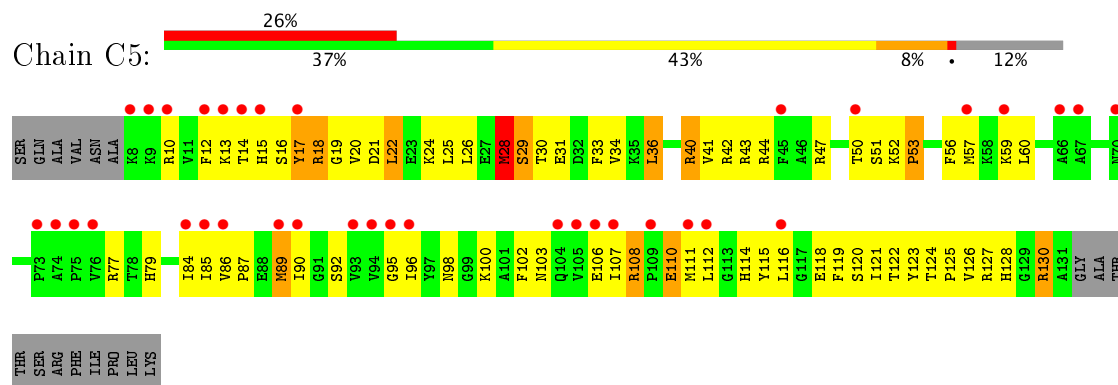
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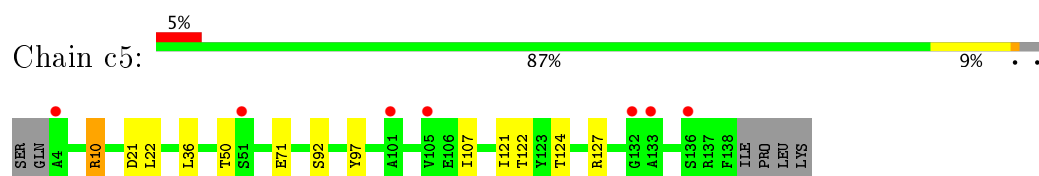
- Molecule 60: 40S ribosomal protein S14-B



- Molecule 61: 40S ribosomal protein S15

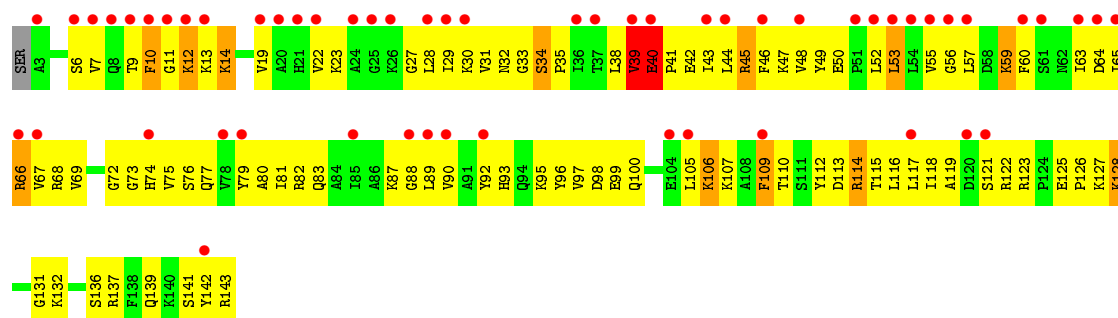


- Molecule 61: 40S ribosomal protein S15

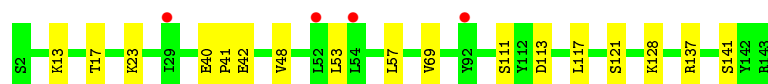
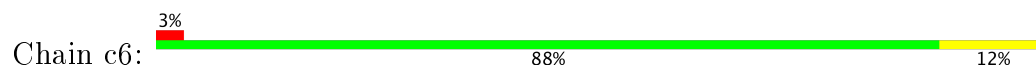


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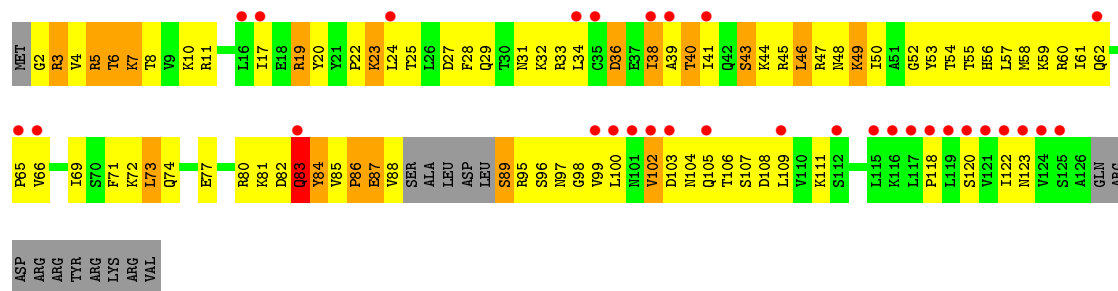




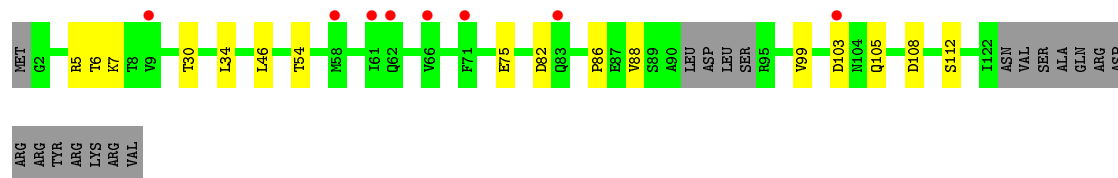
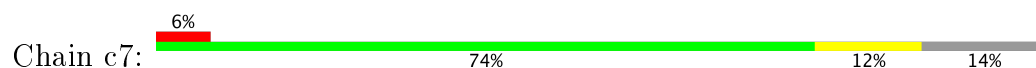
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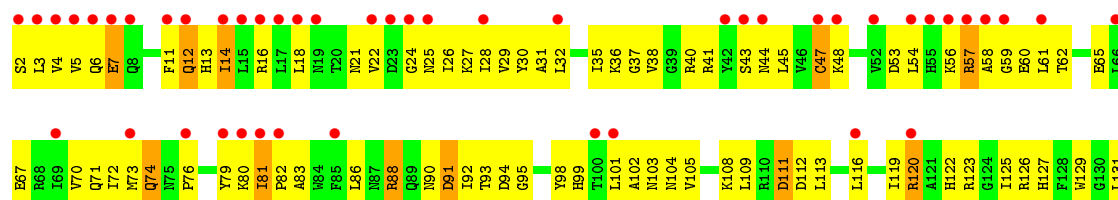
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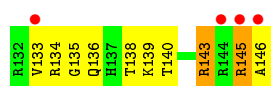


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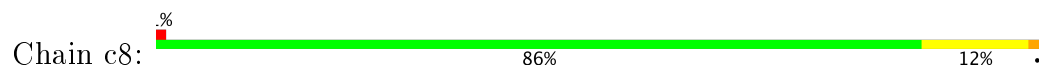


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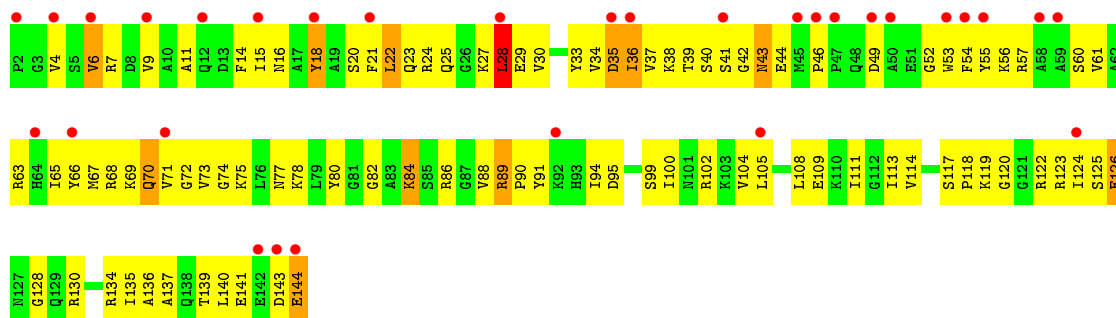




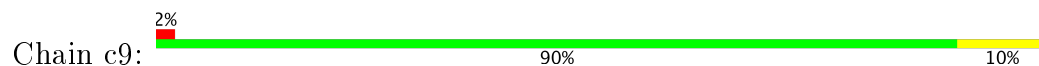
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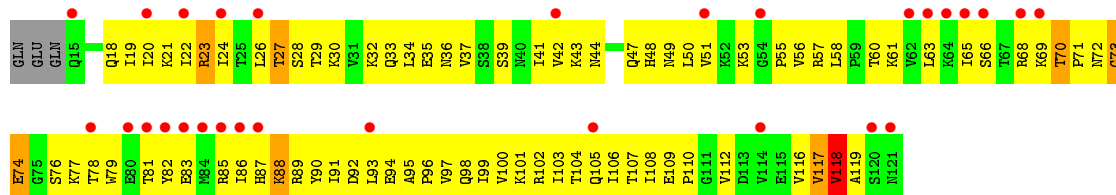
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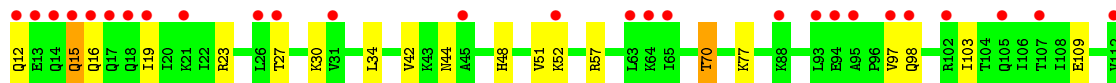
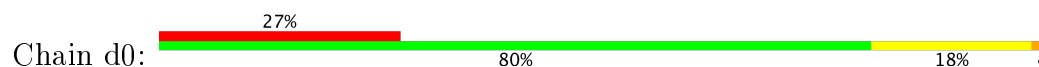
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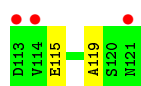


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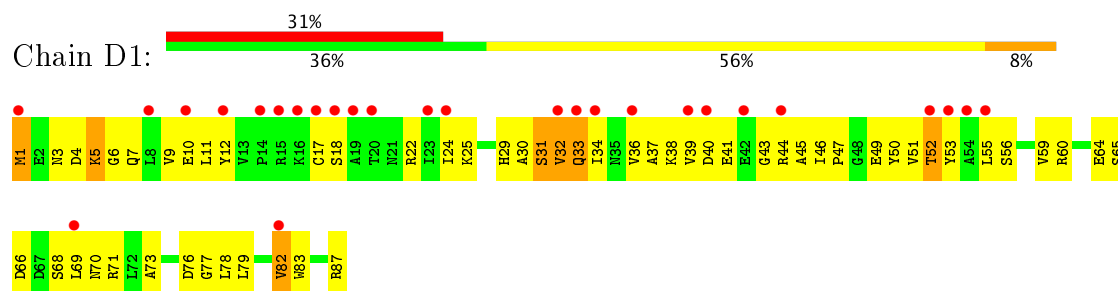


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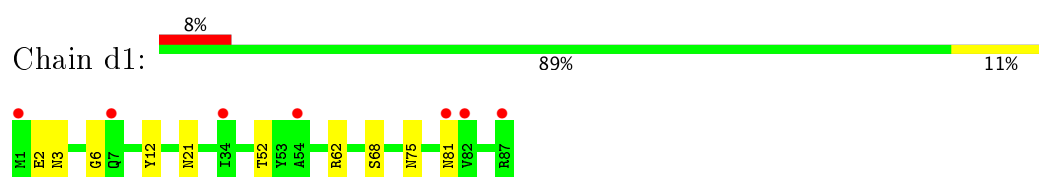




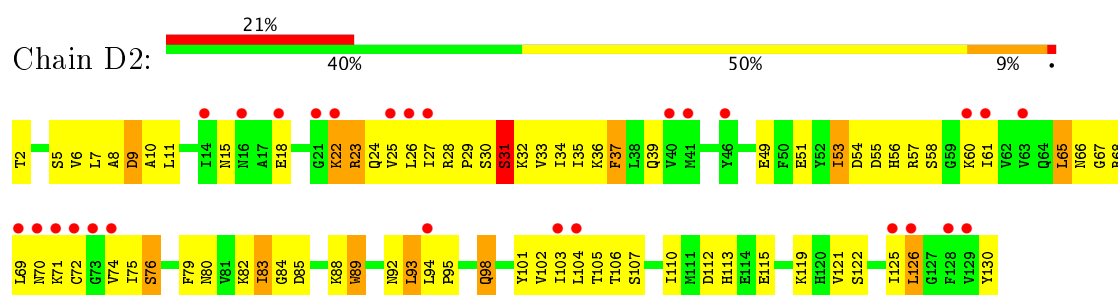
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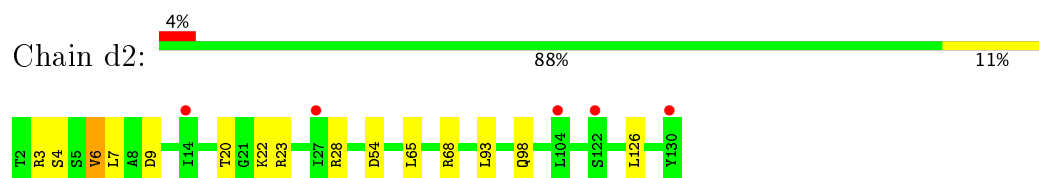
- Molecule 67: 40S ribosomal protein S21-A



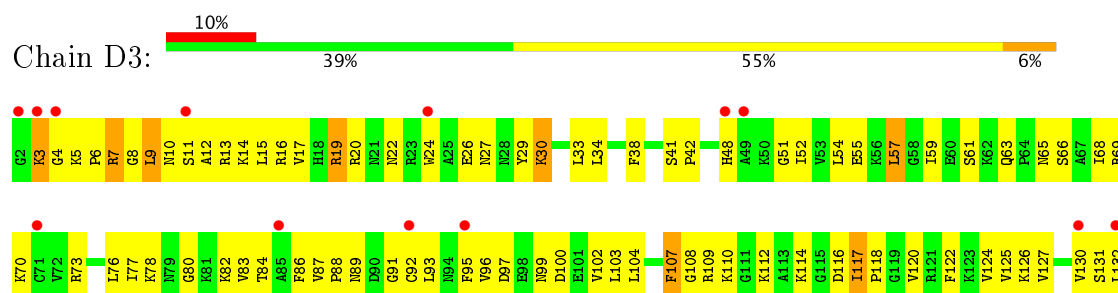
- Molecule 68: 40S ribosomal protein S22-A

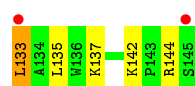


- Molecule 68: 40S ribosomal protein S22-A



- Molecule 69: 40S ribosomal protein S23-A

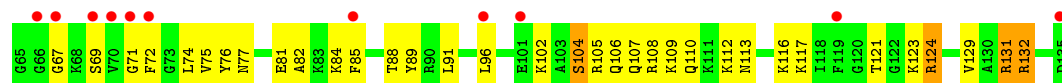
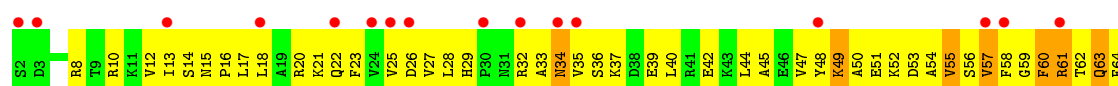
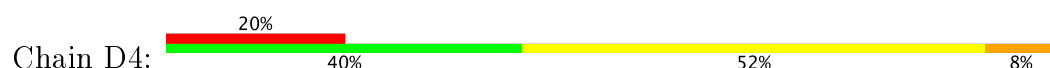




- Molecule 69: 40S ribosomal protein S23-A



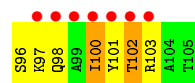
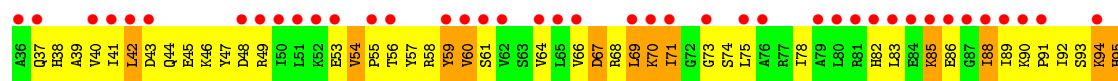
- Molecule 70: 40S ribosomal protein S24-A



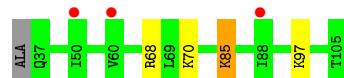
- Molecule 70: 40S ribosomal protein S24-A



- Molecule 71: 40S ribosomal protein S25-A

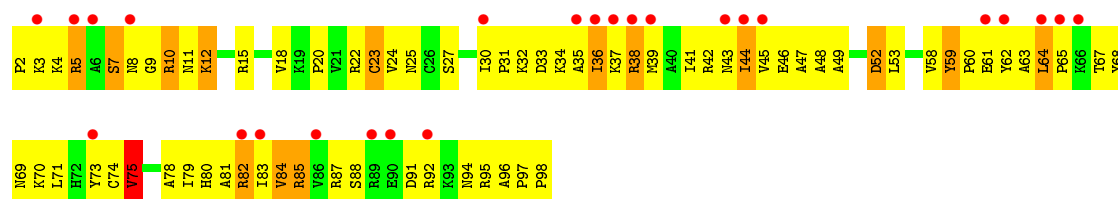


- Molecule 71: 40S ribosomal protein S25-A

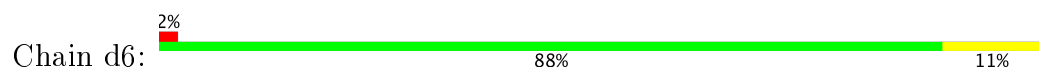


- Molecule 72: 40S ribosomal protein S26-B

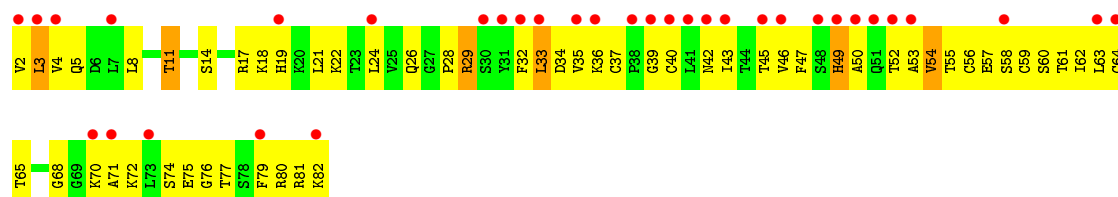




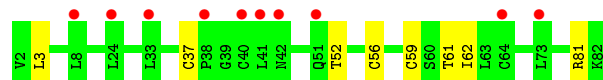
- Molecule 72: 40S ribosomal protein S26-B



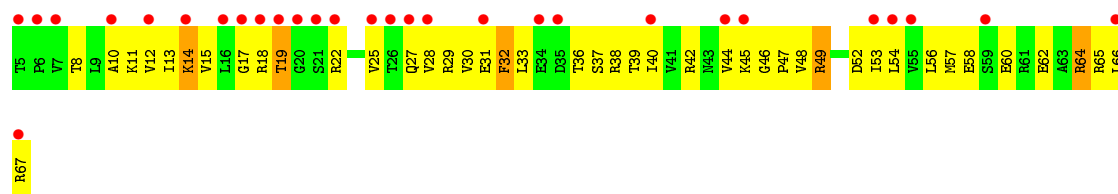
- Molecule 73: 40S ribosomal protein S27-A



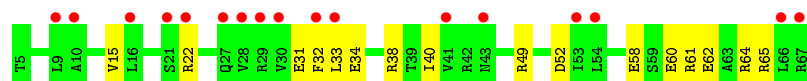
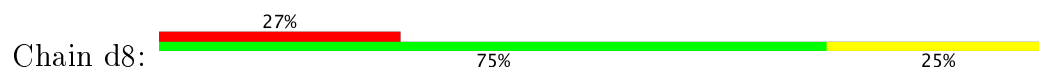
- Molecule 73: 40S ribosomal protein S27-A



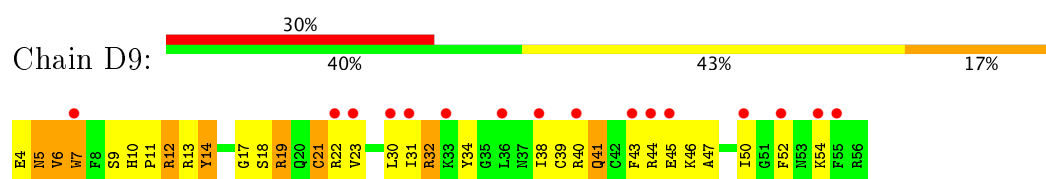
- Molecule 74: 40S ribosomal protein S28-A



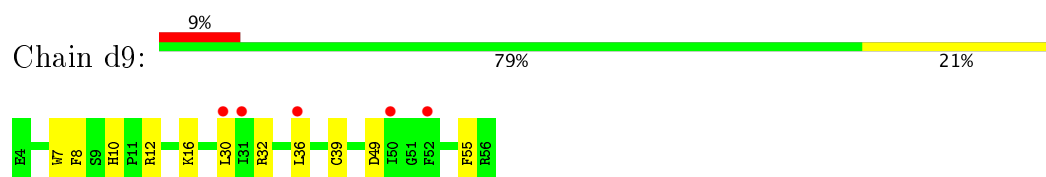
- Molecule 74: 40S ribosomal protein S28-A



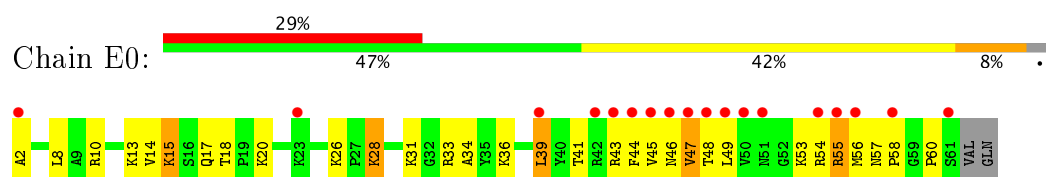
- Molecule 75: 40S ribosomal protein S29-A



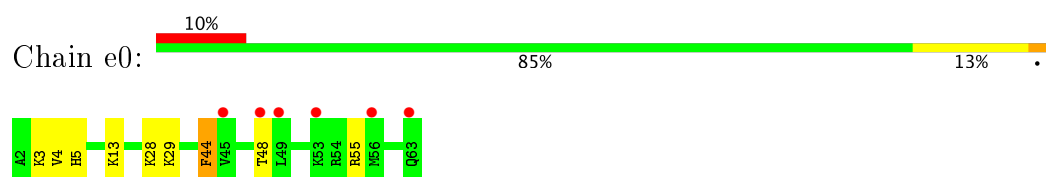
- Molecule 75: 40S ribosomal protein S29-A



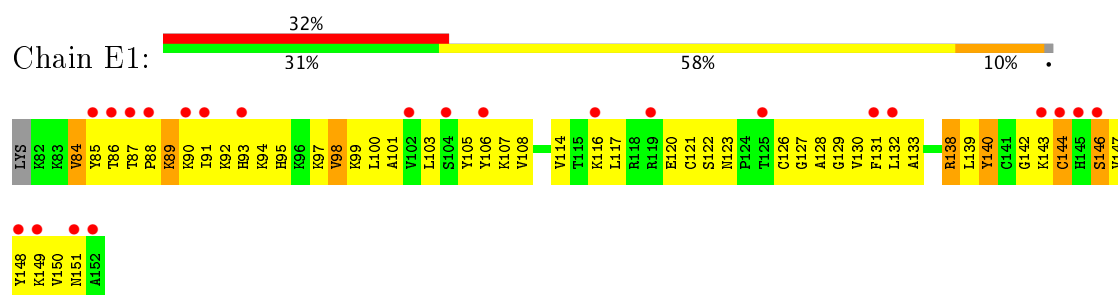
- Molecule 76: 40S ribosomal protein S30-A



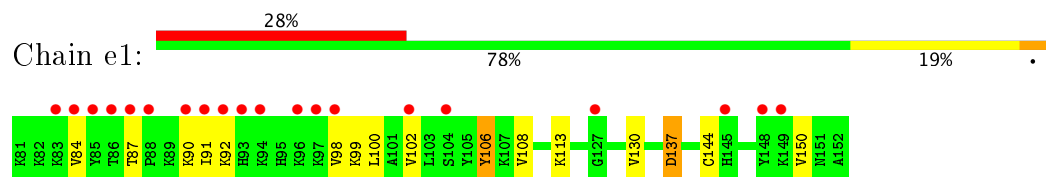
- Molecule 76: 40S ribosomal protein S30-A



- Molecule 77: Ubiquitin-40S ribosomal protein S31

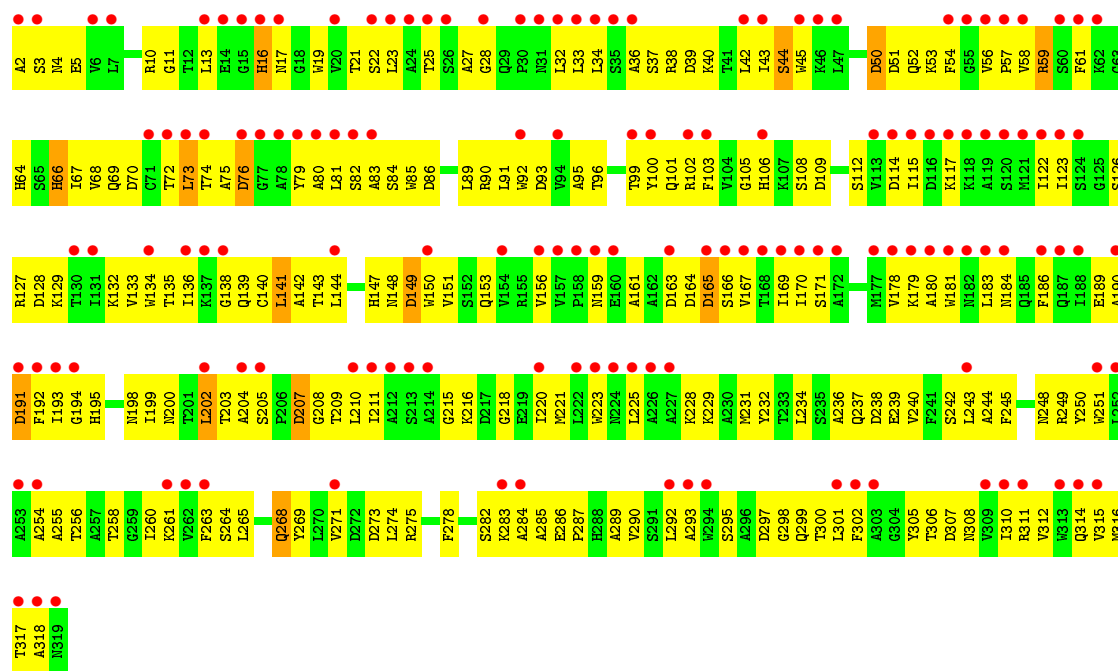


- Molecule 77: Ubiquitin-40S ribosomal protein S31

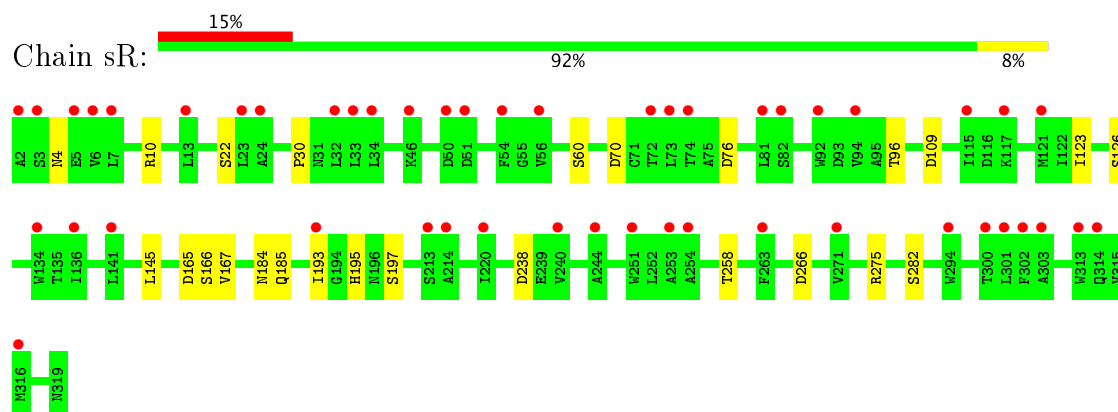


- Molecule 78: Guanine nucleotide-binding protein subunit beta-like protein

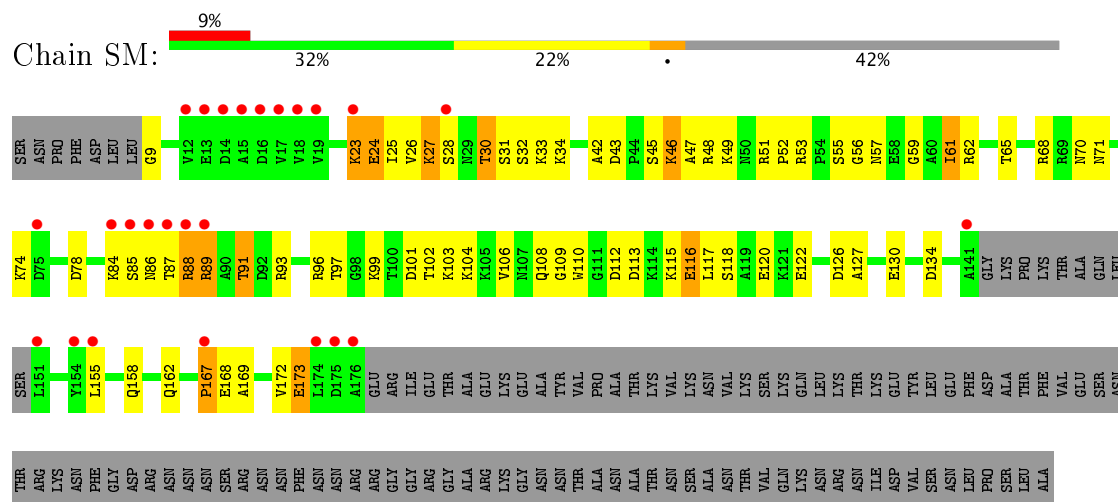




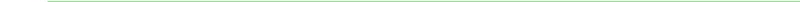
- Molecule 78: Guanine nucleotide-binding protein subunit beta-like protein



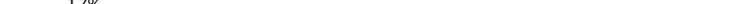
- Molecule 79: Suppressor protein STM1



[illegible]

Chain m2:  89%  9%

| Chain | Category | Value |
|----------|----------|-------|
| Chain m2 | x9 | 1 |
| | x10 | 1 |
| | x117 | 1 |
| | x153 | 1 |
| | x163 | 1 |
| | UNK | 1 |
| | UNK | 1 |
| | UNK | 1 |
| | UNK | 1 |
| | UNK | 1 |
| Chain m3 | x9 | 1 |
| | x10 | 1 |
| | x117 | 1 |
| | x153 | 1 |
| | x163 | 1 |
| | UNK | 1 |
| | UNK | 1 |
| | UNK | 1 |
| | UNK | 1 |
| | UNK | 1 |

Chain n4: 



Chain p0: 

Chain p1: 100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 436.63 Å 287.00 Å 304.73 Å 90.00° 99.08° 90.00° | Depositor |
| Resolution (Å) | 143.72 – 3.40 143.72 – 3.40 | Depositor EDS |
| % Data completeness (in resolution range) | 99.9 (143.72-3.40) 92.9 (143.72-3.40) | Depositor EDS |
| R_{merge} | 0.30 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.64 (at 3.41 Å) | Xtriage |
| Refinement program | PHENIX | Depositor |
| R, R_{free} | 0.189 , 0.238 0.188 , 0.237 | Depositor DCC |
| R_{free} test set | 18827 reflections (2.00%) | DCC |
| Wilson B-factor (Å ²) | 83.7 | Xtriage |
| Anisotropy | 0.132 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.30 , 85.8 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.93 | EDS |
| Total number of atoms | 404238 | wwPDB-VP |
| Average B, all atoms (Å ²) | 108.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% 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: ZN, MG, LLL

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 | 0.73 | 10/74216 (0.0%) | 1.29 | 499/115705 (0.4%) |
| 1 | 5 | 0.83 | 19/75037 (0.0%) | 1.37 | 668/116983 (0.6%) |
| 2 | 3 | 0.62 | 0/2883 | 1.14 | 5/4491 (0.1%) |
| 2 | 7 | 0.81 | 0/2883 | 1.33 | 18/4491 (0.4%) |
| 3 | 4 | 0.66 | 0/3701 | 1.20 | 14/5760 (0.2%) |
| 3 | 8 | 0.63 | 0/3746 | 1.18 | 14/5832 (0.2%) |
| 4 | L2 | 0.42 | 0/1948 | 0.66 | 0/2617 |
| 4 | l2 | 0.44 | 0/1946 | 0.71 | 0/2614 |
| 5 | L3 | 0.49 | 0/3152 | 0.67 | 1/4239 (0.0%) |
| 5 | l3 | 0.56 | 0/3152 | 0.71 | 1/4239 (0.0%) |
| 6 | L4 | 0.49 | 1/2801 (0.0%) | 0.72 | 3/3792 (0.1%) |
| 6 | l4 | 0.47 | 0/2801 | 0.68 | 1/3792 (0.0%) |
| 7 | L5 | 0.41 | 0/2425 | 0.60 | 0/3271 |
| 7 | l5 | 0.53 | 0/2408 | 0.67 | 1/3248 (0.0%) |
| 8 | L6 | 0.49 | 0/1260 | 0.63 | 0/1694 |
| 8 | l6 | 0.53 | 0/1269 | 0.67 | 0/1705 |
| 9 | L7 | 0.45 | 0/1821 | 0.64 | 0/2451 |
| 9 | l7 | 0.54 | 0/1828 | 0.69 | 1/2461 (0.0%) |
| 10 | L8 | 0.38 | 0/1849 | 0.55 | 0/2495 |
| 10 | l8 | 0.43 | 1/1795 (0.1%) | 0.61 | 0/2429 |
| 11 | L9 | 0.46 | 0/1539 | 0.64 | 0/2073 |
| 11 | l9 | 0.60 | 0/1539 | 0.68 | 0/2073 |
| 12 | M0 | 0.52 | 0/1743 | 0.64 | 0/2339 |
| 12 | m0 | 0.63 | 0/1752 | 0.76 | 2/2349 (0.1%) |
| 13 | M1 | 0.40 | 0/1374 | 0.63 | 2/1842 (0.1%) |
| 13 | m1 | 0.54 | 0/1374 | 0.69 | 1/1842 (0.1%) |
| 14 | M3 | 0.47 | 0/1568 | 0.67 | 0/2106 |
| 14 | m3 | 0.45 | 0/1573 | 0.66 | 0/2113 |
| 15 | M4 | 0.48 | 0/1068 | 0.60 | 0/1438 |
| 15 | m4 | 0.55 | 0/1074 | 0.67 | 0/1446 |
| 16 | M5 | 0.43 | 0/1757 | 0.63 | 0/2354 |
| 16 | m5 | 0.44 | 0/1757 | 0.63 | 0/2354 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | M6 | 0.58 | 1/1585 (0.1%) | 0.69 | 0/2128 |
| 17 | m6 | 0.67 | 0/1585 | 0.74 | 3/2128 (0.1%) |
| 18 | M7 | 0.49 | 0/1438 | 0.65 | 0/1937 |
| 18 | m7 | 0.51 | 0/1250 | 0.69 | 0/1683 |
| 19 | M8 | 0.45 | 0/1465 | 0.67 | 0/1965 |
| 19 | m8 | 0.49 | 0/1465 | 0.68 | 0/1965 |
| 20 | M9 | 0.36 | 0/1491 | 0.57 | 0/1987 |
| 20 | m9 | 0.39 | 0/1538 | 0.54 | 0/2050 |
| 21 | N0 | 0.44 | 0/1481 | 0.61 | 0/1990 |
| 21 | n0 | 0.58 | 0/1481 | 0.68 | 2/1990 (0.1%) |
| 22 | N1 | 0.48 | 0/1300 | 0.64 | 0/1743 |
| 22 | n1 | 0.59 | 0/1300 | 0.66 | 0/1743 |
| 23 | N2 | 0.34 | 0/812 | 0.53 | 0/1099 |
| 23 | n2 | 0.39 | 0/794 | 0.56 | 0/1076 |
| 24 | N3 | 0.51 | 0/1018 | 0.65 | 0/1369 |
| 24 | n3 | 0.59 | 0/1018 | 0.74 | 0/1369 |
| 25 | N4 | 0.40 | 0/712 | 0.58 | 0/958 |
| 26 | N5 | 0.39 | 0/979 | 0.60 | 1/1321 (0.1%) |
| 26 | n5 | 0.41 | 0/974 | 0.64 | 0/1314 |
| 27 | N6 | 0.45 | 0/1004 | 0.69 | 0/1341 |
| 27 | n6 | 0.41 | 0/1004 | 0.65 | 0/1341 |
| 28 | N7 | 0.37 | 0/1118 | 0.58 | 0/1497 |
| 28 | n7 | 0.38 | 0/1118 | 0.55 | 0/1497 |
| 29 | N8 | 0.47 | 0/1204 | 0.68 | 0/1612 |
| 29 | n8 | 0.50 | 0/1204 | 0.70 | 0/1612 |
| 30 | N9 | 0.50 | 0/473 | 0.68 | 0/629 |
| 30 | n9 | 0.54 | 0/473 | 0.74 | 0/629 |
| 31 | O0 | 0.34 | 0/751 | 0.56 | 1/1008 (0.1%) |
| 31 | o0 | 0.36 | 0/775 | 0.56 | 0/1040 |
| 32 | O1 | 0.43 | 0/904 | 0.60 | 0/1213 |
| 32 | o1 | 0.51 | 0/904 | 0.65 | 0/1213 |
| 33 | O2 | 0.53 | 0/1041 | 0.67 | 0/1394 |
| 33 | o2 | 0.49 | 0/1041 | 0.66 | 0/1394 |
| 34 | O3 | 0.55 | 0/868 | 0.66 | 0/1168 |
| 34 | o3 | 0.64 | 0/868 | 0.69 | 0/1168 |
| 35 | O4 | 0.39 | 0/891 | 0.57 | 1/1191 (0.1%) |
| 35 | o4 | 0.39 | 0/891 | 0.61 | 0/1191 |
| 36 | O5 | 0.43 | 0/978 | 0.62 | 0/1301 |
| 36 | o5 | 0.39 | 0/978 | 0.58 | 1/1301 (0.1%) |
| 37 | O6 | 0.41 | 0/778 | 0.66 | 0/1034 |
| 37 | o6 | 0.41 | 0/778 | 0.57 | 0/1034 |
| 38 | O7 | 0.46 | 0/696 | 0.72 | 0/923 |
| 38 | o7 | 0.50 | 0/696 | 0.71 | 0/923 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 39 | O8 | 0.35 | 0/618 | 0.55 | 0/826 |
| 39 | o8 | 0.36 | 0/618 | 0.60 | 0/826 |
| 40 | O9 | 0.49 | 0/443 | 0.66 | 0/588 |
| 40 | o9 | 0.48 | 0/443 | 0.67 | 0/588 |
| 41 | Q0 | 0.55 | 0/423 | 0.74 | 0/562 |
| 41 | q0 | 0.77 | 2/423 (0.5%) | 0.80 | 0/562 |
| 42 | Q1 | 0.42 | 0/234 | 0.57 | 0/300 |
| 42 | q1 | 0.56 | 0/234 | 0.77 | 0/300 |
| 43 | Q2 | 0.50 | 0/860 | 0.72 | 1/1136 (0.1%) |
| 43 | q2 | 0.59 | 0/860 | 0.74 | 0/1136 |
| 44 | Q3 | 0.40 | 0/701 | 0.61 | 0/934 |
| 44 | q3 | 0.47 | 0/701 | 0.65 | 0/934 |
| 45 | 2 | 0.50 | 0/40811 | 1.07 | 126/63585 (0.2%) |
| 45 | 6 | 0.66 | 4/41451 (0.0%) | 1.23 | 234/64581 (0.4%) |
| 46 | S0 | 0.35 | 1/1653 (0.1%) | 0.56 | 0/2261 |
| 46 | s0 | 0.37 | 0/1653 | 0.61 | 0/2261 |
| 47 | S1 | 0.33 | 0/1735 | 0.63 | 3/2335 (0.1%) |
| 47 | s1 | 0.37 | 0/1748 | 0.63 | 2/2352 (0.1%) |
| 48 | S2 | 0.37 | 0/1665 | 0.59 | 0/2263 |
| 48 | s2 | 0.41 | 0/1665 | 0.67 | 1/2263 (0.0%) |
| 49 | S3 | 0.34 | 0/1759 | 0.53 | 0/2368 |
| 49 | s3 | 0.40 | 0/1753 | 0.59 | 0/2361 |
| 50 | S4 | 0.36 | 0/2109 | 0.63 | 1/2839 (0.0%) |
| 50 | s4 | 0.39 | 0/2109 | 0.66 | 1/2839 (0.0%) |
| 51 | S5 | 0.59 | 1/1629 (0.1%) | 0.52 | 0/2202 |
| 51 | s5 | 0.42 | 0/1629 | 0.67 | 0/2202 |
| 52 | S6 | 0.37 | 0/1837 | 0.55 | 0/2455 |
| 52 | s6 | 0.40 | 0/1779 | 0.59 | 1/2379 (0.0%) |
| 53 | S7 | 0.34 | 0/1506 | 0.59 | 0/2028 |
| 53 | s7 | 0.36 | 0/1516 | 0.61 | 1/2043 (0.0%) |
| 54 | S8 | 0.36 | 0/1514 | 0.58 | 1/2021 (0.0%) |
| 54 | s8 | 0.40 | 0/1496 | 0.61 | 0/1999 |
| 55 | S9 | 0.34 | 0/1519 | 0.59 | 2/2035 (0.1%) |
| 55 | s9 | 0.38 | 0/1519 | 0.62 | 0/2035 |
| 56 | C0 | 0.34 | 0/789 | 0.62 | 1/1067 (0.1%) |
| 56 | c0 | 0.36 | 0/776 | 0.76 | 4/1047 (0.4%) |
| 57 | C1 | 0.38 | 0/1239 | 0.54 | 0/1673 |
| 57 | c1 | 0.43 | 0/1164 | 0.60 | 0/1569 |
| 58 | C2 | 0.31 | 0/898 | 0.66 | 1/1220 (0.1%) |
| 58 | c2 | 0.33 | 0/898 | 0.65 | 2/1220 (0.2%) |
| 59 | C3 | 0.33 | 0/1215 | 0.52 | 0/1638 |
| 59 | c3 | 0.41 | 0/1215 | 0.62 | 1/1638 (0.1%) |
| 60 | C4 | 0.30 | 0/901 | 0.60 | 0/1217 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 60 | c4 | 0.39 | 0/960 | 0.70 | 0/1290 |
| 61 | C5 | 0.37 | 0/998 | 0.59 | 0/1341 |
| 61 | c5 | 0.45 | 0/1060 | 0.69 | 1/1426 (0.1%) |
| 62 | C6 | 0.32 | 0/1125 | 0.57 | 1/1510 (0.1%) |
| 62 | c6 | 0.46 | 0/1131 | 0.63 | 0/1518 |
| 63 | C7 | 0.35 | 0/975 | 0.61 | 1/1307 (0.1%) |
| 63 | c7 | 0.38 | 0/925 | 0.63 | 0/1239 |
| 64 | C8 | 0.32 | 0/1211 | 0.54 | 0/1628 |
| 64 | c8 | 0.48 | 0/1211 | 0.67 | 1/1628 (0.1%) |
| 65 | C9 | 0.33 | 0/1130 | 0.54 | 1/1517 (0.1%) |
| 65 | c9 | 0.46 | 0/1130 | 0.60 | 0/1517 |
| 66 | D0 | 0.36 | 0/865 | 0.56 | 0/1169 |
| 66 | d0 | 0.43 | 0/892 | 0.65 | 0/1205 |
| 67 | D1 | 0.31 | 0/693 | 0.60 | 0/935 |
| 67 | d1 | 0.37 | 0/693 | 0.60 | 0/935 |
| 68 | D2 | 0.35 | 0/1038 | 0.61 | 0/1395 |
| 68 | d2 | 0.40 | 0/1038 | 0.64 | 1/1395 (0.1%) |
| 69 | D3 | 0.43 | 0/1139 | 0.63 | 1/1518 (0.1%) |
| 69 | d3 | 0.52 | 1/1139 (0.1%) | 0.68 | 0/1518 |
| 70 | D4 | 0.38 | 0/1087 | 0.57 | 0/1449 |
| 70 | d4 | 0.39 | 0/1079 | 0.60 | 0/1438 |
| 71 | D5 | 0.29 | 0/571 | 0.58 | 0/768 |
| 71 | d5 | 0.43 | 0/566 | 0.55 | 0/761 |
| 72 | D6 | 0.48 | 1/782 (0.1%) | 0.66 | 1/1047 (0.1%) |
| 72 | d6 | 0.52 | 0/782 | 0.72 | 0/1047 |
| 73 | D7 | 0.32 | 0/620 | 0.59 | 0/838 |
| 73 | d7 | 0.37 | 0/620 | 0.69 | 1/838 (0.1%) |
| 74 | D8 | 0.30 | 0/499 | 0.52 | 0/670 |
| 74 | d8 | 0.40 | 0/499 | 0.60 | 0/670 |
| 75 | D9 | 0.46 | 0/453 | 0.69 | 0/602 |
| 75 | d9 | 0.44 | 0/453 | 0.68 | 0/602 |
| 76 | E0 | 0.36 | 0/483 | 0.57 | 0/643 |
| 76 | e0 | 0.40 | 0/499 | 0.67 | 0/665 |
| 77 | E1 | 0.34 | 0/577 | 0.66 | 0/770 |
| 77 | e1 | 0.39 | 0/586 | 0.78 | 0/781 |
| 78 | SR | 0.30 | 0/2494 | 0.55 | 0/3394 |
| 78 | sR | 0.34 | 0/2494 | 0.59 | 0/3394 |
| 79 | SM | 0.34 | 0/1113 | 0.64 | 1/1502 (0.1%) |
| 79 | sM | 0.41 | 0/929 | 0.68 | 3/1246 (0.2%) |
| 81 | n4 | 0.42 | 0/1058 | 0.62 | 0/1405 |
| 82 | p0 | 0.36 | 0/1092 | 0.56 | 0/1474 |
| All | All | 0.61 | 42/426558 (0.0%) | 1.06 | 1636/625790 (0.3%) |

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 |
|-----|-------|---------------------|---------------------|
| 4 | L2 | 0 | 1 |
| 4 | l2 | 0 | 2 |
| 5 | l3 | 0 | 1 |
| 6 | L4 | 0 | 1 |
| 6 | l4 | 0 | 2 |
| 7 | L5 | 0 | 1 |
| 7 | l5 | 0 | 2 |
| 9 | L7 | 0 | 1 |
| 9 | l7 | 0 | 2 |
| 11 | L9 | 0 | 1 |
| 12 | M0 | 0 | 1 |
| 12 | m0 | 0 | 1 |
| 13 | M1 | 0 | 1 |
| 13 | m1 | 0 | 1 |
| 14 | M3 | 0 | 1 |
| 15 | M4 | 0 | 1 |
| 16 | m5 | 0 | 1 |
| 18 | M7 | 0 | 1 |
| 19 | M8 | 0 | 1 |
| 21 | N0 | 0 | 2 |
| 23 | n2 | 0 | 1 |
| 24 | n3 | 0 | 1 |
| 25 | N4 | 0 | 2 |
| 27 | N6 | 0 | 1 |
| 28 | N7 | 0 | 1 |
| 28 | n7 | 0 | 2 |
| 29 | N8 | 0 | 3 |
| 29 | n8 | 0 | 1 |
| 30 | N9 | 0 | 1 |
| 32 | o1 | 0 | 1 |
| 33 | o2 | 0 | 2 |
| 34 | o3 | 0 | 1 |
| 35 | o4 | 0 | 1 |
| 37 | o6 | 0 | 1 |
| 40 | O9 | 0 | 1 |
| 46 | s0 | 0 | 3 |
| 47 | S1 | 0 | 1 |
| 48 | S2 | 0 | 2 |
| 49 | s3 | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 50 | S4 | 0 | 3 |
| 51 | S5 | 0 | 1 |
| 51 | s5 | 0 | 2 |
| 52 | S6 | 0 | 1 |
| 52 | s6 | 0 | 1 |
| 53 | S7 | 0 | 5 |
| 53 | s7 | 0 | 3 |
| 54 | s8 | 0 | 2 |
| 55 | s9 | 0 | 2 |
| 58 | c2 | 0 | 1 |
| 59 | c3 | 0 | 1 |
| 60 | C4 | 0 | 2 |
| 60 | c4 | 0 | 4 |
| 61 | C5 | 0 | 2 |
| 61 | c5 | 0 | 2 |
| 62 | C6 | 0 | 1 |
| 63 | C7 | 0 | 2 |
| 63 | c7 | 0 | 2 |
| 64 | C8 | 0 | 1 |
| 66 | D0 | 0 | 2 |
| 66 | d0 | 0 | 5 |
| 67 | D1 | 0 | 1 |
| 68 | D2 | 0 | 1 |
| 68 | d2 | 0 | 1 |
| 69 | d3 | 0 | 1 |
| 70 | D4 | 0 | 1 |
| 70 | d4 | 0 | 2 |
| 71 | D5 | 0 | 3 |
| 71 | d5 | 0 | 1 |
| 72 | D6 | 0 | 2 |
| 72 | d6 | 0 | 1 |
| 73 | D7 | 0 | 1 |
| 76 | e0 | 0 | 1 |
| 77 | E1 | 0 | 3 |
| 77 | e1 | 0 | 2 |
| 78 | sR | 0 | 4 |
| 79 | SM | 0 | 2 |
| 79 | sM | 0 | 2 |
| 80 | m2 | 0 | 3 |
| 82 | p0 | 0 | 1 |
| All | All | 0 | 130 |

The worst 5 of 42 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 51 | S5 | 21 | THR | C-N | 20.19 | 1.72 | 1.34 |
| 1 | 5 | 2971 | A | N9-C4 | 12.79 | 1.45 | 1.37 |
| 1 | 5 | 1152 | G | N9-C4 | -9.61 | 1.30 | 1.38 |
| 6 | L4 | 19 | ALA | C-N | 8.69 | 1.54 | 1.34 |
| 72 | D6 | 59 | TYR | C-N | 8.53 | 1.50 | 1.34 |

The worst 5 of 1636 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | 5 | 1152 | G | N3-C4-N9 | -18.77 | 114.74 | 126.00 |
| 1 | 5 | 1152 | G | N3-C4-C5 | 17.59 | 137.39 | 128.60 |
| 1 | 1 | 1201 | C | C6-N1-C2 | -14.35 | 114.56 | 120.30 |
| 6 | L4 | 182 | LEU | CA-CB-CG | 12.68 | 144.47 | 115.30 |
| 1 | 5 | 420 | G | C5-C6-O6 | -12.32 | 121.21 | 128.60 |

There are no chirality outliers.

5 of 130 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 4 | L2 | 48 | ILE | Peptide |
| 6 | L4 | 318 | LEU | Peptide |
| 7 | L5 | 251 | PRO | Peptide |
| 9 | L7 | 29 | GLU | Peptide |
| 11 | L9 | 21 | LYS | Peptide |

5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 1 | 66304 | 0 | 33321 | 1403 | 0 |
| 1 | 5 | 67039 | 0 | 33693 | 1455 | 0 |
| 2 | 3 | 2579 | 0 | 1304 | 53 | 0 |
| 2 | 7 | 2579 | 0 | 1304 | 78 | 0 |
| 3 | 4 | 3313 | 0 | 1676 | 58 | 0 |
| 3 | 8 | 3353 | 0 | 1695 | 89 | 0 |
| 4 | L2 | 1914 | 0 | 1981 | 181 | 0 |
| 4 | 12 | 1912 | 0 | 1976 | 0 | 0 |
| 5 | L3 | 3081 | 0 | 3165 | 231 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5 | l3 | 3081 | 0 | 3165 | 0 | 0 |
| 6 | L4 | 2749 | 0 | 2863 | 255 | 0 |
| 6 | l4 | 2749 | 0 | 2863 | 0 | 0 |
| 7 | L5 | 2375 | 0 | 2325 | 184 | 0 |
| 7 | l5 | 2359 | 0 | 2311 | 0 | 0 |
| 8 | L6 | 1239 | 0 | 1326 | 101 | 0 |
| 8 | l6 | 1248 | 0 | 1339 | 0 | 0 |
| 9 | L7 | 1784 | 0 | 1862 | 129 | 0 |
| 9 | l7 | 1791 | 0 | 1869 | 0 | 0 |
| 10 | L8 | 1817 | 0 | 1908 | 148 | 0 |
| 10 | l8 | 1763 | 0 | 1818 | 0 | 0 |
| 11 | L9 | 1518 | 0 | 1587 | 153 | 0 |
| 11 | l9 | 1518 | 0 | 1587 | 0 | 0 |
| 12 | M0 | 1707 | 0 | 1731 | 144 | 0 |
| 12 | m0 | 1716 | 0 | 1757 | 0 | 0 |
| 13 | M1 | 1353 | 0 | 1383 | 104 | 0 |
| 13 | m1 | 1353 | 0 | 1383 | 0 | 0 |
| 14 | M3 | 1543 | 0 | 1608 | 153 | 0 |
| 14 | m3 | 1548 | 0 | 1613 | 0 | 0 |
| 15 | M4 | 1053 | 0 | 1149 | 90 | 0 |
| 15 | m4 | 1059 | 0 | 1154 | 0 | 0 |
| 16 | M5 | 1720 | 0 | 1779 | 161 | 0 |
| 16 | m5 | 1720 | 0 | 1779 | 0 | 0 |
| 17 | M6 | 1555 | 0 | 1659 | 101 | 0 |
| 17 | m6 | 1555 | 0 | 1659 | 0 | 0 |
| 18 | M7 | 1415 | 0 | 1421 | 109 | 0 |
| 18 | m7 | 1227 | 0 | 1236 | 0 | 0 |
| 19 | M8 | 1441 | 0 | 1543 | 129 | 0 |
| 19 | m8 | 1441 | 0 | 1543 | 0 | 0 |
| 20 | M9 | 1474 | 0 | 1567 | 101 | 0 |
| 20 | m9 | 1521 | 0 | 1617 | 0 | 0 |
| 21 | N0 | 1445 | 0 | 1487 | 99 | 0 |
| 21 | n0 | 1445 | 0 | 1487 | 0 | 0 |
| 22 | N1 | 1276 | 0 | 1323 | 133 | 0 |
| 22 | n1 | 1276 | 0 | 1323 | 0 | 0 |
| 23 | N2 | 796 | 0 | 812 | 56 | 0 |
| 23 | n2 | 778 | 0 | 791 | 0 | 0 |
| 24 | N3 | 1003 | 0 | 1048 | 78 | 0 |
| 24 | n3 | 1003 | 0 | 1048 | 0 | 0 |
| 25 | N4 | 699 | 0 | 640 | 35 | 0 |
| 26 | N5 | 964 | 0 | 1025 | 83 | 0 |
| 26 | n5 | 959 | 0 | 1023 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 27 | N6 | 993 | 0 | 1081 | 84 | 0 |
| 27 | n6 | 993 | 0 | 1081 | 0 | 0 |
| 28 | N7 | 1092 | 0 | 1155 | 105 | 0 |
| 28 | n7 | 1092 | 0 | 1155 | 0 | 0 |
| 29 | N8 | 1173 | 0 | 1215 | 117 | 0 |
| 29 | n8 | 1173 | 0 | 1215 | 0 | 0 |
| 30 | N9 | 462 | 0 | 491 | 35 | 0 |
| 30 | n9 | 462 | 0 | 491 | 0 | 0 |
| 31 | O0 | 743 | 0 | 797 | 58 | 0 |
| 31 | o0 | 767 | 0 | 816 | 0 | 0 |
| 32 | O1 | 890 | 0 | 938 | 59 | 0 |
| 32 | o1 | 890 | 0 | 938 | 0 | 0 |
| 33 | O2 | 1020 | 0 | 1090 | 78 | 0 |
| 33 | o2 | 1020 | 0 | 1090 | 0 | 0 |
| 34 | O3 | 850 | 0 | 880 | 53 | 0 |
| 34 | o3 | 850 | 0 | 880 | 0 | 0 |
| 35 | O4 | 881 | 0 | 947 | 76 | 0 |
| 35 | o4 | 881 | 0 | 947 | 0 | 0 |
| 36 | O5 | 969 | 0 | 1078 | 98 | 0 |
| 36 | o5 | 969 | 0 | 1078 | 0 | 0 |
| 37 | O6 | 771 | 0 | 849 | 73 | 0 |
| 37 | o6 | 771 | 0 | 849 | 0 | 0 |
| 38 | O7 | 681 | 0 | 683 | 68 | 0 |
| 38 | o7 | 681 | 0 | 684 | 0 | 0 |
| 39 | O8 | 612 | 0 | 682 | 40 | 0 |
| 39 | o8 | 612 | 0 | 682 | 0 | 0 |
| 40 | O9 | 436 | 0 | 475 | 55 | 0 |
| 40 | o9 | 436 | 0 | 475 | 0 | 0 |
| 41 | Q0 | 417 | 0 | 456 | 32 | 0 |
| 41 | q0 | 417 | 0 | 455 | 0 | 0 |
| 42 | Q1 | 233 | 0 | 284 | 16 | 0 |
| 42 | q1 | 233 | 0 | 284 | 0 | 0 |
| 43 | Q2 | 847 | 0 | 915 | 64 | 0 |
| 43 | q2 | 847 | 0 | 914 | 0 | 0 |
| 44 | Q3 | 694 | 0 | 734 | 61 | 0 |
| 44 | q3 | 694 | 0 | 734 | 0 | 0 |
| 45 | 2 | 36488 | 0 | 18357 | 1002 | 1 |
| 45 | 6 | 37060 | 0 | 18648 | 922 | 0 |
| 46 | S0 | 1612 | 0 | 1623 | 180 | 0 |
| 46 | s0 | 1612 | 0 | 1623 | 0 | 0 |
| 47 | S1 | 1709 | 0 | 1784 | 210 | 0 |
| 47 | s1 | 1722 | 0 | 1793 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 48 | S2 | 1635 | 0 | 1723 | 151 | 0 |
| 48 | s2 | 1635 | 0 | 1723 | 0 | 0 |
| 49 | S3 | 1734 | 0 | 1817 | 150 | 0 |
| 49 | s3 | 1728 | 0 | 1806 | 0 | 0 |
| 50 | S4 | 2068 | 0 | 2154 | 184 | 0 |
| 50 | s4 | 2068 | 0 | 2154 | 0 | 0 |
| 51 | S5 | 1609 | 0 | 1675 | 191 | 0 |
| 51 | s5 | 1609 | 0 | 1675 | 0 | 0 |
| 52 | S6 | 1813 | 0 | 1905 | 141 | 0 |
| 52 | s6 | 1755 | 0 | 1846 | 0 | 0 |
| 53 | S7 | 1481 | 0 | 1572 | 131 | 0 |
| 53 | s7 | 1491 | 0 | 1578 | 0 | 0 |
| 54 | S8 | 1489 | 0 | 1525 | 146 | 0 |
| 54 | s8 | 1471 | 0 | 1499 | 0 | 0 |
| 55 | S9 | 1494 | 0 | 1573 | 163 | 0 |
| 55 | s9 | 1494 | 0 | 1573 | 0 | 0 |
| 56 | C0 | 772 | 0 | 727 | 70 | 0 |
| 56 | c0 | 761 | 0 | 697 | 0 | 0 |
| 57 | C1 | 1213 | 0 | 1257 | 105 | 0 |
| 57 | c1 | 1138 | 0 | 1204 | 0 | 0 |
| 58 | C2 | 890 | 0 | 887 | 82 | 0 |
| 58 | c2 | 890 | 0 | 887 | 0 | 0 |
| 59 | C3 | 1192 | 0 | 1255 | 85 | 0 |
| 59 | c3 | 1192 | 0 | 1255 | 0 | 0 |
| 60 | C4 | 891 | 0 | 883 | 84 | 0 |
| 60 | c4 | 949 | 0 | 985 | 0 | 0 |
| 61 | C5 | 977 | 0 | 1002 | 95 | 0 |
| 61 | c5 | 1039 | 0 | 1050 | 0 | 0 |
| 62 | C6 | 1105 | 0 | 1166 | 116 | 0 |
| 62 | c6 | 1111 | 0 | 1171 | 0 | 0 |
| 63 | C7 | 965 | 0 | 1027 | 115 | 0 |
| 63 | c7 | 917 | 0 | 932 | 0 | 0 |
| 64 | C8 | 1192 | 0 | 1222 | 132 | 0 |
| 64 | c8 | 1192 | 0 | 1222 | 0 | 0 |
| 65 | C9 | 1112 | 0 | 1124 | 98 | 0 |
| 65 | c9 | 1112 | 0 | 1124 | 0 | 0 |
| 66 | D0 | 855 | 0 | 917 | 100 | 0 |
| 66 | d0 | 882 | 0 | 939 | 0 | 1 |
| 67 | D1 | 684 | 0 | 672 | 70 | 0 |
| 67 | d1 | 684 | 0 | 672 | 0 | 0 |
| 68 | D2 | 1021 | 0 | 1060 | 102 | 0 |
| 68 | d2 | 1021 | 0 | 1060 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 69 | D3 | 1121 | 0 | 1196 | 98 | 0 |
| 69 | d3 | 1121 | 0 | 1196 | 0 | 0 |
| 70 | D4 | 1073 | 0 | 1132 | 88 | 0 |
| 70 | d4 | 1065 | 0 | 1128 | 0 | 0 |
| 71 | D5 | 563 | 0 | 603 | 78 | 0 |
| 71 | d5 | 558 | 0 | 598 | 0 | 0 |
| 72 | D6 | 769 | 0 | 815 | 110 | 0 |
| 72 | d6 | 769 | 0 | 814 | 0 | 0 |
| 73 | D7 | 610 | 0 | 633 | 55 | 0 |
| 73 | d7 | 610 | 0 | 633 | 0 | 0 |
| 74 | D8 | 497 | 0 | 535 | 59 | 0 |
| 74 | d8 | 497 | 0 | 535 | 0 | 0 |
| 75 | D9 | 443 | 0 | 433 | 55 | 0 |
| 75 | d9 | 443 | 0 | 431 | 0 | 0 |
| 76 | E0 | 475 | 0 | 525 | 53 | 0 |
| 76 | e0 | 491 | 0 | 542 | 0 | 0 |
| 77 | E1 | 566 | 0 | 604 | 60 | 0 |
| 77 | e1 | 575 | 0 | 617 | 0 | 0 |
| 78 | SR | 2441 | 0 | 2393 | 195 | 0 |
| 78 | sR | 2441 | 0 | 2393 | 0 | 0 |
| 79 | SM | 1104 | 0 | 996 | 93 | 0 |
| 79 | sM | 923 | 0 | 868 | 0 | 0 |
| 80 | m2 | 750 | 0 | 167 | 0 | 0 |
| 81 | n4 | 1044 | 0 | 1082 | 0 | 0 |
| 82 | p0 | 1077 | 0 | 1041 | 0 | 0 |
| 83 | p1 | 235 | 0 | 51 | 0 | 0 |
| 84 | 1 | 588 | 0 | 0 | 0 | 0 |
| 84 | 2 | 142 | 0 | 0 | 0 | 0 |
| 84 | 3 | 19 | 0 | 0 | 0 | 0 |
| 84 | 4 | 23 | 0 | 0 | 0 | 0 |
| 84 | 5 | 750 | 0 | 0 | 0 | 0 |
| 84 | 6 | 263 | 0 | 0 | 0 | 0 |
| 84 | 7 | 30 | 0 | 0 | 0 | 0 |
| 84 | 8 | 20 | 0 | 0 | 0 | 0 |
| 84 | C1 | 1 | 0 | 0 | 0 | 0 |
| 84 | C3 | 1 | 0 | 0 | 0 | 0 |
| 84 | C8 | 1 | 0 | 0 | 0 | 0 |
| 84 | D3 | 5 | 0 | 0 | 0 | 0 |
| 84 | L2 | 5 | 0 | 0 | 0 | 0 |
| 84 | L3 | 3 | 0 | 0 | 0 | 0 |
| 84 | L4 | 6 | 0 | 0 | 0 | 0 |
| 84 | L5 | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 84 | L7 | 1 | 0 | 0 | 0 | 0 |
| 84 | L8 | 1 | 0 | 0 | 0 | 0 |
| 84 | L9 | 1 | 0 | 0 | 0 | 0 |
| 84 | M0 | 4 | 0 | 0 | 0 | 0 |
| 84 | M3 | 5 | 0 | 0 | 0 | 0 |
| 84 | M5 | 5 | 0 | 0 | 0 | 0 |
| 84 | M6 | 1 | 0 | 0 | 0 | 0 |
| 84 | M7 | 5 | 0 | 0 | 0 | 0 |
| 84 | M8 | 1 | 0 | 0 | 0 | 0 |
| 84 | N0 | 4 | 0 | 0 | 0 | 0 |
| 84 | N1 | 2 | 0 | 0 | 0 | 0 |
| 84 | N3 | 4 | 0 | 0 | 0 | 0 |
| 84 | N4 | 1 | 0 | 0 | 0 | 0 |
| 84 | N5 | 1 | 0 | 0 | 0 | 0 |
| 84 | N8 | 3 | 0 | 0 | 0 | 0 |
| 84 | O2 | 4 | 0 | 0 | 0 | 0 |
| 84 | O3 | 1 | 0 | 0 | 0 | 0 |
| 84 | O4 | 3 | 0 | 0 | 0 | 0 |
| 84 | O6 | 1 | 0 | 0 | 0 | 0 |
| 84 | O7 | 3 | 0 | 0 | 0 | 0 |
| 84 | Q1 | 1 | 0 | 0 | 0 | 0 |
| 84 | Q2 | 4 | 0 | 0 | 0 | 0 |
| 84 | S1 | 1 | 0 | 0 | 0 | 0 |
| 84 | S2 | 1 | 0 | 0 | 0 | 0 |
| 84 | S3 | 1 | 0 | 0 | 0 | 0 |
| 84 | S4 | 1 | 0 | 0 | 0 | 0 |
| 84 | c1 | 1 | 0 | 0 | 0 | 0 |
| 84 | c3 | 6 | 0 | 0 | 0 | 0 |
| 84 | c4 | 1 | 0 | 0 | 0 | 0 |
| 84 | c8 | 3 | 0 | 0 | 0 | 0 |
| 84 | d1 | 2 | 0 | 0 | 0 | 0 |
| 84 | d2 | 1 | 0 | 0 | 0 | 0 |
| 84 | d3 | 5 | 0 | 0 | 0 | 0 |
| 84 | d5 | 1 | 0 | 0 | 0 | 0 |
| 84 | d6 | 3 | 0 | 0 | 0 | 0 |
| 84 | d7 | 1 | 0 | 0 | 0 | 0 |
| 84 | d9 | 1 | 0 | 0 | 0 | 0 |
| 84 | l2 | 5 | 0 | 0 | 0 | 0 |
| 84 | l3 | 11 | 0 | 0 | 0 | 0 |
| 84 | l4 | 2 | 0 | 0 | 0 | 0 |
| 84 | l5 | 6 | 0 | 0 | 0 | 0 |
| 84 | l6 | 2 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 84 | l7 | 3 | 0 | 0 | 0 | 0 |
| 84 | l8 | 1 | 0 | 0 | 0 | 0 |
| 84 | l9 | 8 | 0 | 0 | 0 | 0 |
| 84 | m0 | 2 | 0 | 0 | 0 | 0 |
| 84 | m3 | 4 | 0 | 0 | 0 | 0 |
| 84 | m4 | 6 | 0 | 0 | 0 | 0 |
| 84 | m5 | 3 | 0 | 0 | 0 | 0 |
| 84 | m6 | 8 | 0 | 0 | 0 | 0 |
| 84 | m7 | 7 | 0 | 0 | 0 | 0 |
| 84 | m8 | 4 | 0 | 0 | 0 | 0 |
| 84 | m9 | 2 | 0 | 0 | 0 | 0 |
| 84 | n0 | 7 | 0 | 0 | 0 | 0 |
| 84 | n1 | 2 | 0 | 0 | 0 | 0 |
| 84 | n3 | 2 | 0 | 0 | 0 | 0 |
| 84 | n5 | 3 | 0 | 0 | 0 | 0 |
| 84 | n8 | 3 | 0 | 0 | 0 | 0 |
| 84 | n9 | 1 | 0 | 0 | 0 | 0 |
| 84 | o1 | 1 | 0 | 0 | 0 | 0 |
| 84 | o2 | 3 | 0 | 0 | 0 | 0 |
| 84 | o3 | 2 | 0 | 0 | 0 | 0 |
| 84 | o4 | 2 | 0 | 0 | 0 | 0 |
| 84 | q0 | 1 | 0 | 0 | 0 | 0 |
| 84 | q1 | 2 | 0 | 0 | 0 | 0 |
| 84 | q2 | 7 | 0 | 0 | 0 | 0 |
| 84 | q3 | 3 | 0 | 0 | 0 | 0 |
| 84 | s0 | 1 | 0 | 0 | 0 | 0 |
| 84 | s2 | 2 | 0 | 0 | 0 | 0 |
| 84 | s3 | 1 | 0 | 0 | 0 | 0 |
| 84 | s4 | 1 | 0 | 0 | 0 | 0 |
| 84 | s5 | 3 | 0 | 0 | 0 | 0 |
| 84 | s6 | 1 | 0 | 0 | 0 | 0 |
| 84 | sR | 1 | 0 | 0 | 0 | 0 |
| 85 | 1 | 496 | 0 | 624 | 28 | 0 |
| 85 | 2 | 93 | 0 | 117 | 9 | 0 |
| 85 | 3 | 31 | 0 | 39 | 2 | 0 |
| 85 | 4 | 31 | 0 | 39 | 9 | 0 |
| 85 | 5 | 868 | 0 | 1092 | 53 | 0 |
| 85 | 6 | 403 | 0 | 507 | 27 | 0 |
| 85 | 7 | 93 | 0 | 117 | 11 | 0 |
| 85 | 8 | 62 | 0 | 78 | 16 | 0 |
| 85 | L3 | 31 | 0 | 39 | 2 | 0 |
| 85 | l3 | 31 | 0 | 39 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 86 | D6 | 1 | 0 | 0 | 0 | 0 |
| 86 | D7 | 1 | 0 | 0 | 0 | 0 |
| 86 | D9 | 1 | 0 | 0 | 0 | 0 |
| 86 | E1 | 1 | 0 | 0 | 0 | 0 |
| 86 | O4 | 1 | 0 | 0 | 0 | 0 |
| 86 | O7 | 1 | 0 | 0 | 0 | 0 |
| 86 | Q0 | 1 | 0 | 0 | 0 | 0 |
| 86 | Q2 | 1 | 0 | 0 | 0 | 0 |
| 86 | Q3 | 1 | 0 | 0 | 0 | 0 |
| 86 | d6 | 1 | 0 | 0 | 0 | 0 |
| 86 | d7 | 1 | 0 | 0 | 0 | 0 |
| 86 | d9 | 1 | 0 | 0 | 0 | 0 |
| 86 | e1 | 1 | 0 | 0 | 0 | 0 |
| 86 | o4 | 1 | 0 | 0 | 0 | 0 |
| 86 | o7 | 1 | 0 | 0 | 0 | 0 |
| 86 | q0 | 1 | 0 | 0 | 0 | 0 |
| 86 | q2 | 1 | 0 | 0 | 0 | 0 |
| 86 | q3 | 1 | 0 | 0 | 0 | 0 |
| 87 | 1 | 473 | 0 | 0 | 38 | 0 |
| 87 | 2 | 111 | 0 | 0 | 2 | 0 |
| 87 | 3 | 15 | 0 | 0 | 0 | 0 |
| 87 | 4 | 5 | 0 | 0 | 0 | 0 |
| 87 | 5 | 514 | 0 | 0 | 34 | 0 |
| 87 | 6 | 224 | 0 | 0 | 8 | 0 |
| 87 | 7 | 33 | 0 | 0 | 2 | 0 |
| 87 | 8 | 11 | 0 | 0 | 1 | 0 |
| 87 | C9 | 2 | 0 | 0 | 0 | 0 |
| 87 | D0 | 1 | 0 | 0 | 0 | 0 |
| 87 | D3 | 1 | 0 | 0 | 0 | 0 |
| 87 | L2 | 1 | 0 | 0 | 0 | 0 |
| 87 | L3 | 7 | 0 | 0 | 2 | 0 |
| 87 | L4 | 2 | 0 | 0 | 0 | 0 |
| 87 | L5 | 2 | 0 | 0 | 1 | 0 |
| 87 | M0 | 1 | 0 | 0 | 1 | 0 |
| 87 | M3 | 2 | 0 | 0 | 0 | 0 |
| 87 | M5 | 3 | 0 | 0 | 0 | 0 |
| 87 | M6 | 6 | 0 | 0 | 0 | 0 |
| 87 | M7 | 5 | 0 | 0 | 1 | 0 |
| 87 | N0 | 4 | 0 | 0 | 1 | 0 |
| 87 | N1 | 3 | 0 | 0 | 1 | 0 |
| 87 | N3 | 5 | 0 | 0 | 3 | 0 |
| 87 | N4 | 2 | 0 | 0 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 87 | N5 | 2 | 0 | 0 | 1 | 0 |
| 87 | N8 | 3 | 0 | 0 | 0 | 0 |
| 87 | N9 | 2 | 0 | 0 | 0 | 0 |
| 87 | O2 | 2 | 0 | 0 | 0 | 0 |
| 87 | O4 | 1 | 0 | 0 | 0 | 0 |
| 87 | O7 | 1 | 0 | 0 | 0 | 0 |
| 87 | Q1 | 1 | 0 | 0 | 2 | 0 |
| 87 | Q2 | 1 | 0 | 0 | 0 | 0 |
| 87 | S1 | 1 | 0 | 0 | 0 | 0 |
| 87 | S3 | 3 | 0 | 0 | 0 | 0 |
| 87 | S4 | 1 | 0 | 0 | 0 | 0 |
| 87 | S8 | 1 | 0 | 0 | 0 | 0 |
| 87 | SR | 2 | 0 | 0 | 0 | 0 |
| 87 | c3 | 5 | 0 | 0 | 0 | 0 |
| 87 | c6 | 1 | 0 | 0 | 0 | 0 |
| 87 | c8 | 3 | 0 | 0 | 0 | 0 |
| 87 | c9 | 5 | 0 | 0 | 0 | 0 |
| 87 | d3 | 5 | 0 | 0 | 0 | 0 |
| 87 | d5 | 3 | 0 | 0 | 0 | 0 |
| 87 | d6 | 3 | 0 | 0 | 0 | 0 |
| 87 | d9 | 2 | 0 | 0 | 0 | 0 |
| 87 | e1 | 1 | 0 | 0 | 0 | 0 |
| 87 | l2 | 7 | 0 | 0 | 0 | 0 |
| 87 | l3 | 6 | 0 | 0 | 0 | 0 |
| 87 | l5 | 5 | 0 | 0 | 0 | 0 |
| 87 | l9 | 3 | 0 | 0 | 0 | 0 |
| 87 | m0 | 1 | 0 | 0 | 0 | 0 |
| 87 | m4 | 1 | 0 | 0 | 0 | 0 |
| 87 | m5 | 2 | 0 | 0 | 0 | 0 |
| 87 | m6 | 8 | 0 | 0 | 0 | 0 |
| 87 | m7 | 4 | 0 | 0 | 0 | 0 |
| 87 | m9 | 3 | 0 | 0 | 0 | 0 |
| 87 | n0 | 4 | 0 | 0 | 0 | 0 |
| 87 | n1 | 2 | 0 | 0 | 0 | 0 |
| 87 | n3 | 2 | 0 | 0 | 0 | 0 |
| 87 | n4 | 1 | 0 | 0 | 0 | 0 |
| 87 | n5 | 2 | 0 | 0 | 0 | 0 |
| 87 | n6 | 1 | 0 | 0 | 0 | 0 |
| 87 | n8 | 4 | 0 | 0 | 0 | 0 |
| 87 | n9 | 1 | 0 | 0 | 0 | 0 |
| 87 | o0 | 1 | 0 | 0 | 0 | 0 |
| 87 | o1 | 2 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 87 | o2 | 4 | 0 | 0 | 0 | 0 |
| 87 | o4 | 2 | 0 | 0 | 0 | 0 |
| 87 | q0 | 1 | 0 | 0 | 0 | 0 |
| 87 | q2 | 2 | 0 | 0 | 0 | 0 |
| 87 | q3 | 3 | 0 | 0 | 0 | 0 |
| 87 | s4 | 1 | 0 | 0 | 0 | 0 |
| 87 | s5 | 1 | 0 | 0 | 0 | 0 |
| 87 | s7 | 1 | 0 | 0 | 0 | 0 |
| 87 | sR | 1 | 0 | 0 | 0 | 0 |
| All | All | 404238 | 0 | 298719 | 11005 | 1 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

The worst 5 of 11005 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) |
|-----------------|--------------------|--------------------------|-------------------|
| 51:S5:21:THR:C | 51:S5:22:PRO:N | 1.72 | 1.42 |
| 45:2:1755:A:C2' | 45:2:1756:A:H5' | 1.74 | 1.17 |
| 45:2:1755:A:H2' | 45:2:1756:A:C5' | 1.76 | 1.16 |
| 54:S8:83:TYR:H | 54:S8:101:ILE:HG21 | 4.57 | 1.11 |
| 45:2:74:U:H1' | 45:2:75:U:H5' | 1.33 | 1.09 |

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

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-------------------------|--------------------------|-------------------|
| 45:2:1491:U:O2' | 66:d0:12:GLN:OE1[1_454] | 2.11 | 0.09 |

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 | L2 | 250/252 (99%) | 233 (93%) | 17 (7%) | 0 | 100 | 100 |
| 4 | l2 | 250/252 (99%) | 227 (91%) | 21 (8%) | 2 (1%) | 22 | 62 |
| 5 | L3 | 384/386 (100%) | 349 (91%) | 32 (8%) | 3 (1%) | 22 | 62 |
| 5 | l3 | 384/386 (100%) | 354 (92%) | 29 (8%) | 1 (0%) | 44 | 79 |
| 6 | L4 | 359/361 (99%) | 323 (90%) | 34 (10%) | 2 (1%) | 28 | 68 |
| 6 | l4 | 359/361 (99%) | 313 (87%) | 43 (12%) | 3 (1%) | 22 | 62 |
| 7 | L5 | 294/296 (99%) | 266 (90%) | 28 (10%) | 0 | 100 | 100 |
| 7 | l5 | 292/296 (99%) | 266 (91%) | 24 (8%) | 2 (1%) | 25 | 65 |
| 8 | L6 | 152/176 (86%) | 141 (93%) | 10 (7%) | 1 (1%) | 25 | 65 |
| 8 | l6 | 153/176 (87%) | 139 (91%) | 12 (8%) | 2 (1%) | 14 | 53 |
| 9 | L7 | 220/223 (99%) | 204 (93%) | 16 (7%) | 0 | 100 | 100 |
| 9 | l7 | 221/223 (99%) | 206 (93%) | 13 (6%) | 2 (1%) | 20 | 61 |
| 10 | L8 | 231/233 (99%) | 199 (86%) | 30 (13%) | 2 (1%) | 20 | 61 |
| 10 | l8 | 229/233 (98%) | 194 (85%) | 33 (14%) | 2 (1%) | 20 | 61 |
| 11 | L9 | 189/191 (99%) | 169 (89%) | 20 (11%) | 0 | 100 | 100 |
| 11 | l9 | 189/191 (99%) | 176 (93%) | 11 (6%) | 2 (1%) | 17 | 57 |
| 12 | M0 | 208/221 (94%) | 188 (90%) | 19 (9%) | 1 (0%) | 32 | 71 |
| 12 | m0 | 207/221 (94%) | 184 (89%) | 23 (11%) | 0 | 100 | 100 |
| 13 | M1 | 167/169 (99%) | 142 (85%) | 25 (15%) | 0 | 100 | 100 |
| 13 | m1 | 167/169 (99%) | 146 (87%) | 19 (11%) | 2 (1%) | 15 | 54 |
| 14 | M3 | 191/194 (98%) | 170 (89%) | 19 (10%) | 2 (1%) | 18 | 59 |
| 14 | m3 | 192/194 (99%) | 164 (85%) | 26 (14%) | 2 (1%) | 18 | 59 |
| 15 | M4 | 134/137 (98%) | 120 (90%) | 14 (10%) | 0 | 100 | 100 |
| 15 | m4 | 135/137 (98%) | 126 (93%) | 9 (7%) | 0 | 100 | 100 |
| 16 | M5 | 201/203 (99%) | 186 (92%) | 15 (8%) | 0 | 100 | 100 |
| 16 | m5 | 201/203 (99%) | 186 (92%) | 15 (8%) | 0 | 100 | 100 |
| 17 | M6 | 195/197 (99%) | 187 (96%) | 7 (4%) | 1 (0%) | 32 | 71 |
| 17 | m6 | 195/197 (99%) | 190 (97%) | 5 (3%) | 0 | 100 | 100 |
| 18 | M7 | 181/184 (98%) | 169 (93%) | 12 (7%) | 0 | 100 | 100 |
| 18 | m7 | 153/184 (83%) | 140 (92%) | 13 (8%) | 0 | 100 | 100 |
| 19 | M8 | 183/185 (99%) | 174 (95%) | 9 (5%) | 0 | 100 | 100 |
| 19 | m8 | 183/185 (99%) | 167 (91%) | 14 (8%) | 2 (1%) | 17 | 57 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 20 | M9 | 180/188 (96%) | 169 (94%) | 11 (6%) | 0 | 100 | 100 |
| 20 | m9 | 186/188 (99%) | 171 (92%) | 15 (8%) | 0 | 100 | 100 |
| 21 | N0 | 170/172 (99%) | 157 (92%) | 13 (8%) | 0 | 100 | 100 |
| 21 | n0 | 170/172 (99%) | 161 (95%) | 9 (5%) | 0 | 100 | 100 |
| 22 | N1 | 157/159 (99%) | 148 (94%) | 6 (4%) | 3 (2%) | 9 | 45 |
| 22 | n1 | 157/159 (99%) | 150 (96%) | 7 (4%) | 0 | 100 | 100 |
| 23 | N2 | 98/100 (98%) | 89 (91%) | 8 (8%) | 1 (1%) | 18 | 59 |
| 23 | n2 | 96/100 (96%) | 84 (88%) | 12 (12%) | 0 | 100 | 100 |
| 24 | N3 | 134/136 (98%) | 130 (97%) | 4 (3%) | 0 | 100 | 100 |
| 24 | n3 | 134/136 (98%) | 130 (97%) | 4 (3%) | 0 | 100 | 100 |
| 25 | N4 | 96/155 (62%) | 83 (86%) | 12 (12%) | 1 (1%) | 18 | 59 |
| 26 | N5 | 119/121 (98%) | 107 (90%) | 12 (10%) | 0 | 100 | 100 |
| 26 | n5 | 118/121 (98%) | 108 (92%) | 10 (8%) | 0 | 100 | 100 |
| 27 | N6 | 124/126 (98%) | 119 (96%) | 5 (4%) | 0 | 100 | 100 |
| 27 | n6 | 124/126 (98%) | 117 (94%) | 5 (4%) | 2 (2%) | 11 | 48 |
| 28 | N7 | 133/135 (98%) | 114 (86%) | 19 (14%) | 0 | 100 | 100 |
| 28 | n7 | 133/135 (98%) | 116 (87%) | 16 (12%) | 1 (1%) | 22 | 62 |
| 29 | N8 | 146/148 (99%) | 126 (86%) | 19 (13%) | 1 (1%) | 25 | 65 |
| 29 | n8 | 146/148 (99%) | 132 (90%) | 13 (9%) | 1 (1%) | 25 | 65 |
| 30 | N9 | 56/58 (97%) | 51 (91%) | 4 (7%) | 1 (2%) | 10 | 46 |
| 30 | n9 | 56/58 (97%) | 49 (88%) | 5 (9%) | 2 (4%) | 4 | 31 |
| 31 | O0 | 95/100 (95%) | 89 (94%) | 5 (5%) | 1 (1%) | 17 | 57 |
| 31 | o0 | 98/100 (98%) | 89 (91%) | 9 (9%) | 0 | 100 | 100 |
| 32 | O1 | 107/109 (98%) | 94 (88%) | 13 (12%) | 0 | 100 | 100 |
| 32 | o1 | 107/109 (98%) | 96 (90%) | 10 (9%) | 1 (1%) | 20 | 61 |
| 33 | O2 | 125/127 (98%) | 117 (94%) | 8 (6%) | 0 | 100 | 100 |
| 33 | o2 | 125/127 (98%) | 111 (89%) | 14 (11%) | 0 | 100 | 100 |
| 34 | O3 | 104/106 (98%) | 97 (93%) | 7 (7%) | 0 | 100 | 100 |
| 34 | o3 | 104/106 (98%) | 99 (95%) | 5 (5%) | 0 | 100 | 100 |
| 35 | O4 | 110/112 (98%) | 100 (91%) | 10 (9%) | 0 | 100 | 100 |
| 35 | o4 | 110/112 (98%) | 99 (90%) | 10 (9%) | 1 (1%) | 20 | 61 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 36 | O5 | 117/119 (98%) | 104 (89%) | 13 (11%) | 0 | 100 | 100 |
| 36 | o5 | 117/119 (98%) | 105 (90%) | 12 (10%) | 0 | 100 | 100 |
| 37 | O6 | 97/99 (98%) | 80 (82%) | 15 (16%) | 2 (2%) | 8 | 43 |
| 37 | o6 | 97/99 (98%) | 86 (89%) | 11 (11%) | 0 | 100 | 100 |
| 38 | O7 | 85/87 (98%) | 77 (91%) | 8 (9%) | 0 | 100 | 100 |
| 38 | o7 | 85/87 (98%) | 77 (91%) | 8 (9%) | 0 | 100 | 100 |
| 39 | O8 | 75/77 (97%) | 69 (92%) | 6 (8%) | 0 | 100 | 100 |
| 39 | o8 | 75/77 (97%) | 71 (95%) | 4 (5%) | 0 | 100 | 100 |
| 40 | O9 | 48/50 (96%) | 43 (90%) | 5 (10%) | 0 | 100 | 100 |
| 40 | o9 | 48/50 (96%) | 46 (96%) | 2 (4%) | 0 | 100 | 100 |
| 41 | Q0 | 50/52 (96%) | 46 (92%) | 4 (8%) | 0 | 100 | 100 |
| 41 | q0 | 50/52 (96%) | 48 (96%) | 1 (2%) | 1 (2%) | 9 | 44 |
| 42 | Q1 | 23/25 (92%) | 22 (96%) | 1 (4%) | 0 | 100 | 100 |
| 42 | q1 | 23/25 (92%) | 20 (87%) | 3 (13%) | 0 | 100 | 100 |
| 43 | Q2 | 103/105 (98%) | 91 (88%) | 12 (12%) | 0 | 100 | 100 |
| 43 | q2 | 103/105 (98%) | 94 (91%) | 8 (8%) | 1 (1%) | 18 | 59 |
| 44 | Q3 | 89/91 (98%) | 77 (86%) | 12 (14%) | 0 | 100 | 100 |
| 44 | q3 | 89/91 (98%) | 81 (91%) | 8 (9%) | 0 | 100 | 100 |
| 46 | S0 | 204/206 (99%) | 176 (86%) | 27 (13%) | 1 (0%) | 32 | 71 |
| 46 | s0 | 204/206 (99%) | 170 (83%) | 30 (15%) | 4 (2%) | 9 | 44 |
| 47 | S1 | 212/216 (98%) | 175 (82%) | 35 (16%) | 2 (1%) | 20 | 61 |
| 47 | s1 | 214/216 (99%) | 188 (88%) | 25 (12%) | 1 (0%) | 32 | 71 |
| 48 | S2 | 215/217 (99%) | 189 (88%) | 25 (12%) | 1 (0%) | 32 | 71 |
| 48 | s2 | 215/217 (99%) | 196 (91%) | 18 (8%) | 1 (0%) | 32 | 71 |
| 49 | S3 | 221/223 (99%) | 201 (91%) | 19 (9%) | 1 (0%) | 32 | 71 |
| 49 | s3 | 221/223 (99%) | 194 (88%) | 25 (11%) | 2 (1%) | 20 | 61 |
| 50 | S4 | 258/260 (99%) | 230 (89%) | 27 (10%) | 1 (0%) | 38 | 75 |
| 50 | s4 | 258/260 (99%) | 225 (87%) | 32 (12%) | 1 (0%) | 38 | 75 |
| 51 | S5 | 204/206 (99%) | 175 (86%) | 26 (13%) | 3 (2%) | 12 | 49 |
| 51 | s5 | 204/206 (99%) | 182 (89%) | 21 (10%) | 1 (0%) | 32 | 71 |
| 52 | S6 | 224/236 (95%) | 207 (92%) | 17 (8%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 52 | s6 | 216/236 (92%) | 198 (92%) | 16 (7%) | 2 (1%) | 20 | 61 |
| 53 | S7 | 182/186 (98%) | 156 (86%) | 22 (12%) | 4 (2%) | 8 | 42 |
| 53 | s7 | 184/186 (99%) | 159 (86%) | 23 (12%) | 2 (1%) | 17 | 57 |
| 54 | S8 | 184/200 (92%) | 158 (86%) | 24 (13%) | 2 (1%) | 17 | 57 |
| 54 | s8 | 182/200 (91%) | 164 (90%) | 16 (9%) | 2 (1%) | 17 | 57 |
| 55 | S9 | 183/185 (99%) | 153 (84%) | 28 (15%) | 2 (1%) | 17 | 57 |
| 55 | s9 | 183/185 (99%) | 158 (86%) | 23 (13%) | 2 (1%) | 17 | 57 |
| 56 | C0 | 94/105 (90%) | 73 (78%) | 17 (18%) | 4 (4%) | 3 | 26 |
| 56 | c0 | 92/105 (88%) | 74 (80%) | 13 (14%) | 5 (5%) | 2 | 19 |
| 57 | C1 | 153/156 (98%) | 138 (90%) | 14 (9%) | 1 (1%) | 25 | 65 |
| 57 | c1 | 140/156 (90%) | 124 (89%) | 15 (11%) | 1 (1%) | 25 | 65 |
| 58 | C2 | 122/143 (85%) | 91 (75%) | 26 (21%) | 5 (4%) | 3 | 27 |
| 58 | c2 | 122/143 (85%) | 88 (72%) | 32 (26%) | 2 (2%) | 11 | 48 |
| 59 | C3 | 148/150 (99%) | 136 (92%) | 12 (8%) | 0 | 100 | 100 |
| 59 | c3 | 148/150 (99%) | 129 (87%) | 15 (10%) | 4 (3%) | 6 | 37 |
| 60 | C4 | 125/128 (98%) | 109 (87%) | 14 (11%) | 2 (2%) | 11 | 48 |
| 60 | c4 | 126/128 (98%) | 107 (85%) | 18 (14%) | 1 (1%) | 22 | 62 |
| 61 | C5 | 122/141 (86%) | 104 (85%) | 15 (12%) | 3 (2%) | 6 | 39 |
| 61 | c5 | 133/141 (94%) | 109 (82%) | 23 (17%) | 1 (1%) | 22 | 62 |
| 62 | C6 | 139/142 (98%) | 123 (88%) | 15 (11%) | 1 (1%) | 25 | 65 |
| 62 | c6 | 140/142 (99%) | 124 (89%) | 14 (10%) | 2 (1%) | 13 | 51 |
| 63 | C7 | 118/136 (87%) | 100 (85%) | 15 (13%) | 3 (2%) | 6 | 39 |
| 63 | c7 | 113/136 (83%) | 97 (86%) | 12 (11%) | 4 (4%) | 4 | 32 |
| 64 | C8 | 143/145 (99%) | 120 (84%) | 21 (15%) | 2 (1%) | 13 | 51 |
| 64 | c8 | 143/145 (99%) | 125 (87%) | 15 (10%) | 3 (2%) | 8 | 43 |
| 65 | C9 | 141/143 (99%) | 127 (90%) | 14 (10%) | 0 | 100 | 100 |
| 65 | c9 | 141/143 (99%) | 132 (94%) | 9 (6%) | 0 | 100 | 100 |
| 66 | D0 | 105/110 (96%) | 96 (91%) | 8 (8%) | 1 (1%) | 18 | 59 |
| 66 | d0 | 108/110 (98%) | 87 (81%) | 17 (16%) | 4 (4%) | 4 | 30 |
| 67 | D1 | 85/87 (98%) | 73 (86%) | 11 (13%) | 1 (1%) | 15 | 54 |
| 67 | d1 | 85/87 (98%) | 72 (85%) | 12 (14%) | 1 (1%) | 15 | 54 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|------------|----------|-------------|-----|
| 68 | D2 | 127/129 (98%) | 114 (90%) | 11 (9%) | 2 (2%) | 11 | 48 |
| 68 | d2 | 127/129 (98%) | 113 (89%) | 13 (10%) | 1 (1%) | 22 | 62 |
| 69 | D3 | 142/144 (99%) | 119 (84%) | 23 (16%) | 0 | 100 | 100 |
| 69 | d3 | 142/144 (99%) | 128 (90%) | 14 (10%) | 0 | 100 | 100 |
| 70 | D4 | 132/134 (98%) | 121 (92%) | 11 (8%) | 0 | 100 | 100 |
| 70 | d4 | 131/134 (98%) | 110 (84%) | 18 (14%) | 3 (2%) | 7 | 41 |
| 71 | D5 | 68/70 (97%) | 53 (78%) | 12 (18%) | 3 (4%) | 3 | 25 |
| 71 | d5 | 67/70 (96%) | 61 (91%) | 6 (9%) | 0 | 100 | 100 |
| 72 | D6 | 95/97 (98%) | 75 (79%) | 17 (18%) | 3 (3%) | 5 | 34 |
| 72 | d6 | 95/97 (98%) | 77 (81%) | 17 (18%) | 1 (1%) | 17 | 57 |
| 73 | D7 | 79/81 (98%) | 71 (90%) | 8 (10%) | 0 | 100 | 100 |
| 73 | d7 | 79/81 (98%) | 71 (90%) | 6 (8%) | 2 (2%) | 6 | 39 |
| 74 | D8 | 61/63 (97%) | 51 (84%) | 10 (16%) | 0 | 100 | 100 |
| 74 | d8 | 61/63 (97%) | 51 (84%) | 9 (15%) | 1 (2%) | 11 | 48 |
| 75 | D9 | 51/53 (96%) | 44 (86%) | 5 (10%) | 2 (4%) | 3 | 28 |
| 75 | d9 | 51/53 (96%) | 46 (90%) | 5 (10%) | 0 | 100 | 100 |
| 76 | E0 | 58/62 (94%) | 46 (79%) | 10 (17%) | 2 (3%) | 4 | 32 |
| 76 | e0 | 60/62 (97%) | 47 (78%) | 13 (22%) | 0 | 100 | 100 |
| 77 | E1 | 69/72 (96%) | 53 (77%) | 15 (22%) | 1 (1%) | 13 | 51 |
| 77 | e1 | 70/72 (97%) | 44 (63%) | 22 (31%) | 4 (6%) | 2 | 18 |
| 78 | SR | 316/318 (99%) | 283 (90%) | 33 (10%) | 0 | 100 | 100 |
| 78 | sR | 316/318 (99%) | 293 (93%) | 21 (7%) | 2 (1%) | 28 | 68 |
| 79 | SM | 155/272 (57%) | 127 (82%) | 26 (17%) | 2 (1%) | 14 | 53 |
| 79 | sM | 123/272 (45%) | 105 (85%) | 15 (12%) | 3 (2%) | 7 | 40 |
| 81 | n4 | 133/135 (98%) | 116 (87%) | 14 (10%) | 3 (2%) | 7 | 41 |
| 82 | p0 | 139/312 (45%) | 124 (89%) | 13 (9%) | 2 (1%) | 13 | 51 |
| All | All | 22342/23454 (95%) | 19892 (89%) | 2273 (10%) | 177 (1%) | 22 | 62 |

5 of 177 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | L4 | 339 | LEU |
| 8 | L6 | 98 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | N4 | 63 | ILE |
| 51 | S5 | 64 | VAL |
| 56 | C0 | 88 | 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 | L2 | 193/194 (100%) | 172 (89%) | 21 (11%) | 7 | 32 |
| 4 | l2 | 192/194 (99%) | 175 (91%) | 17 (9%) | 11 | 42 |
| 5 | L3 | 322/322 (100%) | 273 (85%) | 49 (15%) | 3 | 18 |
| 5 | l3 | 322/322 (100%) | 277 (86%) | 45 (14%) | 4 | 21 |
| 6 | L4 | 288/288 (100%) | 254 (88%) | 34 (12%) | 6 | 27 |
| 6 | l4 | 288/288 (100%) | 253 (88%) | 35 (12%) | 6 | 26 |
| 7 | L5 | 244/244 (100%) | 219 (90%) | 25 (10%) | 8 | 35 |
| 7 | l5 | 243/244 (100%) | 207 (85%) | 36 (15%) | 3 | 19 |
| 8 | L6 | 134/153 (88%) | 115 (86%) | 19 (14%) | 4 | 21 |
| 8 | l6 | 135/153 (88%) | 112 (83%) | 23 (17%) | 2 | 13 |
| 9 | L7 | 186/187 (100%) | 168 (90%) | 18 (10%) | 9 | 37 |
| 9 | l7 | 187/187 (100%) | 168 (90%) | 19 (10%) | 8 | 35 |
| 10 | L8 | 191/191 (100%) | 171 (90%) | 20 (10%) | 8 | 34 |
| 10 | l8 | 177/191 (93%) | 159 (90%) | 18 (10%) | 8 | 35 |
| 11 | L9 | 171/171 (100%) | 143 (84%) | 28 (16%) | 2 | 14 |
| 11 | l9 | 171/171 (100%) | 153 (90%) | 18 (10%) | 8 | 34 |
| 12 | M0 | 176/187 (94%) | 151 (86%) | 25 (14%) | 4 | 21 |
| 12 | m0 | 180/187 (96%) | 143 (79%) | 37 (21%) | 1 | 6 |
| 13 | M1 | 147/147 (100%) | 127 (86%) | 20 (14%) | 4 | 22 |
| 13 | m1 | 147/147 (100%) | 125 (85%) | 22 (15%) | 3 | 18 |
| 14 | M3 | 154/154 (100%) | 127 (82%) | 27 (18%) | 2 | 11 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 14 | m3 | 154/154 (100%) | 137 (89%) | 17 (11%) | 7 | 31 |
| 15 | M4 | 107/108 (99%) | 96 (90%) | 11 (10%) | 8 | 35 |
| 15 | m4 | 108/108 (100%) | 96 (89%) | 12 (11%) | 7 | 31 |
| 16 | M5 | 175/175 (100%) | 151 (86%) | 24 (14%) | 4 | 22 |
| 16 | m5 | 175/175 (100%) | 151 (86%) | 24 (14%) | 4 | 22 |
| 17 | M6 | 160/160 (100%) | 144 (90%) | 16 (10%) | 9 | 36 |
| 17 | m6 | 160/160 (100%) | 141 (88%) | 19 (12%) | 6 | 27 |
| 18 | M7 | 138/146 (94%) | 110 (80%) | 28 (20%) | 1 | 6 |
| 18 | m7 | 125/146 (86%) | 104 (83%) | 21 (17%) | 2 | 13 |
| 19 | M8 | 150/150 (100%) | 134 (89%) | 16 (11%) | 8 | 33 |
| 19 | m8 | 150/150 (100%) | 128 (85%) | 22 (15%) | 3 | 19 |
| 20 | M9 | 148/153 (97%) | 133 (90%) | 15 (10%) | 9 | 35 |
| 20 | m9 | 153/153 (100%) | 138 (90%) | 15 (10%) | 9 | 37 |
| 21 | N0 | 156/156 (100%) | 127 (81%) | 29 (19%) | 2 | 9 |
| 21 | n0 | 156/156 (100%) | 136 (87%) | 20 (13%) | 5 | 24 |
| 22 | N1 | 136/136 (100%) | 118 (87%) | 18 (13%) | 5 | 23 |
| 22 | n1 | 136/136 (100%) | 113 (83%) | 23 (17%) | 2 | 13 |
| 23 | N2 | 87/87 (100%) | 80 (92%) | 7 (8%) | 14 | 48 |
| 23 | n2 | 85/87 (98%) | 76 (89%) | 9 (11%) | 8 | 33 |
| 24 | N3 | 104/104 (100%) | 96 (92%) | 8 (8%) | 15 | 49 |
| 24 | n3 | 104/104 (100%) | 95 (91%) | 9 (9%) | 12 | 43 |
| 25 | N4 | 57/129 (44%) | 53 (93%) | 4 (7%) | 18 | 55 |
| 26 | N5 | 104/105 (99%) | 94 (90%) | 10 (10%) | 10 | 38 |
| 26 | n5 | 104/105 (99%) | 94 (90%) | 10 (10%) | 10 | 38 |
| 27 | N6 | 109/109 (100%) | 95 (87%) | 14 (13%) | 5 | 24 |
| 27 | n6 | 109/109 (100%) | 92 (84%) | 17 (16%) | 3 | 16 |
| 28 | N7 | 115/115 (100%) | 101 (88%) | 14 (12%) | 6 | 26 |
| 28 | n7 | 115/115 (100%) | 103 (90%) | 12 (10%) | 8 | 34 |
| 29 | N8 | 118/118 (100%) | 101 (86%) | 17 (14%) | 4 | 20 |
| 29 | n8 | 118/118 (100%) | 100 (85%) | 18 (15%) | 3 | 17 |
| 30 | N9 | 46/46 (100%) | 41 (89%) | 5 (11%) | 7 | 32 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 30 | n9 | 46/46 (100%) | 39 (85%) | 7 (15%) | 3 | 18 |
| 31 | O0 | 81/84 (96%) | 75 (93%) | 6 (7%) | 16 | 51 |
| 31 | o0 | 84/84 (100%) | 71 (84%) | 13 (16%) | 3 | 17 |
| 32 | O1 | 96/96 (100%) | 82 (85%) | 14 (15%) | 3 | 19 |
| 32 | o1 | 96/96 (100%) | 80 (83%) | 16 (17%) | 2 | 13 |
| 33 | O2 | 109/109 (100%) | 97 (89%) | 12 (11%) | 7 | 31 |
| 33 | o2 | 109/109 (100%) | 93 (85%) | 16 (15%) | 3 | 19 |
| 34 | O3 | 90/90 (100%) | 84 (93%) | 6 (7%) | 19 | 57 |
| 34 | o3 | 90/90 (100%) | 81 (90%) | 9 (10%) | 9 | 36 |
| 35 | O4 | 95/95 (100%) | 84 (88%) | 11 (12%) | 6 | 29 |
| 35 | o4 | 95/95 (100%) | 88 (93%) | 7 (7%) | 16 | 51 |
| 36 | O5 | 104/104 (100%) | 88 (85%) | 16 (15%) | 3 | 17 |
| 36 | o5 | 104/104 (100%) | 91 (88%) | 13 (12%) | 5 | 25 |
| 37 | O6 | 81/81 (100%) | 71 (88%) | 10 (12%) | 5 | 26 |
| 37 | o6 | 81/81 (100%) | 70 (86%) | 11 (14%) | 4 | 22 |
| 38 | O7 | 70/70 (100%) | 62 (89%) | 8 (11%) | 7 | 29 |
| 38 | o7 | 70/70 (100%) | 58 (83%) | 12 (17%) | 2 | 13 |
| 39 | O8 | 68/68 (100%) | 58 (85%) | 10 (15%) | 3 | 19 |
| 39 | o8 | 68/68 (100%) | 60 (88%) | 8 (12%) | 6 | 27 |
| 40 | O9 | 45/45 (100%) | 39 (87%) | 6 (13%) | 4 | 23 |
| 40 | o9 | 45/45 (100%) | 38 (84%) | 7 (16%) | 3 | 16 |
| 41 | Q0 | 47/47 (100%) | 42 (89%) | 5 (11%) | 8 | 33 |
| 41 | q0 | 47/47 (100%) | 39 (83%) | 8 (17%) | 2 | 13 |
| 42 | Q1 | 23/23 (100%) | 19 (83%) | 4 (17%) | 2 | 12 |
| 42 | q1 | 23/23 (100%) | 20 (87%) | 3 (13%) | 5 | 24 |
| 43 | Q2 | 90/90 (100%) | 81 (90%) | 9 (10%) | 9 | 36 |
| 43 | q2 | 90/90 (100%) | 72 (80%) | 18 (20%) | 1 | 7 |
| 44 | Q3 | 71/71 (100%) | 65 (92%) | 6 (8%) | 12 | 45 |
| 44 | q3 | 71/71 (100%) | 65 (92%) | 6 (8%) | 12 | 45 |
| 46 | S0 | 173/173 (100%) | 153 (88%) | 20 (12%) | 6 | 29 |
| 46 | s0 | 173/173 (100%) | 154 (89%) | 19 (11%) | 7 | 31 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 47 | S1 | 191/192 (100%) | 161 (84%) | 30 (16%) | 3 | 16 |
| 47 | s1 | 192/192 (100%) | 174 (91%) | 18 (9%) | 10 | 39 |
| 48 | S2 | 176/176 (100%) | 163 (93%) | 13 (7%) | 16 | 51 |
| 48 | s2 | 176/176 (100%) | 154 (88%) | 22 (12%) | 5 | 25 |
| 49 | S3 | 182/182 (100%) | 162 (89%) | 20 (11%) | 7 | 31 |
| 49 | s3 | 181/182 (100%) | 149 (82%) | 32 (18%) | 2 | 11 |
| 50 | S4 | 221/221 (100%) | 195 (88%) | 26 (12%) | 6 | 27 |
| 50 | s4 | 221/221 (100%) | 195 (88%) | 26 (12%) | 6 | 27 |
| 51 | S5 | 173/173 (100%) | 158 (91%) | 15 (9%) | 12 | 43 |
| 51 | s5 | 173/173 (100%) | 150 (87%) | 23 (13%) | 4 | 23 |
| 52 | S6 | 191/201 (95%) | 167 (87%) | 24 (13%) | 5 | 25 |
| 52 | s6 | 187/201 (93%) | 160 (86%) | 27 (14%) | 4 | 20 |
| 53 | S7 | 165/166 (99%) | 151 (92%) | 14 (8%) | 12 | 45 |
| 53 | s7 | 165/166 (99%) | 152 (92%) | 13 (8%) | 14 | 48 |
| 54 | S8 | 150/161 (93%) | 132 (88%) | 18 (12%) | 6 | 27 |
| 54 | s8 | 148/161 (92%) | 137 (93%) | 11 (7%) | 16 | 51 |
| 55 | S9 | 158/158 (100%) | 140 (89%) | 18 (11%) | 7 | 29 |
| 55 | s9 | 158/158 (100%) | 143 (90%) | 15 (10%) | 10 | 38 |
| 56 | C0 | 77/98 (79%) | 66 (86%) | 11 (14%) | 4 | 20 |
| 56 | c0 | 73/98 (74%) | 65 (89%) | 8 (11%) | 7 | 31 |
| 57 | C1 | 129/137 (94%) | 119 (92%) | 10 (8%) | 15 | 49 |
| 57 | c1 | 125/137 (91%) | 108 (86%) | 17 (14%) | 4 | 22 |
| 58 | C2 | 88/119 (74%) | 80 (91%) | 8 (9%) | 11 | 40 |
| 58 | c2 | 88/119 (74%) | 76 (86%) | 12 (14%) | 4 | 22 |
| 59 | C3 | 127/127 (100%) | 117 (92%) | 10 (8%) | 14 | 48 |
| 59 | c3 | 127/127 (100%) | 110 (87%) | 17 (13%) | 4 | 23 |
| 60 | C4 | 81/97 (84%) | 70 (86%) | 11 (14%) | 4 | 22 |
| 60 | c4 | 97/97 (100%) | 84 (87%) | 13 (13%) | 4 | 23 |
| 61 | C5 | 101/117 (86%) | 91 (90%) | 10 (10%) | 9 | 36 |
| 61 | c5 | 103/117 (88%) | 93 (90%) | 10 (10%) | 9 | 37 |
| 62 | C6 | 117/118 (99%) | 101 (86%) | 16 (14%) | 4 | 22 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 62 | c6 | 118/118 (100%) | 103 (87%) | 15 (13%) | 5 | 25 |
| 63 | C7 | 109/124 (88%) | 91 (84%) | 18 (16%) | 2 | 14 |
| 63 | c7 | 97/124 (78%) | 87 (90%) | 10 (10%) | 8 | 35 |
| 64 | C8 | 128/128 (100%) | 114 (89%) | 14 (11%) | 7 | 32 |
| 64 | c8 | 128/128 (100%) | 108 (84%) | 20 (16%) | 3 | 16 |
| 65 | C9 | 115/115 (100%) | 102 (89%) | 13 (11%) | 7 | 29 |
| 65 | c9 | 115/115 (100%) | 100 (87%) | 15 (13%) | 5 | 24 |
| 66 | D0 | 100/103 (97%) | 89 (89%) | 11 (11%) | 7 | 31 |
| 66 | d0 | 103/103 (100%) | 89 (86%) | 14 (14%) | 4 | 22 |
| 67 | D1 | 74/74 (100%) | 65 (88%) | 9 (12%) | 6 | 26 |
| 67 | d1 | 74/74 (100%) | 65 (88%) | 9 (12%) | 6 | 26 |
| 68 | D2 | 110/110 (100%) | 97 (88%) | 13 (12%) | 6 | 27 |
| 68 | d2 | 110/110 (100%) | 97 (88%) | 13 (12%) | 6 | 27 |
| 69 | D3 | 119/119 (100%) | 107 (90%) | 12 (10%) | 9 | 35 |
| 69 | d3 | 119/119 (100%) | 109 (92%) | 10 (8%) | 13 | 45 |
| 70 | D4 | 112/112 (100%) | 99 (88%) | 13 (12%) | 6 | 29 |
| 70 | d4 | 111/112 (99%) | 100 (90%) | 11 (10%) | 9 | 36 |
| 71 | D5 | 61/61 (100%) | 51 (84%) | 10 (16%) | 2 | 14 |
| 71 | d5 | 61/61 (100%) | 57 (93%) | 4 (7%) | 19 | 57 |
| 72 | D6 | 83/83 (100%) | 71 (86%) | 12 (14%) | 4 | 20 |
| 72 | d6 | 83/83 (100%) | 72 (87%) | 11 (13%) | 4 | 23 |
| 73 | D7 | 70/70 (100%) | 62 (89%) | 8 (11%) | 7 | 29 |
| 73 | d7 | 70/70 (100%) | 65 (93%) | 5 (7%) | 17 | 54 |
| 74 | D8 | 56/56 (100%) | 50 (89%) | 6 (11%) | 8 | 33 |
| 74 | d8 | 56/56 (100%) | 41 (73%) | 15 (27%) | 0 | 3 |
| 75 | D9 | 47/47 (100%) | 39 (83%) | 8 (17%) | 2 | 13 |
| 75 | d9 | 47/47 (100%) | 36 (77%) | 11 (23%) | 1 | 4 |
| 76 | E0 | 51/53 (96%) | 46 (90%) | 5 (10%) | 9 | 37 |
| 76 | e0 | 53/53 (100%) | 44 (83%) | 9 (17%) | 2 | 13 |
| 77 | E1 | 62/63 (98%) | 56 (90%) | 6 (10%) | 9 | 37 |
| 77 | e1 | 63/63 (100%) | 51 (81%) | 12 (19%) | 2 | 8 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|------------|-------------|----|
| 78 | SR | 260/260 (100%) | 239 (92%) | 21 (8%) | 14 | 47 |
| 78 | sR | 260/260 (100%) | 241 (93%) | 19 (7%) | 16 | 52 |
| 79 | SM | 97/227 (43%) | 81 (84%) | 16 (16%) | 2 | 14 |
| 79 | sM | 88/227 (39%) | 77 (88%) | 11 (12%) | 5 | 25 |
| 81 | n4 | 101/114 (89%) | 92 (91%) | 9 (9%) | 11 | 42 |
| 82 | p0 | 105/254 (41%) | 90 (86%) | 15 (14%) | 4 | 20 |
| All | All | 18802/19697 (96%) | 16495 (88%) | 2307 (12%) | 5 | 26 |

5 of 2307 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 72 | D6 | 85 | ARG |
| 10 | l8 | 79 | GLN |
| 64 | c8 | 101 | LEU |
| 77 | E1 | 144 | CYS |
| 5 | l3 | 316 | GLU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 70 | D4 | 63 | GLN |
| 7 | l5 | 81 | HIS |
| 67 | d1 | 3 | ASN |
| 71 | D5 | 95 | HIS |
| 5 | l3 | 211 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------------|-------------------|-----------------|
| 1 | 1 | 3095/3396 (91%) | 696 (22%) | 86 (2%) |
| 1 | 5 | 3129/3396 (92%) | 752 (24%) | 83 (2%) |
| 2 | 3 | 120/121 (99%) | 22 (18%) | 1 (0%) |
| 2 | 7 | 120/121 (99%) | 24 (20%) | 1 (0%) |
| 3 | 4 | 154/158 (97%) | 36 (23%) | 2 (1%) |
| 3 | 8 | 157/158 (99%) | 43 (27%) | 1 (0%) |
| 45 | 2 | 1708/1800 (94%) | 481 (28%) | 59 (3%) |
| 45 | 6 | 1733/1800 (96%) | 485 (27%) | 62 (3%) |
| All | All | 10216/10950 (93%) | 2539 (24%) | 295 (2%) |

5 of 2539 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 1 | 13 | A |
| 1 | 1 | 14 | U |
| 1 | 1 | 16 | A |
| 1 | 1 | 26 | A |
| 1 | 1 | 30 | G |

5 of 295 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 45 | 2 | 1226 | A |
| 1 | 5 | 1160 | C |
| 45 | 6 | 832 | U |
| 45 | 2 | 1344 | A |
| 1 | 5 | 242 | C |

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2153 ligands modelled in this entry, 2084 are monoatomic - leaving 69 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 85 | LLL | 1 | 3989 | - | 30,33,33 | 0.24 | 0 | 33,49,49 | 1.44 | 3 (9%) |
| 85 | LLL | 1 | 3990 | - | 30,33,33 | 0.25 | 0 | 33,49,49 | 1.83 | 1 (3%) |
| 85 | LLL | 1 | 3991 | - | 30,33,33 | 0.19 | 0 | 33,49,49 | 0.85 | 2 (6%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 85 | LLL | 1 | 3992 | - | 30,33,33 | 0.20 | 0 | 33,49,49 | 1.34 | 3 (9%) |
| 85 | LLL | 1 | 3993 | - | 30,33,33 | 0.24 | 0 | 33,49,49 | 1.38 | 4 (12%) |
| 85 | LLL | 1 | 3994 | - | 30,33,33 | 0.19 | 0 | 33,49,49 | 1.20 | 3 (9%) |
| 85 | LLL | 1 | 3995 | - | 30,33,33 | 0.15 | 0 | 33,49,49 | 2.14 | 2 (6%) |
| 85 | LLL | 1 | 3996 | - | 30,33,33 | 0.20 | 0 | 33,49,49 | 0.91 | 3 (9%) |
| 85 | LLL | 1 | 3997 | - | 30,33,33 | 0.18 | 0 | 33,49,49 | 1.24 | 3 (9%) |
| 85 | LLL | 1 | 3998 | - | 30,33,33 | 0.14 | 0 | 33,49,49 | 0.81 | 2 (6%) |
| 85 | LLL | 1 | 3999 | - | 30,33,33 | 0.16 | 0 | 33,49,49 | 1.06 | 4 (12%) |
| 85 | LLL | 1 | 4000 | - | 30,33,33 | 0.17 | 0 | 33,49,49 | 2.14 | 4 (12%) |
| 85 | LLL | 1 | 4001 | - | 30,33,33 | 0.16 | 0 | 33,49,49 | 1.13 | 2 (6%) |
| 85 | LLL | 1 | 4002 | - | 30,33,33 | 0.20 | 0 | 33,49,49 | 2.15 | 3 (9%) |
| 85 | LLL | 1 | 4003 | - | 30,33,33 | 0.18 | 0 | 33,49,49 | 1.44 | 3 (9%) |
| 85 | LLL | 1 | 4004 | - | 30,33,33 | 0.19 | 0 | 33,49,49 | 1.10 | 1 (3%) |
| 85 | LLL | 2 | 2043 | - | 30,33,33 | 0.17 | 0 | 33,49,49 | 0.84 | 3 (9%) |
| 85 | LLL | 2 | 2044 | - | 30,33,33 | 0.19 | 0 | 33,49,49 | 1.54 | 4 (12%) |
| 85 | LLL | 2 | 2045 | - | 30,33,33 | 0.19 | 0 | 33,49,49 | 1.59 | 4 (12%) |
| 85 | LLL | 3 | 220 | - | 30,33,33 | 0.21 | 0 | 33,49,49 | 1.53 | 3 (9%) |
| 85 | LLL | 4 | 224 | - | 30,33,33 | 0.20 | 0 | 33,49,49 | 1.62 | 3 (9%) |
| 85 | LLL | 5 | 4151 | - | 30,33,33 | 0.30 | 0 | 33,49,49 | 1.69 | 3 (9%) |
| 85 | LLL | 5 | 4152 | - | 30,33,33 | 0.17 | 0 | 33,49,49 | 1.54 | 2 (6%) |
| 85 | LLL | 5 | 4153 | - | 30,33,33 | 0.24 | 0 | 33,49,49 | 1.81 | 2 (6%) |
| 85 | LLL | 5 | 4154 | - | 30,33,33 | 0.25 | 0 | 33,49,49 | 0.67 | 0 |
| 85 | LLL | 5 | 4155 | - | 30,33,33 | 0.26 | 0 | 33,49,49 | 1.10 | 3 (9%) |
| 85 | LLL | 5 | 4156 | - | 30,33,33 | 0.21 | 0 | 33,49,49 | 1.34 | 3 (9%) |
| 85 | LLL | 5 | 4157 | - | 30,33,33 | 0.25 | 0 | 33,49,49 | 1.11 | 2 (6%) |
| 85 | LLL | 5 | 4158 | - | 30,33,33 | 0.20 | 0 | 33,49,49 | 2.04 | 5 (15%) |
| 85 | LLL | 5 | 4159 | - | 30,33,33 | 0.21 | 0 | 33,49,49 | 1.11 | 3 (9%) |
| 85 | LLL | 5 | 4160 | - | 30,33,33 | 0.25 | 0 | 33,49,49 | 1.90 | 3 (9%) |
| 85 | LLL | 5 | 4161 | - | 30,33,33 | 0.19 | 0 | 33,49,49 | 1.30 | 3 (9%) |
| 85 | LLL | 5 | 4162 | - | 30,33,33 | 0.17 | 0 | 33,49,49 | 0.86 | 1 (3%) |
| 85 | LLL | 5 | 4163 | - | 30,33,33 | 0.15 | 0 | 33,49,49 | 1.10 | 3 (9%) |
| 85 | LLL | 5 | 4164 | - | 30,33,33 | 0.20 | 0 | 33,49,49 | 1.97 | 3 (9%) |
| 85 | LLL | 5 | 4165 | - | 30,33,33 | 0.16 | 0 | 33,49,49 | 1.12 | 2 (6%) |
| 85 | LLL | 5 | 4166 | - | 30,33,33 | 0.14 | 0 | 33,49,49 | 1.24 | 2 (6%) |
| 85 | LLL | 5 | 4167 | - | 30,33,33 | 0.15 | 0 | 33,49,49 | 1.03 | 2 (6%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 85 | LLL | 5 | 4168 | - | 30,33,33 | 0.21 | 0 | 33,49,49 | 1.70 | 3 (9%) |
| 85 | LLL | 5 | 4169 | - | 30,33,33 | 0.21 | 0 | 33,49,49 | 1.56 | 4 (12%) |
| 85 | LLL | 5 | 4170 | - | 30,33,33 | 0.24 | 0 | 33,49,49 | 1.57 | 2 (6%) |
| 85 | LLL | 5 | 4171 | - | 30,33,33 | 0.19 | 0 | 33,49,49 | 1.09 | 1 (3%) |
| 85 | LLL | 5 | 4172 | - | 30,33,33 | 0.21 | 0 | 33,49,49 | 1.44 | 4 (12%) |
| 85 | LLL | 5 | 4173 | - | 30,33,33 | 0.15 | 0 | 33,49,49 | 1.22 | 4 (12%) |
| 85 | LLL | 5 | 4174 | - | 30,33,33 | 0.25 | 0 | 33,49,49 | 1.63 | 4 (12%) |
| 85 | LLL | 5 | 4175 | - | 30,33,33 | 0.23 | 0 | 33,49,49 | 1.52 | 2 (6%) |
| 85 | LLL | 5 | 4176 | - | 30,33,33 | 0.22 | 0 | 33,49,49 | 1.22 | 2 (6%) |
| 85 | LLL | 5 | 4177 | - | 30,33,33 | 0.26 | 0 | 33,49,49 | 1.88 | 4 (12%) |
| 85 | LLL | 5 | 4178 | - | 30,33,33 | 0.20 | 0 | 33,49,49 | 0.94 | 1 (3%) |
| 85 | LLL | 6 | 2164 | - | 30,33,33 | 0.19 | 0 | 33,49,49 | 1.85 | 2 (6%) |
| 85 | LLL | 6 | 2165 | - | 30,33,33 | 0.22 | 0 | 33,49,49 | 1.18 | 2 (6%) |
| 85 | LLL | 6 | 2166 | - | 30,33,33 | 0.20 | 0 | 33,49,49 | 1.10 | 3 (9%) |
| 85 | LLL | 6 | 2167 | - | 30,33,33 | 0.20 | 0 | 33,49,49 | 1.98 | 5 (15%) |
| 85 | LLL | 6 | 2168 | - | 30,33,33 | 0.21 | 0 | 33,49,49 | 1.50 | 5 (15%) |
| 85 | LLL | 6 | 2169 | - | 30,33,33 | 0.15 | 0 | 33,49,49 | 0.94 | 2 (6%) |
| 85 | LLL | 6 | 2170 | - | 30,33,33 | 0.22 | 0 | 33,49,49 | 1.40 | 3 (9%) |
| 85 | LLL | 6 | 2171 | - | 30,33,33 | 0.14 | 0 | 33,49,49 | 1.17 | 1 (3%) |
| 85 | LLL | 6 | 2172 | - | 30,33,33 | 0.18 | 0 | 33,49,49 | 1.16 | 2 (6%) |
| 85 | LLL | 6 | 2173 | - | 30,33,33 | 0.19 | 0 | 33,49,49 | 1.19 | 5 (15%) |
| 85 | LLL | 6 | 2174 | - | 30,33,33 | 0.26 | 0 | 33,49,49 | 1.32 | 3 (9%) |
| 85 | LLL | 6 | 2175 | - | 30,33,33 | 0.17 | 0 | 33,49,49 | 1.62 | 3 (9%) |
| 85 | LLL | 6 | 2176 | - | 30,33,33 | 0.21 | 0 | 33,49,49 | 1.41 | 4 (12%) |
| 85 | LLL | 7 | 231 | - | 30,33,33 | 0.16 | 0 | 33,49,49 | 2.11 | 7 (21%) |
| 85 | LLL | 7 | 232 | - | 30,33,33 | 0.16 | 0 | 33,49,49 | 0.92 | 2 (6%) |
| 85 | LLL | 7 | 233 | - | 30,33,33 | 0.21 | 0 | 33,49,49 | 1.02 | 2 (6%) |
| 85 | LLL | 8 | 221 | - | 30,33,33 | 0.20 | 0 | 33,49,49 | 1.83 | 2 (6%) |
| 85 | LLL | 8 | 222 | - | 30,33,33 | 0.15 | 0 | 33,49,49 | 0.89 | 1 (3%) |
| 85 | LLL | L3 | 404 | - | 30,33,33 | 0.22 | 0 | 33,49,49 | 1.37 | 3 (9%) |
| 85 | LLL | l3 | 412 | - | 30,33,33 | 0.26 | 0 | 33,49,49 | 1.88 | 3 (9%) |

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 |
|-----|------|-------|------|------|---------|------------|---------|
| 85 | LLL | 1 | 3989 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 1 | 3990 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 1 | 3991 | - | - | 1/11/65/65 | 0/3/3/3 |
| 85 | LLL | 1 | 3992 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 1 | 3993 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 1 | 3994 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 1 | 3995 | - | - | 1/11/65/65 | 0/3/3/3 |
| 85 | LLL | 1 | 3996 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 1 | 3997 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 1 | 3998 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 1 | 3999 | - | - | 1/11/65/65 | 0/3/3/3 |
| 85 | LLL | 1 | 4000 | - | - | 1/11/65/65 | 0/3/3/3 |
| 85 | LLL | 1 | 4001 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 1 | 4002 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 1 | 4003 | - | - | 0/11/65/65 | 2/3/3/3 |
| 85 | LLL | 1 | 4004 | - | - | 0/11/65/65 | 1/3/3/3 |
| 85 | LLL | 2 | 2043 | - | - | 0/11/65/65 | 1/3/3/3 |
| 85 | LLL | 2 | 2044 | - | - | 1/11/65/65 | 1/3/3/3 |
| 85 | LLL | 2 | 2045 | - | - | 1/11/65/65 | 0/3/3/3 |
| 85 | LLL | 3 | 220 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 4 | 224 | - | - | 1/11/65/65 | 0/3/3/3 |
| 85 | LLL | 5 | 4151 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 5 | 4152 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 5 | 4153 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 5 | 4154 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 5 | 4155 | - | - | 2/11/65/65 | 1/3/3/3 |
| 85 | LLL | 5 | 4156 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 5 | 4157 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 5 | 4158 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 5 | 4159 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 5 | 4160 | - | - | 1/11/65/65 | 0/3/3/3 |
| 85 | LLL | 5 | 4161 | - | - | 0/11/65/65 | 1/3/3/3 |
| 85 | LLL | 5 | 4162 | - | - | 1/11/65/65 | 1/3/3/3 |
| 85 | LLL | 5 | 4163 | - | - | 1/11/65/65 | 2/3/3/3 |
| 85 | LLL | 5 | 4164 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 5 | 4165 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 5 | 4166 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 5 | 4167 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 5 | 4168 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 5 | 4169 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 5 | 4170 | - | - | 0/11/65/65 | 1/3/3/3 |
| 85 | LLL | 5 | 4171 | - | - | 1/11/65/65 | 0/3/3/3 |
| 85 | LLL | 5 | 4172 | - | - | 1/11/65/65 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 85 | LLL | 5 | 4173 | - | - | 0/11/65/65 | 1/3/3/3 |
| 85 | LLL | 5 | 4174 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 5 | 4175 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 5 | 4176 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 5 | 4177 | - | - | 1/11/65/65 | 0/3/3/3 |
| 85 | LLL | 5 | 4178 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 6 | 2164 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 6 | 2165 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 6 | 2166 | - | - | 1/11/65/65 | 0/3/3/3 |
| 85 | LLL | 6 | 2167 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 6 | 2168 | - | - | 0/11/65/65 | 1/3/3/3 |
| 85 | LLL | 6 | 2169 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 6 | 2170 | - | - | 1/11/65/65 | 0/3/3/3 |
| 85 | LLL | 6 | 2171 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 6 | 2172 | - | - | 1/11/65/65 | 1/3/3/3 |
| 85 | LLL | 6 | 2173 | - | - | 1/11/65/65 | 1/3/3/3 |
| 85 | LLL | 6 | 2174 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 6 | 2175 | - | - | 1/11/65/65 | 1/3/3/3 |
| 85 | LLL | 6 | 2176 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 7 | 231 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 7 | 232 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 7 | 233 | - | - | 0/11/65/65 | 2/3/3/3 |
| 85 | LLL | 8 | 221 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | 8 | 222 | - | - | 0/11/65/65 | 2/3/3/3 |
| 85 | LLL | L3 | 404 | - | - | 0/11/65/65 | 0/3/3/3 |
| 85 | LLL | l3 | 412 | - | - | 0/11/65/65 | 0/3/3/3 |

There are no bond length outliers.

The worst 5 of 193 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 85 | 2 | 2045 | LLL | O11-C42-C32 | -5.33 | 96.64 | 108.96 |
| 85 | 1 | 3993 | LLL | O11-C11-C21 | -4.75 | 99.36 | 108.21 |
| 85 | 7 | 231 | LLL | O11-C42-C32 | -4.52 | 98.51 | 108.96 |
| 85 | 5 | 4164 | LLL | O11-C42-C32 | -4.45 | 98.67 | 108.96 |
| 85 | 5 | 4151 | LLL | C43-C33-C23 | -4.37 | 100.64 | 112.46 |

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 85 | 5 | 4171 | LLL | O51-C51-C61-N61 |
| 85 | 6 | 2175 | LLL | C42-O11-C11-C21 |
| 85 | 5 | 4163 | LLL | O51-C51-C61-N61 |
| 85 | 5 | 4155 | LLL | C42-O11-C11-C21 |
| 85 | 2 | 2044 | LLL | O51-C51-C61-N61 |

5 of 20 ring outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-------------------------|
| 85 | 6 | 2172 | LLL | C12-C22-C32-C42-C52-C62 |
| 85 | 5 | 4155 | LLL | C11-C21-C31-C41-C51-O51 |
| 85 | 1 | 4004 | LLL | C11-C21-C31-C41-C51-O51 |
| 85 | 5 | 4170 | LLL | C11-C21-C31-C41-C51-O51 |
| 85 | 6 | 2168 | LLL | C11-C21-C31-C41-C51-O51 |

60 monomers are involved in 157 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 85 | 1 | 3989 | LLL | 2 | 0 |
| 85 | 1 | 3990 | LLL | 1 | 0 |
| 85 | 1 | 3991 | LLL | 3 | 0 |
| 85 | 1 | 3992 | LLL | 3 | 0 |
| 85 | 1 | 3993 | LLL | 1 | 0 |
| 85 | 1 | 3994 | LLL | 1 | 0 |
| 85 | 1 | 3996 | LLL | 2 | 0 |
| 85 | 1 | 3997 | LLL | 2 | 0 |
| 85 | 1 | 3998 | LLL | 1 | 0 |
| 85 | 1 | 3999 | LLL | 3 | 0 |
| 85 | 1 | 4000 | LLL | 3 | 0 |
| 85 | 1 | 4001 | LLL | 1 | 0 |
| 85 | 1 | 4002 | LLL | 4 | 0 |
| 85 | 1 | 4003 | LLL | 1 | 0 |
| 85 | 2 | 2043 | LLL | 5 | 0 |
| 85 | 2 | 2044 | LLL | 2 | 0 |
| 85 | 2 | 2045 | LLL | 2 | 0 |
| 85 | 3 | 220 | LLL | 2 | 0 |
| 85 | 4 | 224 | LLL | 9 | 0 |
| 85 | 5 | 4151 | LLL | 2 | 0 |
| 85 | 5 | 4152 | LLL | 2 | 0 |
| 85 | 5 | 4153 | LLL | 1 | 0 |
| 85 | 5 | 4154 | LLL | 3 | 0 |
| 85 | 5 | 4155 | LLL | 2 | 0 |
| 85 | 5 | 4156 | LLL | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 85 | 5 | 4157 | LLL | 1 | 0 |
| 85 | 5 | 4158 | LLL | 2 | 0 |
| 85 | 5 | 4159 | LLL | 1 | 0 |
| 85 | 5 | 4160 | LLL | 2 | 0 |
| 85 | 5 | 4162 | LLL | 4 | 0 |
| 85 | 5 | 4163 | LLL | 2 | 0 |
| 85 | 5 | 4164 | LLL | 1 | 0 |
| 85 | 5 | 4166 | LLL | 1 | 0 |
| 85 | 5 | 4168 | LLL | 4 | 0 |
| 85 | 5 | 4169 | LLL | 1 | 0 |
| 85 | 5 | 4170 | LLL | 1 | 0 |
| 85 | 5 | 4171 | LLL | 3 | 0 |
| 85 | 5 | 4172 | LLL | 3 | 0 |
| 85 | 5 | 4173 | LLL | 2 | 0 |
| 85 | 5 | 4174 | LLL | 3 | 0 |
| 85 | 5 | 4175 | LLL | 2 | 0 |
| 85 | 5 | 4176 | LLL | 1 | 0 |
| 85 | 5 | 4177 | LLL | 3 | 0 |
| 85 | 5 | 4178 | LLL | 4 | 0 |
| 85 | 6 | 2166 | LLL | 3 | 0 |
| 85 | 6 | 2167 | LLL | 6 | 0 |
| 85 | 6 | 2168 | LLL | 4 | 0 |
| 85 | 6 | 2169 | LLL | 3 | 0 |
| 85 | 6 | 2170 | LLL | 1 | 0 |
| 85 | 6 | 2171 | LLL | 2 | 0 |
| 85 | 6 | 2172 | LLL | 2 | 0 |
| 85 | 6 | 2173 | LLL | 3 | 0 |
| 85 | 6 | 2175 | LLL | 2 | 0 |
| 85 | 6 | 2176 | LLL | 1 | 0 |
| 85 | 7 | 231 | LLL | 4 | 0 |
| 85 | 7 | 232 | LLL | 4 | 0 |
| 85 | 7 | 233 | LLL | 3 | 0 |
| 85 | 8 | 221 | LLL | 6 | 0 |
| 85 | 8 | 222 | LLL | 10 | 0 |
| 85 | L3 | 404 | LLL | 2 | 0 |

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 80 | m2 | 2 |
| 51 | S5 | 1 |
| 10 | l8 | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | m2 | 23:UNK | C | 28:UNK | N | 6.26 |
| 1 | m2 | 52:UNK | C | 54:UNK | N | 3.26 |
| 1 | S5 | 21:THR | C | 22:PRO | N | 1.72 |
| 1 | l8 | 51:LYS | C | 52:TRP | N | 1.16 |

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 | 3100/3396 (91%) | 0.02 | 23 (0%) 87 85 | 47, 83, 190, 354 | 0 |
| 1 | 5 | 3134/3396 (92%) | 0.06 | 13 (0%) 92 90 | 37, 76, 173, 292 | 0 |
| 2 | 3 | 121/121 (100%) | -0.29 | 0 100 100 | 58, 107, 135, 155 | 0 |
| 2 | 7 | 121/121 (100%) | -0.24 | 0 100 100 | 45, 72, 94, 160 | 0 |
| 3 | 4 | 156/158 (98%) | -0.02 | 0 100 100 | 54, 94, 152, 260 | 0 |
| 3 | 8 | 158/158 (100%) | 0.02 | 0 100 100 | 61, 102, 164, 234 | 0 |
| 4 | L2 | 252/252 (100%) | 0.40 | 7 (2%) 53 50 | 51, 88, 124, 174 | 0 |
| 4 | 12 | 252/252 (100%) | 0.48 | 6 (2%) 59 55 | 51, 84, 121, 177 | 0 |
| 5 | L3 | 386/386 (100%) | 0.22 | 3 (0%) 86 82 | 41, 77, 104, 170 | 0 |
| 5 | 13 | 386/386 (100%) | 0.08 | 1 (0%) 93 92 | 34, 60, 91, 165 | 0 |
| 6 | L4 | 361/361 (100%) | 0.19 | 0 100 100 | 45, 85, 119, 142 | 0 |
| 6 | 14 | 361/361 (100%) | 0.23 | 6 (1%) 70 66 | 44, 90, 128, 167 | 0 |
| 7 | L5 | 296/296 (100%) | 0.59 | 23 (7%) 14 14 | 74, 120, 162, 214 | 0 |
| 7 | 15 | 294/296 (99%) | 0.21 | 5 (1%) 70 66 | 51, 80, 124, 155 | 0 |
| 8 | L6 | 156/176 (88%) | 0.14 | 1 (0%) 89 86 | 61, 84, 119, 149 | 0 |
| 8 | 16 | 157/176 (89%) | 0.18 | 1 (0%) 89 86 | 53, 81, 129, 204 | 0 |
| 9 | L7 | 222/223 (99%) | 0.14 | 3 (1%) 75 71 | 47, 76, 119, 219 | 0 |
| 9 | 17 | 223/223 (100%) | 0.03 | 0 100 100 | 39, 66, 123, 205 | 0 |
| 10 | L8 | 233/233 (100%) | 0.96 | 33 (14%) 3 3 | 96, 131, 183, 250 | 0 |
| 10 | 18 | 231/233 (99%) | 0.95 | 38 (16%) 2 2 | 96, 137, 184, 229 | 0 |
| 11 | L9 | 191/191 (100%) | 0.35 | 6 (3%) 49 46 | 60, 91, 121, 162 | 0 |
| 11 | 19 | 191/191 (100%) | 0.00 | 1 (0%) 90 88 | 41, 60, 92, 148 | 0 |
| 12 | M0 | 212/221 (95%) | 0.34 | 7 (3%) 47 43 | 52, 84, 129, 242 | 0 |
| 12 | m0 | 211/221 (95%) | 0.24 | 4 (1%) 67 63 | 32, 65, 120, 192 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 13 | M1 | 169/169 (100%) | 1.06 | 32 (18%) 1 2 | 88, 124, 153, 166 | 0 |
| 13 | m1 | 169/169 (100%) | 0.16 | 2 (1%) 79 75 | 51, 77, 104, 125 | 0 |
| 14 | M3 | 193/194 (99%) | 0.55 | 11 (5%) 24 23 | 55, 102, 161, 213 | 0 |
| 14 | m3 | 194/194 (100%) | 0.59 | 16 (8%) 12 13 | 53, 113, 167, 220 | 0 |
| 15 | M4 | 136/137 (99%) | 0.25 | 2 (1%) 74 69 | 61, 88, 115, 151 | 0 |
| 15 | m4 | 137/137 (100%) | -0.10 | 0 100 100 | 45, 67, 96, 170 | 0 |
| 16 | M5 | 203/203 (100%) | 0.79 | 19 (9%) 9 10 | 52, 88, 116, 130 | 0 |
| 16 | m5 | 203/203 (100%) | 0.88 | 18 (8%) 10 11 | 58, 97, 120, 136 | 0 |
| 17 | M6 | 197/197 (100%) | 0.14 | 1 (0%) 90 88 | 45, 64, 104, 140 | 0 |
| 17 | m6 | 197/197 (100%) | -0.08 | 0 100 100 | 34, 50, 93, 123 | 0 |
| 18 | M7 | 183/184 (99%) | 0.91 | 25 (13%) 3 4 | 50, 70, 209, 262 | 0 |
| 18 | m7 | 155/184 (84%) | 0.12 | 1 (0%) 89 86 | 49, 67, 96, 136 | 0 |
| 19 | M8 | 185/185 (100%) | 0.48 | 2 (1%) 80 76 | 62, 83, 102, 160 | 0 |
| 19 | m8 | 185/185 (100%) | 0.42 | 3 (1%) 72 67 | 47, 83, 108, 135 | 0 |
| 20 | M9 | 182/188 (96%) | 0.42 | 7 (3%) 41 37 | 77, 106, 198, 250 | 0 |
| 20 | m9 | 188/188 (100%) | 0.46 | 11 (5%) 23 22 | 63, 95, 190, 264 | 0 |
| 21 | N0 | 172/172 (100%) | 0.56 | 13 (7%) 15 15 | 59, 80, 108, 150 | 0 |
| 21 | n0 | 172/172 (100%) | 0.08 | 2 (1%) 79 75 | 40, 57, 88, 123 | 0 |
| 22 | N1 | 159/159 (100%) | 0.53 | 8 (5%) 30 27 | 56, 84, 149, 195 | 0 |
| 22 | n1 | 159/159 (100%) | 0.32 | 5 (3%) 49 46 | 43, 68, 130, 165 | 0 |
| 23 | N2 | 100/100 (100%) | 0.79 | 13 (13%) 4 4 | 115, 150, 198, 212 | 0 |
| 23 | n2 | 98/100 (98%) | 1.42 | 26 (26%) 1 1 | 92, 136, 165, 200 | 0 |
| 24 | N3 | 136/136 (100%) | 0.41 | 4 (2%) 52 48 | 47, 75, 111, 159 | 0 |
| 24 | n3 | 136/136 (100%) | 0.44 | 2 (1%) 74 69 | 34, 55, 87, 130 | 0 |
| 25 | N4 | 98/155 (63%) | 1.76 | 27 (27%) 1 1 | 67, 97, 245, 294 | 0 |
| 26 | N5 | 121/121 (100%) | 0.92 | 12 (9%) 8 8 | 76, 107, 137, 228 | 0 |
| 26 | n5 | 120/121 (99%) | 0.69 | 9 (7%) 15 15 | 73, 116, 150, 171 | 0 |
| 27 | N6 | 126/126 (100%) | 0.98 | 15 (11%) 5 5 | 60, 96, 132, 163 | 0 |
| 27 | n6 | 126/126 (100%) | 0.74 | 11 (8%) 11 11 | 75, 110, 146, 183 | 0 |
| 28 | N7 | 135/135 (100%) | 2.24 | 70 (51%) 0 0 | 114, 145, 176, 223 | 0 |
| 28 | n7 | 135/135 (100%) | 1.48 | 36 (26%) 1 1 | 106, 144, 172, 207 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 29 | N8 | 148/148 (100%) | 0.74 | 21 (14%) 3 3 | 46, 84, 125, 154 | 0 |
| 29 | n8 | 148/148 (100%) | 0.40 | 6 (4%) 38 34 | 46, 85, 128, 156 | 0 |
| 30 | N9 | 58/58 (100%) | 0.75 | 8 (13%) 3 4 | 50, 90, 159, 165 | 0 |
| 30 | n9 | 58/58 (100%) | 0.36 | 1 (1%) 70 66 | 43, 87, 136, 176 | 0 |
| 31 | O0 | 97/100 (97%) | 0.78 | 13 (13%) 4 4 | 96, 132, 178, 188 | 0 |
| 31 | o0 | 100/100 (100%) | 0.61 | 8 (8%) 13 13 | 93, 124, 178, 229 | 0 |
| 32 | O1 | 109/109 (100%) | 1.04 | 12 (11%) 6 6 | 65, 92, 156, 210 | 0 |
| 32 | o1 | 109/109 (100%) | 0.58 | 5 (4%) 33 30 | 57, 80, 146, 186 | 0 |
| 33 | O2 | 127/127 (100%) | 0.14 | 3 (2%) 59 55 | 42, 67, 95, 128 | 0 |
| 33 | o2 | 127/127 (100%) | 0.13 | 1 (0%) 86 82 | 42, 76, 105, 157 | 0 |
| 34 | O3 | 106/106 (100%) | 0.11 | 0 100 100 | 51, 68, 106, 147 | 0 |
| 34 | o3 | 106/106 (100%) | 0.07 | 0 100 100 | 41, 60, 94, 133 | 0 |
| 35 | O4 | 112/112 (100%) | 0.85 | 15 (13%) 4 4 | 73, 114, 163, 223 | 0 |
| 35 | o4 | 112/112 (100%) | 0.60 | 9 (8%) 13 13 | 69, 104, 163, 198 | 0 |
| 36 | O5 | 119/119 (100%) | 0.60 | 5 (4%) 37 34 | 81, 111, 140, 163 | 0 |
| 36 | o5 | 119/119 (100%) | 0.60 | 5 (4%) 37 34 | 78, 123, 152, 162 | 0 |
| 37 | O6 | 99/99 (100%) | 0.44 | 7 (7%) 17 17 | 85, 111, 160, 197 | 0 |
| 37 | o6 | 99/99 (100%) | 0.87 | 15 (15%) 2 3 | 89, 117, 162, 193 | 0 |
| 38 | O7 | 87/87 (100%) | 0.32 | 2 (2%) 61 56 | 56, 76, 125, 211 | 0 |
| 38 | o7 | 87/87 (100%) | 0.47 | 2 (2%) 61 56 | 54, 82, 153, 163 | 0 |
| 39 | O8 | 77/77 (100%) | 0.79 | 9 (11%) 5 6 | 114, 147, 172, 230 | 0 |
| 39 | o8 | 77/77 (100%) | 1.37 | 22 (28%) 1 1 | 106, 136, 170, 181 | 0 |
| 40 | O9 | 50/50 (100%) | 0.50 | 2 (4%) 39 35 | 63, 84, 106, 116 | 0 |
| 40 | o9 | 50/50 (100%) | 0.48 | 1 (2%) 65 61 | 70, 91, 106, 108 | 0 |
| 41 | Q0 | 52/52 (100%) | 0.81 | 6 (11%) 5 6 | 61, 79, 108, 126 | 0 |
| 41 | q0 | 52/52 (100%) | 0.15 | 0 100 100 | 37, 51, 72, 118 | 0 |
| 42 | Q1 | 25/25 (100%) | 0.49 | 0 100 100 | 71, 84, 103, 104 | 0 |
| 42 | q1 | 25/25 (100%) | -0.04 | 0 100 100 | 55, 70, 90, 100 | 0 |
| 43 | Q2 | 105/105 (100%) | 0.72 | 11 (10%) 7 7 | 59, 84, 123, 165 | 0 |
| 43 | q2 | 105/105 (100%) | 0.20 | 1 (0%) 82 78 | 45, 74, 105, 179 | 0 |
| 44 | Q3 | 91/91 (100%) | 0.26 | 2 (2%) 62 57 | 54, 96, 128, 162 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | OWAB(Å ²) | Q<0.9 | |
|-----|-------|-----------------|--------|----------|-----|-----------------------|--------------------|---|
| 44 | q3 | 91/91 (100%) | 0.25 | 0 | 100 | 100 | 44, 85, 112, 130 | 0 |
| 45 | 2 | 1712/1800 (95%) | -0.02 | 23 (1%) | 77 | 73 | 70, 132, 242, 320 | 0 |
| 45 | 6 | 1739/1800 (96%) | -0.05 | 22 (1%) | 77 | 73 | 49, 95, 249, 344 | 0 |
| 46 | S0 | 206/206 (100%) | 1.38 | 57 (27%) | 1 | 1 | 109, 161, 224, 271 | 0 |
| 46 | s0 | 206/206 (100%) | 0.54 | 10 (4%) | 30 | 28 | 81, 124, 166, 215 | 0 |
| 47 | S1 | 214/216 (99%) | 1.06 | 48 (22%) | 1 | 1 | 114, 173, 227, 252 | 0 |
| 47 | s1 | 216/216 (100%) | 0.59 | 16 (7%) | 15 | 16 | 81, 117, 159, 193 | 0 |
| 48 | S2 | 217/217 (100%) | 0.90 | 32 (14%) | 3 | 3 | 84, 131, 171, 200 | 0 |
| 48 | s2 | 217/217 (100%) | 0.49 | 13 (5%) | 23 | 22 | 71, 104, 138, 174 | 0 |
| 49 | S3 | 223/223 (100%) | 1.21 | 50 (22%) | 1 | 1 | 82, 139, 193, 260 | 0 |
| 49 | s3 | 223/223 (100%) | 0.88 | 29 (13%) | 4 | 4 | 78, 116, 163, 223 | 0 |
| 50 | S4 | 260/260 (100%) | 1.46 | 84 (32%) | 0 | 0 | 97, 142, 169, 225 | 0 |
| 50 | s4 | 260/260 (100%) | 0.86 | 37 (14%) | 3 | 3 | 72, 127, 165, 189 | 0 |
| 51 | S5 | 206/206 (100%) | 1.64 | 56 (27%) | 1 | 1 | 131, 172, 213, 237 | 0 |
| 51 | s5 | 206/206 (100%) | 0.49 | 14 (6%) | 18 | 18 | 64, 97, 147, 197 | 0 |
| 52 | S6 | 226/236 (95%) | 0.88 | 30 (13%) | 4 | 4 | 82, 145, 214, 373 | 0 |
| 52 | s6 | 218/236 (92%) | 0.69 | 18 (8%) | 12 | 13 | 73, 120, 168, 213 | 0 |
| 53 | S7 | 184/186 (98%) | 0.96 | 29 (15%) | 2 | 2 | 115, 179, 224, 251 | 0 |
| 53 | s7 | 186/186 (100%) | 0.77 | 21 (11%) | 6 | 6 | 99, 157, 207, 271 | 0 |
| 54 | S8 | 188/200 (94%) | 1.59 | 63 (33%) | 0 | 0 | 84, 125, 176, 199 | 0 |
| 54 | s8 | 186/200 (93%) | 0.73 | 20 (10%) | 6 | 7 | 70, 113, 164, 198 | 0 |
| 55 | S9 | 185/185 (100%) | 1.51 | 60 (32%) | 0 | 0 | 111, 152, 192, 244 | 0 |
| 55 | s9 | 185/185 (100%) | 0.83 | 20 (10%) | 6 | 7 | 87, 134, 188, 215 | 0 |
| 56 | C0 | 96/105 (91%) | 1.32 | 25 (26%) | 1 | 1 | 127, 170, 212, 235 | 0 |
| 56 | c0 | 96/105 (91%) | 1.22 | 21 (21%) | 1 | 1 | 93, 137, 193, 217 | 0 |
| 57 | C1 | 155/156 (99%) | 1.89 | 62 (40%) | 0 | 0 | 84, 122, 201, 267 | 0 |
| 57 | c1 | 142/156 (91%) | 0.98 | 14 (9%) | 8 | 8 | 69, 111, 169, 198 | 0 |
| 58 | C2 | 124/143 (86%) | 2.46 | 62 (50%) | 0 | 0 | 175, 223, 267, 294 | 0 |
| 58 | c2 | 124/143 (86%) | 1.74 | 51 (41%) | 0 | 0 | 132, 190, 233, 259 | 0 |
| 59 | C3 | 150/150 (100%) | 0.72 | 12 (8%) | 13 | 13 | 95, 139, 177, 206 | 0 |
| 59 | c3 | 150/150 (100%) | 0.10 | 2 (1%) | 77 | 73 | 67, 111, 148, 173 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 60 | C4 | 127/128 (99%) | 1.16 | 37 (29%) 1 1 | 93, 164, 207, 215 | 0 |
| 60 | c4 | 128/128 (100%) | 0.81 | 11 (8%) 11 12 | 63, 103, 135, 156 | 0 |
| 61 | C5 | 124/141 (87%) | 1.25 | 36 (29%) 1 1 | 108, 165, 211, 236 | 0 |
| 61 | c5 | 135/141 (95%) | 0.40 | 7 (5%) 28 26 | 61, 96, 162, 201 | 0 |
| 62 | C6 | 141/142 (99%) | 1.94 | 56 (39%) 0 0 | 105, 157, 196, 212 | 0 |
| 62 | c6 | 142/142 (100%) | 0.38 | 4 (2%) 53 50 | 59, 91, 128, 197 | 0 |
| 63 | C7 | 120/136 (88%) | 1.34 | 31 (25%) 1 1 | 110, 161, 290, 384 | 0 |
| 63 | c7 | 117/136 (86%) | 0.58 | 8 (6%) 18 18 | 81, 123, 194, 239 | 0 |
| 64 | C8 | 145/145 (100%) | 1.46 | 51 (35%) 0 0 | 102, 165, 211, 235 | 0 |
| 64 | c8 | 145/145 (100%) | 0.02 | 2 (1%) 75 71 | 64, 82, 128, 184 | 0 |
| 65 | C9 | 143/143 (100%) | 1.17 | 31 (21%) 1 1 | 128, 159, 204, 232 | 0 |
| 65 | c9 | 143/143 (100%) | 0.18 | 3 (2%) 64 60 | 61, 84, 117, 154 | 0 |
| 66 | D0 | 107/110 (97%) | 1.38 | 29 (27%) 1 1 | 101, 156, 232, 270 | 0 |
| 66 | d0 | 110/110 (100%) | 1.31 | 30 (27%) 1 1 | 68, 121, 203, 223 | 0 |
| 67 | D1 | 87/87 (100%) | 1.48 | 27 (31%) 0 1 | 112, 151, 183, 198 | 0 |
| 67 | d1 | 87/87 (100%) | 0.48 | 7 (8%) 13 13 | 87, 117, 158, 188 | 0 |
| 68 | D2 | 129/129 (100%) | 1.09 | 27 (20%) 1 1 | 99, 127, 155, 176 | 0 |
| 68 | d2 | 129/129 (100%) | 0.64 | 5 (3%) 40 36 | 74, 99, 120, 137 | 0 |
| 69 | D3 | 144/144 (100%) | 0.77 | 15 (10%) 7 7 | 76, 102, 127, 174 | 0 |
| 69 | d3 | 144/144 (100%) | 0.08 | 1 (0%) 87 85 | 51, 73, 99, 157 | 0 |
| 70 | D4 | 134/134 (100%) | 1.13 | 27 (20%) 1 1 | 106, 152, 191, 215 | 0 |
| 70 | d4 | 133/134 (99%) | 0.61 | 15 (11%) 6 6 | 80, 134, 173, 195 | 0 |
| 71 | D5 | 70/70 (100%) | 2.71 | 48 (68%) 0 0 | 151, 189, 233, 266 | 0 |
| 71 | d5 | 69/70 (98%) | 0.48 | 3 (4%) 36 33 | 77, 108, 142, 162 | 0 |
| 72 | D6 | 97/97 (100%) | 1.20 | 25 (25%) 1 1 | 86, 126, 189, 239 | 0 |
| 72 | d6 | 97/97 (100%) | 0.31 | 2 (2%) 64 60 | 63, 88, 136, 238 | 0 |
| 73 | D7 | 81/81 (100%) | 1.67 | 34 (41%) 0 0 | 117, 161, 215, 267 | 0 |
| 73 | d7 | 81/81 (100%) | 0.69 | 10 (12%) 5 5 | 92, 124, 199, 227 | 0 |
| 74 | D8 | 63/63 (100%) | 1.95 | 29 (46%) 0 0 | 136, 175, 215, 257 | 0 |
| 74 | d8 | 63/63 (100%) | 1.33 | 17 (26%) 1 1 | 81, 117, 146, 165 | 0 |
| 75 | D9 | 53/53 (100%) | 1.32 | 16 (30%) 1 1 | 104, 128, 154, 187 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 75 | d9 | 53/53 (100%) | 0.57 | 5 (9%) 9 10 | 64, 86, 109, 148 | 0 |
| 76 | E0 | 60/62 (96%) | 1.42 | 18 (30%) 1 1 | 98, 144, 215, 237 | 0 |
| 76 | e0 | 62/62 (100%) | 0.65 | 6 (9%) 8 9 | 64, 118, 179, 202 | 0 |
| 77 | E1 | 71/72 (98%) | 1.72 | 23 (32%) 0 0 | 143, 199, 243, 257 | 0 |
| 77 | e1 | 72/72 (100%) | 1.32 | 20 (27%) 1 1 | 125, 174, 212, 236 | 0 |
| 78 | SR | 318/318 (100%) | 2.13 | 147 (46%) 0 0 | 131, 175, 225, 269 | 0 |
| 78 | sR | 318/318 (100%) | 0.88 | 48 (15%) 3 3 | 88, 125, 174, 226 | 0 |
| 79 | SM | 159/272 (58%) | 0.85 | 25 (15%) 2 2 | 88, 153, 237, 268 | 0 |
| 79 | sM | 129/272 (47%) | 0.53 | 10 (7%) 14 14 | 76, 118, 187, 220 | 0 |
| 80 | m2 | 0/165 | - | - | - | - |
| 81 | n4 | 135/135 (100%) | 1.00 | 23 (17%) 2 2 | 42, 139, 211, 238 | 0 |
| 82 | p0 | 143/312 (45%) | 0.94 | 23 (16%) 2 2 | 84, 138, 215, 261 | 0 |
| 83 | p1 | 0/47 | - | - | - | - |
| All | All | 32909/34616 (95%) | 0.50 | 2769 (8%) 12 12 | 32, 103, 196, 384 | 0 |

The worst 5 of 2769 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 25 | N4 | 75 | THR | 15.4 |
| 25 | N4 | 76 | VAL | 12.9 |
| 18 | M7 | 167 | ARG | 12.4 |
| 57 | C1 | 146 | ALA | 12.4 |
| 57 | C1 | 145 | ALA | 11.3 |

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|-------|----------------------------|-------|
| 84 | MG | 5 | 4048 | 1/1 | 0.93 | 0.56 | 60.88 | 64,64,64,64 | 0 |
| 84 | MG | 1 | 3529 | 1/1 | 0.81 | 0.76 | 51.58 | 66,66,66,66 | 0 |
| 84 | MG | 5 | 3634 | 1/1 | -0.07 | 1.24 | 50.74 | 57,57,57,57 | 0 |
| 84 | MG | 5 | 3667 | 1/1 | 0.95 | 0.56 | 48.93 | 49,49,49,49 | 0 |
| 84 | MG | 5 | 3868 | 1/1 | 0.70 | 0.74 | 38.76 | 57,57,57,57 | 0 |
| 84 | MG | 5 | 3577 | 1/1 | 0.75 | 0.57 | 36.10 | 54,54,54,54 | 0 |
| 84 | MG | 1 | 3605 | 1/1 | 0.92 | 0.72 | 35.75 | 46,46,46,46 | 0 |
| 84 | MG | 5 | 3535 | 1/1 | 0.93 | 0.44 | 35.68 | 57,57,57,57 | 0 |
| 84 | MG | 1 | 3695 | 1/1 | 0.83 | 0.64 | 35.42 | 67,67,67,67 | 0 |
| 84 | MG | 5 | 3964 | 1/1 | 0.89 | 0.59 | 32.52 | 82,82,82,82 | 0 |
| 84 | MG | 5 | 3904 | 1/1 | 0.64 | 0.62 | 31.61 | 59,59,59,59 | 0 |
| 84 | MG | 1 | 3508 | 1/1 | 0.79 | 0.90 | 30.00 | 60,60,60,60 | 0 |
| 84 | MG | 1 | 3526 | 1/1 | 0.94 | 0.57 | 28.34 | 65,65,65,65 | 0 |
| 84 | MG | 5 | 3743 | 1/1 | 0.87 | 0.44 | 27.07 | 61,61,61,61 | 0 |
| 84 | MG | 1 | 3767 | 1/1 | 0.90 | 0.56 | 25.87 | 57,57,57,57 | 0 |
| 84 | MG | 2 | 1980 | 1/1 | 0.46 | 0.54 | 25.28 | 77,77,77,77 | 0 |
| 84 | MG | 5 | 3881 | 1/1 | 0.85 | 0.43 | 24.55 | 63,63,63,63 | 0 |
| 84 | MG | 5 | 3993 | 1/1 | 0.93 | 0.44 | 24.18 | 56,56,56,56 | 0 |
| 84 | MG | 6 | 2127 | 1/1 | 0.84 | 0.44 | 22.96 | 76,76,76,76 | 0 |
| 84 | MG | 5 | 3449 | 1/1 | 0.89 | 0.42 | 22.77 | 50,50,50,50 | 0 |
| 84 | MG | 5 | 3768 | 1/1 | 0.68 | 0.41 | 22.49 | 73,73,73,73 | 0 |
| 84 | MG | 1 | 3430 | 1/1 | 0.80 | 0.38 | 21.91 | 54,54,54,54 | 0 |
| 84 | MG | 1 | 3690 | 1/1 | 0.97 | 0.40 | 21.67 | 58,58,58,58 | 0 |
| 84 | MG | 1 | 3545 | 1/1 | 0.70 | 0.55 | 21.36 | 62,62,62,62 | 0 |
| 84 | MG | 1 | 3432 | 1/1 | 0.96 | 0.43 | 20.98 | 46,46,46,46 | 0 |
| 84 | MG | 5 | 3954 | 1/1 | 0.77 | 0.62 | 20.81 | 58,58,58,58 | 0 |
| 84 | MG | 1 | 3875 | 1/1 | 0.86 | 0.38 | 18.24 | 64,64,64,64 | 0 |
| 84 | MG | 1 | 3532 | 1/1 | 0.93 | 0.66 | 17.82 | 68,68,68,68 | 0 |
| 84 | MG | 5 | 3668 | 1/1 | 0.95 | 0.44 | 17.78 | 49,49,49,49 | 0 |
| 84 | MG | 6 | 1943 | 1/1 | 0.70 | 0.35 | 17.59 | 65,65,65,65 | 0 |
| 84 | MG | 5 | 3407 | 1/1 | 0.98 | 0.37 | 17.42 | 43,43,43,43 | 0 |
| 84 | MG | 1 | 3962 | 1/1 | 0.92 | 0.28 | 17.12 | 78,78,78,78 | 0 |
| 84 | MG | 1 | 3441 | 1/1 | 0.89 | 0.33 | 15.42 | 62,62,62,62 | 0 |
| 84 | MG | 6 | 2079 | 1/1 | 0.83 | 0.38 | 15.38 | 63,63,63,63 | 0 |
| 84 | MG | 1 | 3612 | 1/1 | 0.96 | 0.37 | 15.29 | 55,55,55,55 | 0 |
| 84 | MG | 1 | 3826 | 1/1 | 0.97 | 0.42 | 15.27 | 65,65,65,65 | 0 |
| 84 | MG | 1 | 3522 | 1/1 | 0.99 | 0.34 | 15.26 | 63,63,63,63 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 84 | MG | 5 | 3417 | 1/1 | 0.97 | 0.38 | 15.23 | 43,43,43,43 | 0 |
| 84 | MG | 2 | 1926 | 1/1 | 0.97 | 0.52 | 15.15 | 89,89,89,89 | 0 |
| 84 | MG | 5 | 3483 | 1/1 | 0.79 | 0.36 | 14.94 | 57,57,57,57 | 0 |
| 84 | MG | 1 | 3827 | 1/1 | 0.76 | 0.47 | 14.54 | 61,61,61,61 | 0 |
| 84 | MG | 1 | 3930 | 1/1 | 0.84 | 0.38 | 14.52 | 73,73,73,73 | 0 |
| 84 | MG | 5 | 4064 | 1/1 | 0.93 | 0.36 | 14.32 | 44,44,44,44 | 0 |
| 84 | MG | 5 | 3592 | 1/1 | 0.89 | 0.34 | 14.30 | 57,57,57,57 | 0 |
| 84 | MG | 5 | 3418 | 1/1 | 0.98 | 0.29 | 13.80 | 44,44,44,44 | 0 |
| 84 | MG | 1 | 3894 | 1/1 | 0.93 | 0.35 | 13.58 | 60,60,60,60 | 0 |
| 84 | MG | 5 | 3448 | 1/1 | 0.89 | 0.35 | 13.11 | 49,49,49,49 | 0 |
| 84 | MG | 5 | 3738 | 1/1 | 0.99 | 0.30 | 13.07 | 50,50,50,50 | 0 |
| 84 | MG | 6 | 2038 | 1/1 | 0.89 | 0.30 | 13.00 | 85,85,85,85 | 0 |
| 84 | MG | 1 | 3611 | 1/1 | 0.88 | 0.40 | 12.98 | 47,47,47,47 | 0 |
| 84 | MG | 5 | 3693 | 1/1 | 0.76 | 0.32 | 12.83 | 81,81,81,81 | 0 |
| 84 | MG | 5 | 4012 | 1/1 | 0.79 | 0.31 | 12.55 | 61,61,61,61 | 0 |
| 84 | MG | 6 | 2096 | 1/1 | 0.91 | 0.40 | 12.52 | 65,65,65,65 | 0 |
| 84 | MG | 5 | 3569 | 1/1 | 0.95 | 0.43 | 12.50 | 64,64,64,64 | 0 |
| 84 | MG | 5 | 3585 | 1/1 | 0.97 | 0.38 | 12.33 | 48,48,48,48 | 0 |
| 84 | MG | 1 | 3795 | 1/1 | 0.97 | 0.41 | 12.33 | 56,56,56,56 | 0 |
| 84 | MG | 5 | 3587 | 1/1 | 0.96 | 0.35 | 12.23 | 55,55,55,55 | 0 |
| 84 | MG | 1 | 3820 | 1/1 | 0.79 | 0.45 | 12.18 | 76,76,76,76 | 0 |
| 84 | MG | 1 | 3701 | 1/1 | 0.96 | 0.29 | 12.09 | 59,59,59,59 | 0 |
| 84 | MG | 1 | 3937 | 1/1 | 0.81 | 0.42 | 12.02 | 73,73,73,73 | 0 |
| 84 | MG | 5 | 3957 | 1/1 | 0.96 | 0.30 | 11.95 | 57,57,57,57 | 0 |
| 84 | MG | 1 | 3509 | 1/1 | 0.82 | 0.54 | 11.80 | 60,60,60,60 | 0 |
| 84 | MG | M5 | 305 | 1/1 | 0.64 | 0.33 | 11.69 | 72,72,72,72 | 0 |
| 84 | MG | 1 | 3516 | 1/1 | 0.97 | 0.34 | 11.68 | 54,54,54,54 | 0 |
| 84 | MG | 5 | 3454 | 1/1 | 0.87 | 0.42 | 11.32 | 46,46,46,46 | 0 |
| 84 | MG | 5 | 3416 | 1/1 | 0.95 | 0.31 | 11.07 | 45,45,45,45 | 0 |
| 84 | MG | 1 | 3438 | 1/1 | 0.96 | 0.30 | 11.06 | 51,51,51,51 | 0 |
| 84 | MG | 6 | 2029 | 1/1 | 0.94 | 0.27 | 10.99 | 75,75,75,75 | 0 |
| 84 | MG | 2 | 1995 | 1/1 | 0.95 | 0.40 | 10.88 | 100,100,100,100 | 0 |
| 84 | MG | 5 | 3478 | 1/1 | 0.94 | 0.42 | 10.83 | 50,50,50,50 | 0 |
| 84 | MG | 5 | 3639 | 1/1 | 0.97 | 0.30 | 10.78 | 42,42,42,42 | 0 |
| 84 | MG | 5 | 3848 | 1/1 | 0.97 | 0.26 | 10.64 | 44,44,44,44 | 0 |
| 84 | MG | 2 | 1923 | 1/1 | 0.84 | 0.41 | 10.63 | 87,87,87,87 | 0 |
| 84 | MG | 5 | 3485 | 1/1 | 0.91 | 0.29 | 10.57 | 57,57,57,57 | 0 |
| 84 | MG | 1 | 3601 | 1/1 | 0.94 | 0.35 | 10.30 | 53,53,53,53 | 0 |
| 85 | LLL | 7 | 232 | 31/31 | 0.86 | 0.34 | 10.28 | 81,81,81,81 | 31 |
| 84 | MG | 5 | 3405 | 1/1 | 0.98 | 0.42 | 10.27 | 47,47,47,47 | 0 |
| 84 | MG | 1 | 3678 | 1/1 | 0.97 | 0.28 | 10.27 | 69,69,69,69 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 84 | MG | 1 | 3917 | 1/1 | 0.42 | 0.35 | 10.11 | 74,74,74,74 | 0 |
| 84 | MG | 1 | 3517 | 1/1 | 0.95 | 0.42 | 9.99 | 54,54,54,54 | 0 |
| 84 | MG | 5 | 3745 | 1/1 | 0.95 | 0.34 | 9.92 | 52,52,52,52 | 0 |
| 85 | LLL | 5 | 4174 | 31/31 | 0.87 | 0.33 | 9.52 | 47,47,47,47 | 31 |
| 84 | MG | 1 | 3521 | 1/1 | 0.63 | 0.43 | 9.49 | 69,69,69,69 | 0 |
| 84 | MG | 5 | 3956 | 1/1 | 0.98 | 0.29 | 9.47 | 55,55,55,55 | 0 |
| 84 | MG | 1 | 3544 | 1/1 | 0.97 | 0.38 | 9.44 | 54,54,54,54 | 0 |
| 84 | MG | 2 | 1908 | 1/1 | 0.84 | 0.36 | 9.29 | 104,104,104,104 | 0 |
| 84 | MG | 5 | 3905 | 1/1 | 0.94 | 0.45 | 9.26 | 44,44,44,44 | 0 |
| 84 | MG | 5 | 3531 | 1/1 | 0.94 | 0.35 | 9.22 | 43,43,43,43 | 0 |
| 84 | MG | N3 | 202 | 1/1 | 0.97 | 0.32 | 9.07 | 55,55,55,55 | 0 |
| 84 | MG | 1 | 3839 | 1/1 | 0.98 | 0.34 | 9.01 | 57,57,57,57 | 0 |
| 84 | MG | 1 | 3590 | 1/1 | 0.65 | 0.39 | 8.98 | 58,58,58,58 | 0 |
| 84 | MG | 5 | 3546 | 1/1 | 0.82 | 0.37 | 8.96 | 63,63,63,63 | 0 |
| 84 | MG | 5 | 3429 | 1/1 | 0.92 | 0.36 | 8.89 | 48,48,48,48 | 0 |
| 84 | MG | 1 | 3838 | 1/1 | 0.88 | 0.32 | 8.86 | 50,50,50,50 | 0 |
| 84 | MG | 6 | 1929 | 1/1 | 0.85 | 0.38 | 8.84 | 69,69,69,69 | 0 |
| 84 | MG | 1 | 3535 | 1/1 | 0.92 | 0.48 | 8.82 | 62,62,62,62 | 0 |
| 84 | MG | 5 | 3613 | 1/1 | 0.92 | 0.32 | 8.80 | 79,79,79,79 | 0 |
| 84 | MG | 6 | 2099 | 1/1 | 0.97 | 0.31 | 8.79 | 57,57,57,57 | 0 |
| 84 | MG | 5 | 3411 | 1/1 | 0.97 | 0.38 | 8.73 | 46,46,46,46 | 0 |
| 84 | MG | 2 | 1985 | 1/1 | 0.94 | 0.28 | 8.70 | 122,122,122,122 | 0 |
| 84 | MG | 5 | 3611 | 1/1 | 0.47 | 0.38 | 8.67 | 104,104,104,104 | 0 |
| 84 | MG | 1 | 3739 | 1/1 | 0.81 | 0.42 | 8.65 | 72,72,72,72 | 0 |
| 84 | MG | 6 | 2080 | 1/1 | 0.91 | 0.31 | 8.56 | 62,62,62,62 | 0 |
| 84 | MG | 5 | 3551 | 1/1 | 0.84 | 0.48 | 8.55 | 56,56,56,56 | 0 |
| 84 | MG | 1 | 3824 | 1/1 | 0.83 | 0.37 | 8.47 | 62,62,62,62 | 0 |
| 84 | MG | 8 | 207 | 1/1 | 0.77 | 0.31 | 8.35 | 74,74,74,74 | 0 |
| 84 | MG | 1 | 3770 | 1/1 | 0.96 | 0.36 | 8.20 | 55,55,55,55 | 0 |
| 84 | MG | 5 | 4052 | 1/1 | 0.80 | 0.43 | 8.09 | 77,77,77,77 | 0 |
| 84 | MG | 1 | 3405 | 1/1 | 0.96 | 0.35 | 8.06 | 53,53,53,53 | 0 |
| 84 | MG | 1 | 3619 | 1/1 | 0.97 | 0.32 | 8.02 | 59,59,59,59 | 0 |
| 84 | MG | 5 | 3939 | 1/1 | 0.83 | 0.24 | 7.92 | 76,76,76,76 | 0 |
| 84 | MG | 1 | 3924 | 1/1 | 0.91 | 0.35 | 7.90 | 65,65,65,65 | 0 |
| 84 | MG | 1 | 3925 | 1/1 | 0.85 | 0.30 | 7.88 | 83,83,83,83 | 0 |
| 84 | MG | 5 | 3832 | 1/1 | 0.93 | 0.24 | 7.86 | 50,50,50,50 | 0 |
| 84 | MG | 1 | 3596 | 1/1 | 0.96 | 0.36 | 7.84 | 55,55,55,55 | 0 |
| 84 | MG | 5 | 3673 | 1/1 | 0.99 | 0.33 | 7.82 | 55,55,55,55 | 0 |
| 84 | MG | 5 | 3986 | 1/1 | 0.96 | 0.34 | 7.81 | 45,45,45,45 | 1 |
| 84 | MG | 5 | 3690 | 1/1 | 0.73 | 0.31 | 7.79 | 65,65,65,65 | 0 |
| 84 | MG | 1 | 3831 | 1/1 | 0.85 | 0.38 | 7.73 | 59,59,59,59 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 5 | 4059 | 1/1 | 0.86 | 0.37 | 7.66 | 66,66,66,66 | 0 |
| 84 | MG | 5 | 3663 | 1/1 | 0.96 | 0.31 | 7.58 | 46,46,46,46 | 0 |
| 84 | MG | 1 | 3760 | 1/1 | 0.93 | 0.34 | 7.54 | 69,69,69,69 | 0 |
| 84 | MG | 1 | 3549 | 1/1 | 0.87 | 0.27 | 7.53 | 67,67,67,67 | 0 |
| 84 | MG | 5 | 3895 | 1/1 | 0.91 | 0.32 | 7.52 | 57,57,57,57 | 0 |
| 84 | MG | 5 | 3530 | 1/1 | 0.89 | 0.37 | 7.46 | 47,47,47,47 | 1 |
| 84 | MG | 5 | 3413 | 1/1 | 0.97 | 0.30 | 7.45 | 46,46,46,46 | 0 |
| 84 | MG | 6 | 2095 | 1/1 | 0.93 | 0.33 | 7.40 | 65,65,65,65 | 0 |
| 84 | MG | 6 | 2098 | 1/1 | 0.94 | 0.32 | 7.38 | 63,63,63,63 | 0 |
| 84 | MG | 1 | 3401 | 1/1 | 0.98 | 0.31 | 7.27 | 56,56,56,56 | 0 |
| 84 | MG | 5 | 3700 | 1/1 | 0.90 | 0.32 | 7.20 | 65,65,65,65 | 0 |
| 84 | MG | 1 | 3587 | 1/1 | 0.97 | 0.31 | 7.20 | 58,58,58,58 | 0 |
| 84 | MG | 6 | 2077 | 1/1 | 0.93 | 0.32 | 7.14 | 65,65,65,65 | 0 |
| 84 | MG | D3 | 203 | 1/1 | 0.83 | 0.36 | 7.05 | 85,85,85,85 | 0 |
| 84 | MG | 1 | 3559 | 1/1 | 0.82 | 0.24 | 6.95 | 73,73,73,73 | 0 |
| 84 | MG | 1 | 3499 | 1/1 | 0.76 | 0.46 | 6.91 | 61,61,61,61 | 0 |
| 84 | MG | 6 | 2034 | 1/1 | 0.66 | 0.39 | 6.88 | 69,69,69,69 | 0 |
| 84 | MG | 5 | 3835 | 1/1 | 0.94 | 0.30 | 6.86 | 62,62,62,62 | 0 |
| 84 | MG | 5 | 3401 | 1/1 | 0.95 | 0.36 | 6.78 | 49,49,49,49 | 0 |
| 84 | MG | 5 | 3949 | 1/1 | 0.97 | 0.36 | 6.77 | 56,56,56,56 | 0 |
| 84 | MG | 1 | 3473 | 1/1 | 0.99 | 0.37 | 6.76 | 59,59,59,59 | 0 |
| 84 | MG | 1 | 3465 | 1/1 | 0.79 | 0.37 | 6.65 | 56,56,56,56 | 0 |
| 84 | MG | 5 | 3987 | 1/1 | 0.92 | 0.35 | 6.61 | 48,48,48,48 | 0 |
| 84 | MG | 1 | 3417 | 1/1 | 0.96 | 0.28 | 6.57 | 52,52,52,52 | 0 |
| 84 | MG | 5 | 3852 | 1/1 | 0.93 | 0.31 | 6.56 | 57,57,57,57 | 0 |
| 84 | MG | N3 | 204 | 1/1 | 0.49 | 0.39 | 6.51 | 87,87,87,87 | 0 |
| 84 | MG | 1 | 3599 | 1/1 | 0.99 | 0.28 | 6.45 | 52,52,52,52 | 0 |
| 84 | MG | 5 | 3764 | 1/1 | 0.73 | 0.32 | 6.38 | 78,78,78,78 | 0 |
| 85 | LLL | 5 | 4177 | 31/31 | 0.86 | 0.32 | 6.35 | 51,51,51,51 | 31 |
| 85 | LLL | 5 | 4169 | 31/31 | 0.87 | 0.31 | 6.35 | 51,51,51,51 | 31 |
| 84 | MG | 1 | 3449 | 1/1 | 0.91 | 0.26 | 6.34 | 56,56,56,56 | 0 |
| 84 | MG | 5 | 3811 | 1/1 | 0.98 | 0.30 | 6.18 | 44,44,44,44 | 0 |
| 84 | MG | 1 | 3833 | 1/1 | 0.95 | 0.27 | 6.18 | 64,64,64,64 | 0 |
| 84 | MG | 1 | 3403 | 1/1 | 0.97 | 0.35 | 6.16 | 58,58,58,58 | 0 |
| 84 | MG | 6 | 2022 | 1/1 | 0.92 | 0.26 | 6.15 | 88,88,88,88 | 0 |
| 84 | MG | 1 | 3856 | 1/1 | 0.97 | 0.26 | 6.14 | 55,55,55,55 | 0 |
| 84 | MG | 1 | 3929 | 1/1 | 0.83 | 0.55 | 6.13 | 63,63,63,63 | 0 |
| 84 | MG | o2 | 201 | 1/1 | 0.97 | 0.30 | 6.13 | 55,55,55,55 | 0 |
| 84 | MG | 1 | 3436 | 1/1 | 0.99 | 0.28 | 6.05 | 49,49,49,49 | 0 |
| 84 | MG | 2 | 1971 | 1/1 | 0.97 | 0.26 | 5.98 | 102,102,102,102 | 0 |
| 84 | MG | 1 | 3644 | 1/1 | 0.98 | 0.32 | 5.97 | 49,49,49,49 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | n3 | 201 | 1/1 | 0.96 | 0.25 | 5.97 | 43,43,43,43 | 0 |
| 85 | LLL | 1 | 3997 | 31/31 | 0.88 | 0.36 | 5.94 | 108,108,108,108 | 0 |
| 84 | MG | 1 | 3423 | 1/1 | 0.95 | 0.30 | 5.93 | 51,51,51,51 | 0 |
| 84 | MG | 5 | 3694 | 1/1 | 0.82 | 0.22 | 5.90 | 84,84,84,84 | 0 |
| 84 | MG | 1 | 3686 | 1/1 | 0.78 | 0.34 | 5.83 | 57,57,57,57 | 0 |
| 84 | MG | 5 | 4009 | 1/1 | 0.96 | 0.38 | 5.79 | 53,53,53,53 | 0 |
| 84 | MG | 6 | 1950 | 1/1 | 0.82 | 0.28 | 5.73 | 72,72,72,72 | 0 |
| 84 | MG | 4 | 219 | 1/1 | 0.91 | 0.26 | 5.70 | 68,68,68,68 | 0 |
| 84 | MG | 2 | 1925 | 1/1 | 0.94 | 0.28 | 5.67 | 90,90,90,90 | 0 |
| 84 | MG | 5 | 4029 | 1/1 | 0.97 | 0.27 | 5.62 | 52,52,52,52 | 0 |
| 84 | MG | 1 | 3502 | 1/1 | 0.83 | 0.37 | 5.59 | 64,64,64,64 | 0 |
| 85 | LLL | 6 | 2175 | 31/31 | 0.85 | 0.30 | 5.58 | 66,66,66,66 | 31 |
| 84 | MG | 1 | 3606 | 1/1 | 0.97 | 0.29 | 5.48 | 52,52,52,52 | 0 |
| 84 | MG | 5 | 3420 | 1/1 | 0.89 | 0.29 | 5.43 | 50,50,50,50 | 0 |
| 84 | MG | 5 | 3817 | 1/1 | 0.92 | 0.25 | 5.37 | 41,41,41,41 | 0 |
| 85 | LLL | 6 | 2167 | 31/31 | 0.91 | 0.35 | 5.28 | 97,98,98,98 | 0 |
| 84 | MG | 6 | 1925 | 1/1 | 0.95 | 0.28 | 5.28 | 68,68,68,68 | 0 |
| 84 | MG | 1 | 3408 | 1/1 | 0.96 | 0.27 | 5.26 | 51,51,51,51 | 0 |
| 84 | MG | 5 | 3959 | 1/1 | 0.93 | 0.36 | 5.22 | 51,51,51,51 | 0 |
| 84 | MG | 5 | 4047 | 1/1 | 0.88 | 0.33 | 5.19 | 52,52,52,52 | 0 |
| 84 | MG | 5 | 3610 | 1/1 | 0.85 | 0.24 | 5.17 | 110,110,110,110 | 0 |
| 84 | MG | 6 | 2043 | 1/1 | 0.96 | 0.21 | 5.11 | 96,96,96,96 | 0 |
| 84 | MG | 5 | 3412 | 1/1 | 0.98 | 0.27 | 5.09 | 47,47,47,47 | 0 |
| 85 | LLL | 1 | 4000 | 31/31 | 0.84 | 0.29 | 4.98 | 84,85,85,85 | 31 |
| 85 | LLL | 5 | 4166 | 31/31 | 0.89 | 0.26 | 4.98 | 77,78,78,78 | 31 |
| 84 | MG | 5 | 3465 | 1/1 | 0.93 | 0.29 | 4.94 | 41,41,41,41 | 0 |
| 84 | MG | 1 | 3540 | 1/1 | 0.94 | 0.27 | 4.91 | 54,54,54,54 | 0 |
| 84 | MG | 6 | 2026 | 1/1 | 0.79 | 0.28 | 4.90 | 78,78,78,78 | 0 |
| 84 | MG | 5 | 3737 | 1/1 | 0.97 | 0.27 | 4.86 | 49,49,49,49 | 0 |
| 84 | MG | 1 | 3586 | 1/1 | 0.88 | 0.28 | 4.84 | 58,58,58,58 | 0 |
| 85 | LLL | 5 | 4175 | 31/31 | 0.85 | 0.29 | 4.72 | 60,60,60,60 | 31 |
| 84 | MG | 5 | 3589 | 1/1 | 0.97 | 0.35 | 4.68 | 58,58,58,58 | 0 |
| 85 | LLL | 2 | 2044 | 31/31 | 0.86 | 0.28 | 4.59 | 116,116,116,116 | 0 |
| 84 | MG | 1 | 3446 | 1/1 | 0.82 | 0.23 | 4.57 | 62,62,62,62 | 0 |
| 85 | LLL | 1 | 3995 | 31/31 | 0.88 | 0.24 | 4.51 | 124,125,125,125 | 0 |
| 84 | MG | 1 | 3536 | 1/1 | 0.90 | 0.31 | 4.47 | 64,64,64,64 | 0 |
| 84 | MG | O3 | 201 | 1/1 | 0.82 | 0.41 | 4.45 | 64,64,64,64 | 0 |
| 84 | MG | 1 | 3914 | 1/1 | 0.83 | 0.26 | 4.45 | 59,59,59,59 | 0 |
| 85 | LLL | 5 | 4178 | 31/31 | 0.79 | 0.35 | 4.44 | 69,69,69,69 | 31 |
| 84 | MG | 1 | 3737 | 1/1 | 0.90 | 0.33 | 4.41 | 73,73,73,73 | 0 |
| 84 | MG | m4 | 204 | 1/1 | 0.89 | 0.38 | 4.40 | 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 | MG | 5 | 3981 | 1/1 | 0.86 | 0.31 | 4.38 | 46,46,46,46 | 0 |
| 85 | LLL | 5 | 4152 | 31/31 | 0.92 | 0.27 | 4.22 | 79,79,79,79 | 31 |
| 85 | LLL | 5 | 4153 | 31/31 | 0.91 | 0.28 | 4.07 | 64,64,65,65 | 0 |
| 84 | MG | 6 | 1928 | 1/1 | 0.99 | 0.31 | 4.06 | 68,68,68,68 | 0 |
| 84 | MG | 5 | 3427 | 1/1 | 0.93 | 0.30 | 4.03 | 45,45,45,45 | 0 |
| 84 | MG | 2 | 1927 | 1/1 | 0.98 | 0.26 | 4.00 | 95,95,95,95 | 0 |
| 84 | MG | 6 | 1904 | 1/1 | 0.93 | 0.29 | 3.99 | 65,65,65,65 | 0 |
| 84 | MG | 5 | 3446 | 1/1 | 0.87 | 0.33 | 3.97 | 53,53,53,53 | 0 |
| 84 | MG | 5 | 3466 | 1/1 | 0.87 | 0.34 | 3.90 | 50,50,50,50 | 0 |
| 84 | MG | 5 | 3740 | 1/1 | 0.95 | 0.28 | 3.86 | 56,56,56,56 | 0 |
| 84 | MG | n8 | 201 | 1/1 | 0.96 | 0.30 | 3.80 | 54,54,54,54 | 0 |
| 84 | MG | 5 | 4123 | 1/1 | 0.94 | 0.28 | 3.79 | 53,53,53,53 | 0 |
| 84 | MG | 5 | 3561 | 1/1 | 0.96 | 0.29 | 3.71 | 57,57,57,57 | 0 |
| 84 | MG | 1 | 3977 | 1/1 | 0.76 | 0.16 | 3.70 | 87,87,87,87 | 0 |
| 84 | MG | 1 | 3412 | 1/1 | 0.85 | 0.31 | 3.68 | 51,51,51,51 | 0 |
| 84 | MG | 4 | 223 | 1/1 | 0.77 | 0.26 | 3.68 | 72,72,72,72 | 0 |
| 84 | MG | 5 | 3503 | 1/1 | 0.91 | 0.31 | 3.64 | 42,42,42,42 | 0 |
| 84 | MG | 1 | 3680 | 1/1 | 0.90 | 0.35 | 3.60 | 59,59,59,59 | 0 |
| 84 | MG | 1 | 3588 | 1/1 | 0.99 | 0.26 | 3.57 | 58,58,58,58 | 0 |
| 84 | MG | 6 | 1948 | 1/1 | 0.97 | 0.27 | 3.54 | 66,66,66,66 | 0 |
| 84 | MG | 5 | 4055 | 1/1 | 0.97 | 0.24 | 3.53 | 103,103,103,103 | 0 |
| 84 | MG | 2 | 1975 | 1/1 | 0.82 | 0.46 | 3.52 | 87,87,87,87 | 0 |
| 84 | MG | 1 | 3407 | 1/1 | 0.97 | 0.28 | 3.52 | 59,59,59,59 | 0 |
| 85 | LLL | 5 | 4173 | 31/31 | 0.83 | 0.30 | 3.51 | 106,106,107,107 | 31 |
| 84 | MG | 5 | 3968 | 1/1 | 0.81 | 0.25 | 3.50 | 56,56,56,56 | 0 |
| 84 | MG | m8 | 202 | 1/1 | 0.77 | 0.53 | 3.43 | 63,63,63,63 | 0 |
| 85 | LLL | 5 | 4151 | 31/31 | 0.96 | 0.22 | 3.43 | 48,48,49,49 | 0 |
| 85 | LLL | 2 | 2045 | 31/31 | 0.86 | 0.42 | 3.42 | 117,117,117,118 | 0 |
| 84 | MG | 5 | 3618 | 1/1 | 0.87 | 0.44 | 3.42 | 83,83,83,83 | 0 |
| 84 | MG | 1 | 3474 | 1/1 | 0.97 | 0.29 | 3.42 | 59,59,59,59 | 0 |
| 84 | MG | 1 | 3687 | 1/1 | 0.87 | 0.36 | 3.41 | 51,51,51,51 | 0 |
| 84 | MG | 5 | 4042 | 1/1 | 0.95 | 0.27 | 3.40 | 46,46,46,46 | 0 |
| 84 | MG | 1 | 3756 | 1/1 | 0.99 | 0.24 | 3.37 | 62,62,62,62 | 0 |
| 84 | MG | l3 | 405 | 1/1 | 0.95 | 0.30 | 3.36 | 43,43,43,43 | 0 |
| 84 | MG | 6 | 1921 | 1/1 | 0.87 | 0.22 | 3.32 | 76,76,76,76 | 0 |
| 84 | MG | 1 | 3688 | 1/1 | 0.98 | 0.26 | 3.32 | 61,61,61,61 | 0 |
| 85 | LLL | 5 | 4176 | 31/31 | 0.84 | 0.27 | 3.31 | 74,74,74,74 | 31 |
| 84 | MG | 1 | 3433 | 1/1 | 0.98 | 0.30 | 3.30 | 49,49,49,49 | 0 |
| 84 | MG | 5 | 3643 | 1/1 | 0.98 | 0.26 | 3.29 | 55,55,55,55 | 0 |
| 84 | MG | 2 | 1943 | 1/1 | 0.94 | 0.27 | 3.28 | 95,95,95,95 | 0 |
| 85 | LLL | 1 | 3998 | 31/31 | 0.89 | 0.35 | 3.27 | 99,100,100,100 | 31 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 6 | 2158 | 1/1 | 0.91 | 0.22 | 3.26 | 77,77,77,77 | 0 |
| 84 | MG | 5 | 3955 | 1/1 | 0.92 | 0.32 | 3.24 | 52,52,52,52 | 0 |
| 84 | MG | 5 | 3437 | 1/1 | 0.79 | 0.25 | 3.24 | 59,59,59,59 | 0 |
| 84 | MG | 5 | 3560 | 1/1 | 0.97 | 0.24 | 3.24 | 51,51,51,51 | 0 |
| 84 | MG | 6 | 1906 | 1/1 | 0.84 | 0.29 | 3.19 | 76,76,76,76 | 0 |
| 84 | MG | 1 | 3531 | 1/1 | 0.91 | 0.30 | 3.15 | 68,68,68,68 | 0 |
| 84 | MG | l3 | 408 | 1/1 | 0.80 | 0.41 | 3.10 | 64,64,64,64 | 0 |
| 84 | MG | Q2 | 505 | 1/1 | 0.91 | 0.35 | 3.07 | 59,59,59,59 | 0 |
| 84 | MG | 6 | 1917 | 1/1 | 0.84 | 0.28 | 3.03 | 89,89,89,89 | 0 |
| 84 | MG | 1 | 3674 | 1/1 | 0.96 | 0.25 | 3.01 | 63,63,63,63 | 0 |
| 84 | MG | l3 | 401 | 1/1 | 0.93 | 0.29 | 3.00 | 57,57,57,57 | 0 |
| 85 | LLL | 3 | 220 | 31/31 | 0.91 | 0.24 | 2.99 | 98,98,99,99 | 0 |
| 84 | MG | 6 | 2084 | 1/1 | 0.96 | 0.27 | 2.97 | 67,67,67,67 | 0 |
| 84 | MG | 1 | 3548 | 1/1 | 0.93 | 0.33 | 2.96 | 70,70,70,70 | 0 |
| 84 | MG | 1 | 3518 | 1/1 | 0.95 | 0.28 | 2.95 | 64,64,64,64 | 0 |
| 84 | MG | 2 | 1932 | 1/1 | 0.97 | 0.25 | 2.93 | 91,91,91,91 | 0 |
| 84 | MG | m6 | 204 | 1/1 | 0.92 | 0.35 | 2.84 | 48,48,48,48 | 0 |
| 84 | MG | 5 | 3845 | 1/1 | 0.89 | 0.24 | 2.83 | 48,48,48,48 | 1 |
| 85 | LLL | 5 | 4161 | 31/31 | 0.95 | 0.22 | 2.82 | 69,70,70,70 | 0 |
| 84 | MG | 8 | 214 | 1/1 | 0.77 | 0.39 | 2.82 | 54,54,54,54 | 0 |
| 84 | MG | 1 | 3931 | 1/1 | 0.89 | 0.25 | 2.80 | 79,79,79,79 | 0 |
| 84 | MG | 2 | 1931 | 1/1 | 0.55 | 0.47 | 2.80 | 90,90,90,90 | 0 |
| 84 | MG | 6 | 1999 | 1/1 | 0.97 | 0.24 | 2.65 | 87,87,87,87 | 0 |
| 84 | MG | 6 | 2057 | 1/1 | 0.98 | 0.24 | 2.55 | 81,81,81,81 | 0 |
| 85 | LLL | 6 | 2174 | 31/31 | 0.83 | 0.29 | 2.55 | 81,81,81,81 | 31 |
| 85 | LLL | 5 | 4156 | 31/31 | 0.86 | 0.28 | 2.53 | 83,84,84,84 | 31 |
| 84 | MG | 5 | 4098 | 1/1 | 0.79 | 0.36 | 2.51 | 81,81,81,81 | 0 |
| 84 | MG | 5 | 3602 | 1/1 | 0.90 | 0.26 | 2.44 | 81,81,81,81 | 0 |
| 84 | MG | 1 | 3537 | 1/1 | 0.97 | 0.30 | 2.40 | 60,60,60,60 | 0 |
| 84 | MG | 5 | 3435 | 1/1 | 0.89 | 0.20 | 2.39 | 50,50,50,50 | 0 |
| 84 | MG | 1 | 3967 | 1/1 | 0.93 | 0.20 | 2.36 | 72,72,72,72 | 0 |
| 84 | MG | 5 | 3871 | 1/1 | 0.91 | 0.24 | 2.34 | 71,71,71,71 | 0 |
| 84 | MG | 1 | 3484 | 1/1 | 0.95 | 0.31 | 2.33 | 60,60,60,60 | 0 |
| 84 | MG | 5 | 4045 | 1/1 | 0.96 | 0.21 | 2.33 | 71,71,71,71 | 0 |
| 84 | MG | 1 | 3766 | 1/1 | 0.82 | 0.27 | 2.33 | 58,58,58,58 | 0 |
| 85 | LLL | 6 | 2172 | 31/31 | 0.90 | 0.26 | 2.26 | 103,104,104,104 | 0 |
| 84 | MG | 1 | 3634 | 1/1 | 0.79 | 0.26 | 2.26 | 105,105,105,105 | 0 |
| 84 | MG | L2 | 305 | 1/1 | 0.90 | 0.31 | 2.21 | 60,60,60,60 | 0 |
| 85 | LLL | 6 | 2173 | 31/31 | 0.86 | 0.35 | 2.20 | 102,102,103,103 | 31 |
| 84 | MG | m5 | 301 | 1/1 | 0.88 | 0.29 | 2.19 | 62,62,62,62 | 0 |
| 85 | LLL | 1 | 3994 | 31/31 | 0.93 | 0.23 | 2.12 | 68,69,69,69 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 6 | 1935 | 1/1 | 0.95 | 0.24 | 2.08 | 73,73,73,73 | 0 |
| 84 | MG | 1 | 3604 | 1/1 | 0.94 | 0.26 | 2.02 | 52,52,52,52 | 0 |
| 84 | MG | 17 | 302 | 1/1 | 0.95 | 0.30 | 2.00 | 55,55,55,55 | 0 |
| 84 | MG | 1 | 3850 | 1/1 | 0.98 | 0.29 | 1.99 | 57,57,57,57 | 0 |
| 85 | LLL | 5 | 4154 | 31/31 | 0.94 | 0.25 | 1.97 | 67,67,67,67 | 0 |
| 84 | MG | L7 | 301 | 1/1 | 0.93 | 0.34 | 1.95 | 58,58,58,58 | 0 |
| 84 | MG | 6 | 1954 | 1/1 | 0.88 | 0.28 | 1.92 | 80,80,80,80 | 0 |
| 84 | MG | 1 | 3525 | 1/1 | 0.98 | 0.23 | 1.91 | 69,69,69,69 | 0 |
| 84 | MG | 1 | 3684 | 1/1 | 0.99 | 0.25 | 1.89 | 58,58,58,58 | 0 |
| 85 | LLL | 5 | 4158 | 31/31 | 0.89 | 0.28 | 1.89 | 60,60,60,60 | 31 |
| 84 | MG | 1 | 3944 | 1/1 | 0.95 | 0.20 | 1.88 | 67,67,67,67 | 0 |
| 84 | MG | 6 | 2149 | 1/1 | 0.65 | 0.18 | 1.86 | 73,73,73,73 | 0 |
| 84 | MG | 1 | 3472 | 1/1 | 0.98 | 0.32 | 1.85 | 57,57,57,57 | 0 |
| 84 | MG | 5 | 3604 | 1/1 | 0.84 | 0.23 | 1.85 | 78,78,78,78 | 0 |
| 84 | MG | 5 | 3856 | 1/1 | 0.74 | 0.34 | 1.84 | 61,61,61,61 | 0 |
| 85 | LLL | 6 | 2164 | 31/31 | 0.91 | 0.27 | 1.84 | 73,74,74,74 | 0 |
| 84 | MG | 2 | 1976 | 1/1 | 0.93 | 0.35 | 1.84 | 92,92,92,92 | 0 |
| 85 | LLL | 5 | 4162 | 31/31 | 0.90 | 0.16 | 1.79 | 117,118,118,118 | 0 |
| 84 | MG | n0 | 207 | 1/1 | 0.95 | 0.23 | 1.77 | 56,56,56,56 | 0 |
| 84 | MG | 5 | 3831 | 1/1 | 0.97 | 0.26 | 1.75 | 44,44,44,44 | 0 |
| 84 | MG | 5 | 3826 | 1/1 | 0.94 | 0.21 | 1.75 | 56,56,56,56 | 0 |
| 84 | MG | 1 | 3553 | 1/1 | 0.96 | 0.20 | 1.71 | 71,71,71,71 | 0 |
| 84 | MG | 1 | 3946 | 1/1 | 0.99 | 0.27 | 1.69 | 54,54,54,54 | 0 |
| 84 | MG | 6 | 2023 | 1/1 | 0.86 | 0.18 | 1.67 | 79,79,79,79 | 0 |
| 84 | MG | 1 | 3920 | 1/1 | 0.92 | 0.29 | 1.65 | 53,53,53,53 | 0 |
| 84 | MG | 5 | 4102 | 1/1 | 0.91 | 0.32 | 1.64 | 47,47,47,47 | 0 |
| 84 | MG | m6 | 207 | 1/1 | 0.79 | 0.29 | 1.64 | 47,47,47,47 | 0 |
| 84 | MG | 1 | 3434 | 1/1 | 0.98 | 0.24 | 1.61 | 53,53,53,53 | 0 |
| 84 | MG | L3 | 403 | 1/1 | 0.92 | 0.27 | 1.60 | 62,62,62,62 | 0 |
| 85 | LLL | 1 | 3996 | 31/31 | 0.88 | 0.28 | 1.59 | 107,107,108,108 | 31 |
| 84 | MG | m7 | 201 | 1/1 | 0.97 | 0.25 | 1.57 | 57,57,57,57 | 0 |
| 84 | MG | L4 | 401 | 1/1 | 0.86 | 0.31 | 1.56 | 69,69,69,69 | 0 |
| 84 | MG | s5 | 302 | 1/1 | 0.89 | 0.31 | 1.56 | 76,76,76,76 | 0 |
| 84 | MG | 5 | 3415 | 1/1 | 0.94 | 0.24 | 1.54 | 48,48,48,48 | 1 |
| 84 | MG | 5 | 3641 | 1/1 | 0.94 | 0.24 | 1.53 | 51,51,51,51 | 0 |
| 84 | MG | 1 | 3539 | 1/1 | 0.98 | 0.24 | 1.53 | 52,52,52,52 | 0 |
| 85 | LLL | 4 | 224 | 31/31 | 0.85 | 0.36 | 1.52 | 99,99,99,99 | 0 |
| 85 | LLL | 5 | 4170 | 31/31 | 0.93 | 0.21 | 1.51 | 61,61,61,61 | 31 |
| 84 | MG | 1 | 3844 | 1/1 | 0.95 | 0.22 | 1.50 | 56,56,56,56 | 0 |
| 85 | LLL | 6 | 2170 | 31/31 | 0.92 | 0.19 | 1.50 | 82,82,83,83 | 0 |
| 85 | LLL | 8 | 222 | 31/31 | 0.90 | 0.36 | 1.50 | 102,102,102,102 | 31 |
| 84 | MG | 5 | 3996 | 1/1 | 0.92 | 0.26 | 1.46 | 44,44,44,44 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 5 | 3793 | 1/1 | 0.75 | 0.37 | 1.46 | 68,68,68,68 | 0 |
| 84 | MG | 5 | 3408 | 1/1 | 0.98 | 0.26 | 1.41 | 45,45,45,45 | 0 |
| 84 | MG | 12 | 301 | 1/1 | 0.92 | 0.30 | 1.40 | 59,59,59,59 | 0 |
| 85 | LLL | 1 | 3990 | 31/31 | 0.94 | 0.20 | 1.38 | 75,75,75,75 | 0 |
| 84 | MG | 1 | 3498 | 1/1 | 0.98 | 0.19 | 1.37 | 62,62,62,62 | 0 |
| 84 | MG | 5 | 3727 | 1/1 | 0.99 | 0.25 | 1.37 | 46,46,46,46 | 0 |
| 84 | MG | 2 | 1983 | 1/1 | 0.96 | 0.22 | 1.35 | 112,112,112,112 | 0 |
| 85 | LLL | 1 | 4004 | 31/31 | 0.90 | 0.23 | 1.34 | 100,101,101,101 | 31 |
| 84 | MG | M7 | 204 | 1/1 | 0.95 | 0.26 | 1.32 | 60,60,60,60 | 0 |
| 85 | LLL | 5 | 4155 | 31/31 | 0.87 | 0.30 | 1.30 | 81,81,82,82 | 0 |
| 84 | MG | o4 | 502 | 1/1 | 0.97 | 0.41 | 1.29 | 87,87,87,87 | 0 |
| 84 | MG | 2 | 1997 | 1/1 | 0.69 | 0.35 | 1.29 | 98,98,98,98 | 0 |
| 84 | MG | 5 | 3480 | 1/1 | 0.96 | 0.25 | 1.24 | 49,49,49,49 | 0 |
| 84 | MG | 1 | 3435 | 1/1 | 0.99 | 0.23 | 1.22 | 53,53,53,53 | 0 |
| 84 | MG | 5 | 3819 | 1/1 | 0.77 | 0.24 | 1.22 | 57,57,57,57 | 0 |
| 84 | MG | 1 | 3520 | 1/1 | 0.99 | 0.22 | 1.20 | 69,69,69,69 | 0 |
| 84 | MG | 5 | 3625 | 1/1 | 0.97 | 0.27 | 1.20 | 54,54,54,54 | 0 |
| 84 | MG | 2 | 1987 | 1/1 | 0.93 | 0.17 | 1.20 | 110,110,110,110 | 0 |
| 84 | MG | 1 | 3891 | 1/1 | 0.96 | 0.21 | 1.19 | 60,60,60,60 | 0 |
| 85 | LLL | 1 | 4003 | 31/31 | 0.93 | 0.23 | 1.19 | 79,80,80,80 | 31 |
| 84 | MG | 5 | 3940 | 1/1 | 0.84 | 0.36 | 1.19 | 71,71,71,71 | 0 |
| 84 | MG | O2 | 204 | 1/1 | 0.81 | 0.32 | 1.18 | 58,58,58,58 | 0 |
| 84 | MG | 6 | 1997 | 1/1 | 0.78 | 0.28 | 1.18 | 78,78,78,78 | 0 |
| 85 | LLL | 5 | 4159 | 31/31 | 0.93 | 0.23 | 1.18 | 59,59,60,60 | 0 |
| 84 | MG | m0 | 301 | 1/1 | 0.99 | 0.26 | 1.17 | 49,49,49,49 | 1 |
| 84 | MG | 6 | 2050 | 1/1 | 0.88 | 0.17 | 1.17 | 71,71,71,71 | 0 |
| 84 | MG | n0 | 202 | 1/1 | 0.97 | 0.26 | 1.14 | 52,52,52,52 | 0 |
| 84 | MG | 19 | 202 | 1/1 | 0.88 | 0.35 | 1.10 | 58,58,58,58 | 0 |
| 85 | LLL | 5 | 4157 | 31/31 | 0.96 | 0.25 | 1.09 | 49,49,49,49 | 0 |
| 84 | MG | 1 | 3969 | 1/1 | 0.86 | 0.34 | 1.08 | 72,72,72,72 | 0 |
| 85 | LLL | 1 | 3992 | 31/31 | 0.93 | 0.32 | 1.02 | 78,79,79,79 | 31 |
| 85 | LLL | 1 | 3989 | 31/31 | 0.95 | 0.21 | 1.02 | 69,69,69,69 | 0 |
| 84 | MG | 1 | 3806 | 1/1 | 0.89 | 0.24 | 1.02 | 65,65,65,65 | 0 |
| 85 | LLL | 5 | 4160 | 31/31 | 0.95 | 0.28 | 1.00 | 49,50,50,50 | 31 |
| 85 | LLL | 6 | 2171 | 31/31 | 0.93 | 0.21 | 0.97 | 87,88,88,88 | 0 |
| 84 | MG | 17 | 301 | 1/1 | 0.98 | 0.24 | 0.95 | 45,45,45,45 | 0 |
| 84 | MG | 5 | 3889 | 1/1 | 0.91 | 0.21 | 0.93 | 55,55,55,55 | 0 |
| 84 | MG | m5 | 302 | 1/1 | 0.87 | 0.33 | 0.89 | 71,71,71,71 | 0 |
| 85 | LLL | 6 | 2169 | 31/31 | 0.93 | 0.20 | 0.87 | 89,89,90,90 | 0 |
| 85 | LLL | 6 | 2166 | 31/31 | 0.94 | 0.26 | 0.85 | 77,77,77,77 | 31 |
| 84 | MG | 1 | 3419 | 1/1 | 0.96 | 0.22 | 0.81 | 55,55,55,55 | 0 |
| 84 | MG | 1 | 3801 | 1/1 | 0.92 | 0.19 | 0.78 | 69,69,69,69 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | l2 | 305 | 1/1 | 0.92 | 0.27 | 0.74 | 50,50,50,50 | 0 |
| 85 | LLL | 5 | 4164 | 31/31 | 0.91 | 0.23 | 0.72 | 62,62,62,62 | 31 |
| 84 | MG | 3 | 213 | 1/1 | 0.87 | 0.14 | 0.71 | 90,90,90,90 | 0 |
| 85 | LLL | 5 | 4171 | 31/31 | 0.87 | 0.24 | 0.70 | 107,107,107,107 | 0 |
| 84 | MG | d6 | 102 | 1/1 | 0.50 | 0.28 | 0.68 | 76,76,76,76 | 0 |
| 85 | LLL | 7 | 233 | 31/31 | 0.84 | 0.23 | 0.67 | 82,82,82,82 | 31 |
| 84 | MG | 5 | 3995 | 1/1 | 0.99 | 0.22 | 0.66 | 47,47,47,47 | 0 |
| 84 | MG | 1 | 3656 | 1/1 | 0.94 | 0.24 | 0.65 | 52,52,52,52 | 0 |
| 84 | MG | 6 | 1959 | 1/1 | 0.94 | 0.22 | 0.64 | 68,68,68,68 | 0 |
| 85 | LLL | 6 | 2176 | 31/31 | 0.91 | 0.24 | 0.62 | 80,80,80,80 | 31 |
| 84 | MG | 6 | 2012 | 1/1 | 0.90 | 0.21 | 0.61 | 61,61,61,61 | 0 |
| 84 | MG | 5 | 3857 | 1/1 | 0.77 | 0.21 | 0.60 | 65,65,65,65 | 0 |
| 84 | MG | 1 | 3885 | 1/1 | 0.95 | 0.19 | 0.59 | 80,80,80,80 | 0 |
| 84 | MG | 5 | 3513 | 1/1 | 0.98 | 0.22 | 0.59 | 48,48,48,48 | 0 |
| 84 | MG | 2 | 2025 | 1/1 | 0.87 | 0.20 | 0.59 | 123,123,123,123 | 0 |
| 84 | MG | l6 | 201 | 1/1 | 0.89 | 0.26 | 0.56 | 60,60,60,60 | 0 |
| 85 | LLL | 1 | 3999 | 31/31 | 0.89 | 0.29 | 0.55 | 85,86,86,86 | 31 |
| 84 | MG | 1 | 3558 | 1/1 | 0.84 | 0.20 | 0.55 | 68,68,68,68 | 0 |
| 84 | MG | 5 | 3788 | 1/1 | 0.98 | 0.22 | 0.54 | 50,50,50,50 | 0 |
| 84 | MG | 2 | 1918 | 1/1 | 0.94 | 0.22 | 0.53 | 91,91,91,91 | 0 |
| 85 | LLL | 2 | 2043 | 31/31 | 0.94 | 0.31 | 0.49 | 101,101,101,101 | 0 |
| 85 | LLL | 1 | 4002 | 31/31 | 0.85 | 0.36 | 0.49 | 136,137,137,137 | 0 |
| 84 | MG | 6 | 2033 | 1/1 | 0.97 | 0.18 | 0.48 | 74,74,74,74 | 0 |
| 85 | LLL | 5 | 4165 | 31/31 | 0.93 | 0.21 | 0.35 | 84,84,84,84 | 0 |
| 85 | LLL | 1 | 3993 | 31/31 | 0.96 | 0.22 | 0.33 | 61,61,61,61 | 0 |
| 84 | MG | M3 | 203 | 1/1 | 0.47 | 0.24 | 0.32 | 92,92,92,92 | 0 |
| 85 | LLL | 5 | 4163 | 31/31 | 0.92 | 0.17 | 0.31 | 112,112,112,112 | 0 |
| 84 | MG | 1 | 3428 | 1/1 | 0.99 | 0.22 | 0.30 | 54,54,54,54 | 0 |
| 84 | MG | d6 | 104 | 1/1 | 0.76 | 0.30 | 0.28 | 76,76,76,76 | 0 |
| 85 | LLL | 1 | 4001 | 31/31 | 0.88 | 0.22 | 0.25 | 121,121,121,121 | 0 |
| 84 | MG | d9 | 102 | 1/1 | 0.74 | 0.22 | 0.25 | 94,94,94,94 | 0 |
| 84 | MG | 5 | 3930 | 1/1 | 0.97 | 0.20 | 0.24 | 45,45,45,45 | 0 |
| 84 | MG | 6 | 2152 | 1/1 | 0.87 | 0.19 | 0.24 | 68,68,68,68 | 0 |
| 84 | MG | 5 | 3842 | 1/1 | 0.94 | 0.24 | 0.24 | 46,46,46,46 | 0 |
| 84 | MG | 4 | 218 | 1/1 | 0.88 | 0.23 | 0.22 | 60,60,60,60 | 0 |
| 84 | MG | 5 | 3683 | 1/1 | 0.98 | 0.23 | 0.18 | 73,73,73,73 | 0 |
| 84 | MG | 1 | 3851 | 1/1 | 0.96 | 0.19 | 0.18 | 57,57,57,57 | 0 |
| 84 | MG | M7 | 201 | 1/1 | 0.86 | 0.29 | 0.18 | 59,59,59,59 | 0 |
| 84 | MG | d3 | 204 | 1/1 | 0.86 | 0.27 | 0.16 | 66,66,66,66 | 0 |
| 84 | MG | 5 | 3488 | 1/1 | 0.82 | 0.21 | 0.15 | 55,55,55,55 | 0 |
| 85 | LLL | 6 | 2165 | 31/31 | 0.92 | 0.22 | 0.14 | 76,77,77,77 | 31 |
| 85 | LLL | 6 | 2168 | 31/31 | 0.90 | 0.24 | 0.14 | 86,86,86,87 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 85 | LLL | 5 | 4168 | 31/31 | 0.93 | 0.27 | 0.13 | 76,76,76,76 | 0 |
| 84 | MG | N3 | 201 | 1/1 | 0.94 | 0.31 | 0.12 | 67,67,67,67 | 0 |
| 84 | MG | 6 | 2004 | 1/1 | 0.99 | 0.22 | 0.11 | 67,67,67,67 | 0 |
| 84 | MG | 2 | 1972 | 1/1 | 0.90 | 0.22 | 0.11 | 88,88,88,88 | 0 |
| 84 | MG | 1 | 3762 | 1/1 | 0.98 | 0.26 | 0.11 | 70,70,70,70 | 0 |
| 85 | LLL | 1 | 3991 | 31/31 | 0.96 | 0.21 | 0.10 | 67,67,67,67 | 0 |
| 84 | MG | 2 | 2011 | 1/1 | 0.94 | 0.19 | 0.05 | 102,102,102,102 | 0 |
| 85 | LLL | 7 | 231 | 31/31 | 0.88 | 0.20 | 0.02 | 81,82,82,82 | 31 |
| 84 | MG | 1 | 3471 | 1/1 | 0.98 | 0.20 | 0.01 | 63,63,63,63 | 0 |
| 84 | MG | 1 | 3974 | 1/1 | 0.96 | 0.19 | -0.00 | 79,79,79,79 | 0 |
| 84 | MG | 5 | 3906 | 1/1 | 0.98 | 0.22 | -0.01 | 50,50,50,50 | 0 |
| 84 | MG | 1 | 3649 | 1/1 | 0.91 | 0.19 | -0.01 | 61,61,61,61 | 0 |
| 84 | MG | 5 | 3462 | 1/1 | 0.94 | 0.21 | -0.07 | 53,53,53,53 | 0 |
| 85 | LLL | 8 | 221 | 31/31 | 0.90 | 0.22 | -0.07 | 100,100,100,100 | 31 |
| 84 | MG | 6 | 1984 | 1/1 | 0.87 | 0.18 | -0.08 | 89,89,89,89 | 0 |
| 84 | MG | 8 | 217 | 1/1 | 0.95 | 0.22 | -0.09 | 64,64,64,64 | 0 |
| 86 | ZN | o4 | 501 | 1/1 | 0.98 | 0.17 | -0.10 | 127,127,127,127 | 0 |
| 84 | MG | 1 | 3561 | 1/1 | 0.95 | 0.15 | -0.11 | 79,79,79,79 | 0 |
| 84 | MG | 6 | 2151 | 1/1 | 0.95 | 0.20 | -0.11 | 67,67,67,67 | 0 |
| 84 | MG | 1 | 3715 | 1/1 | 0.80 | 0.18 | -0.12 | 83,83,83,83 | 0 |
| 84 | MG | 1 | 3616 | 1/1 | 0.93 | 0.21 | -0.12 | 54,54,54,54 | 0 |
| 85 | LLL | l3 | 412 | 31/31 | 0.94 | 0.20 | -0.12 | 69,69,70,70 | 0 |
| 84 | MG | 5 | 3677 | 1/1 | 0.98 | 0.22 | -0.13 | 59,59,59,59 | 0 |
| 84 | MG | 5 | 3622 | 1/1 | 0.76 | 0.19 | -0.15 | 84,84,84,84 | 0 |
| 85 | LLL | 5 | 4172 | 31/31 | 0.91 | 0.18 | -0.15 | 77,77,77,77 | 31 |
| 84 | MG | 5 | 3445 | 1/1 | 0.95 | 0.21 | -0.17 | 50,50,50,50 | 0 |
| 84 | MG | 5 | 4110 | 1/1 | 0.94 | 0.17 | -0.18 | 47,47,47,47 | 0 |
| 84 | MG | 5 | 4017 | 1/1 | 0.96 | 0.19 | -0.19 | 63,63,63,63 | 0 |
| 84 | MG | 6 | 2031 | 1/1 | 0.96 | 0.18 | -0.19 | 73,73,73,73 | 0 |
| 84 | MG | M5 | 303 | 1/1 | 0.94 | 0.19 | -0.21 | 65,65,65,65 | 0 |
| 84 | MG | m7 | 205 | 1/1 | 0.90 | 0.20 | -0.23 | 53,53,53,53 | 0 |
| 84 | MG | 5 | 4083 | 1/1 | 0.82 | 0.15 | -0.27 | 88,88,88,88 | 0 |
| 84 | MG | 5 | 3473 | 1/1 | 0.96 | 0.22 | -0.28 | 63,63,63,63 | 0 |
| 84 | MG | C3 | 201 | 1/1 | 0.72 | 0.20 | -0.29 | 102,102,102,102 | 0 |
| 84 | MG | 6 | 2039 | 1/1 | 0.88 | 0.20 | -0.29 | 83,83,83,83 | 0 |
| 84 | MG | 6 | 2055 | 1/1 | 0.97 | 0.17 | -0.32 | 77,77,77,77 | 0 |
| 85 | LLL | L3 | 404 | 31/31 | 0.92 | 0.22 | -0.33 | 82,82,82,82 | 0 |
| 84 | MG | 5 | 3631 | 1/1 | 0.90 | 0.21 | -0.33 | 55,55,55,55 | 0 |
| 84 | MG | 5 | 3572 | 1/1 | 0.98 | 0.23 | -0.33 | 67,67,67,67 | 0 |
| 84 | MG | 7 | 207 | 1/1 | 0.96 | 0.16 | -0.33 | 62,62,62,62 | 0 |
| 84 | MG | 5 | 3501 | 1/1 | 0.93 | 0.19 | -0.36 | 54,54,54,54 | 0 |
| 84 | MG | l7 | 303 | 1/1 | 0.90 | 0.20 | -0.36 | 56,56,56,56 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 84 | MG | n0 | 203 | 1/1 | 0.96 | 0.19 | -0.37 | 49,49,49,49 | 0 |
| 84 | MG | 5 | 3568 | 1/1 | 0.97 | 0.20 | -0.38 | 67,67,67,67 | 0 |
| 84 | MG | 5 | 3505 | 1/1 | 0.91 | 0.19 | -0.39 | 50,50,50,50 | 0 |
| 84 | MG | 6 | 2040 | 1/1 | 0.98 | 0.16 | -0.40 | 78,78,78,78 | 0 |
| 84 | MG | 6 | 2136 | 1/1 | 0.90 | 0.16 | -0.41 | 85,85,85,85 | 0 |
| 84 | MG | m0 | 302 | 1/1 | 0.98 | 0.21 | -0.42 | 53,53,53,53 | 0 |
| 84 | MG | m9 | 201 | 1/1 | 0.83 | 0.24 | -0.43 | 74,74,74,74 | 0 |
| 84 | MG | 6 | 2051 | 1/1 | 0.94 | 0.16 | -0.43 | 69,69,69,69 | 0 |
| 85 | LLL | 5 | 4167 | 31/31 | 0.90 | 0.16 | -0.44 | 125,126,126,126 | 0 |
| 84 | MG | 1 | 3921 | 1/1 | 0.92 | 0.18 | -0.44 | 72,72,72,72 | 0 |
| 84 | MG | 1 | 3740 | 1/1 | 0.97 | 0.17 | -0.45 | 74,74,74,74 | 0 |
| 84 | MG | 2 | 2036 | 1/1 | 0.65 | 0.18 | -0.45 | 113,113,113,113 | 0 |
| 84 | MG | L2 | 301 | 1/1 | 0.95 | 0.20 | -0.45 | 55,55,55,55 | 0 |
| 84 | MG | 5 | 4053 | 1/1 | 0.89 | 0.15 | -0.50 | 94,94,94,94 | 0 |
| 84 | MG | m4 | 203 | 1/1 | 0.85 | 0.21 | -0.54 | 59,59,59,59 | 0 |
| 84 | MG | c4 | 201 | 1/1 | 0.89 | 0.20 | -0.55 | 87,87,87,87 | 0 |
| 84 | MG | 6 | 2019 | 1/1 | 0.96 | 0.18 | -0.55 | 81,81,81,81 | 0 |
| 84 | MG | m3 | 202 | 1/1 | 0.79 | 0.23 | -0.62 | 82,82,82,82 | 0 |
| 86 | ZN | o7 | 501 | 1/1 | 0.99 | 0.19 | -0.64 | 80,80,80,80 | 0 |
| 84 | MG | 1 | 3744 | 1/1 | 0.60 | 0.17 | -0.65 | 82,82,82,82 | 0 |
| 84 | MG | 2 | 1994 | 1/1 | 0.92 | 0.14 | -0.66 | 109,109,109,109 | 0 |
| 84 | MG | 1 | 3564 | 1/1 | 0.90 | 0.14 | -0.68 | 71,71,71,71 | 0 |
| 84 | MG | 1 | 3832 | 1/1 | 0.98 | 0.21 | -0.68 | 58,58,58,58 | 0 |
| 84 | MG | 5 | 3402 | 1/1 | 0.99 | 0.22 | -0.72 | 47,47,47,47 | 0 |
| 84 | MG | 5 | 4062 | 1/1 | 0.91 | 0.16 | -0.72 | 86,86,86,86 | 0 |
| 84 | MG | 1 | 3697 | 1/1 | 0.97 | 0.19 | -0.75 | 56,56,56,56 | 0 |
| 84 | MG | 1 | 3761 | 1/1 | 0.94 | 0.17 | -0.75 | 73,73,73,73 | 1 |
| 84 | MG | 6 | 1953 | 1/1 | 0.91 | 0.17 | -0.76 | 83,83,83,83 | 0 |
| 84 | MG | 1 | 3712 | 1/1 | 0.92 | 0.17 | -0.79 | 82,82,82,82 | 0 |
| 86 | ZN | d6 | 101 | 1/1 | 0.99 | 0.16 | -0.79 | 82,82,82,82 | 0 |
| 86 | ZN | q3 | 501 | 1/1 | 0.99 | 0.14 | -0.79 | 102,102,102,102 | 0 |
| 84 | MG | D3 | 205 | 1/1 | 0.82 | 0.23 | -0.81 | 86,86,86,86 | 0 |
| 84 | MG | 6 | 1923 | 1/1 | 0.93 | 0.17 | -0.81 | 71,71,71,71 | 0 |
| 84 | MG | 5 | 3500 | 1/1 | 0.99 | 0.19 | -0.81 | 51,51,51,51 | 0 |
| 84 | MG | 6 | 2020 | 1/1 | 0.92 | 0.13 | -0.83 | 85,85,85,85 | 0 |
| 84 | MG | 5 | 3659 | 1/1 | 0.94 | 0.13 | -0.83 | 98,98,98,98 | 0 |
| 84 | MG | 1 | 3469 | 1/1 | 0.80 | 0.21 | -0.84 | 59,59,59,59 | 1 |
| 84 | MG | m3 | 201 | 1/1 | 0.79 | 0.28 | -0.85 | 88,88,88,88 | 0 |
| 84 | MG | 5 | 3497 | 1/1 | 0.95 | 0.17 | -0.87 | 49,49,49,49 | 0 |
| 84 | MG | 2 | 1988 | 1/1 | 0.98 | 0.14 | -0.89 | 112,112,112,112 | 0 |
| 86 | ZN | Q0 | 500 | 1/1 | 0.99 | 0.17 | -0.90 | 72,72,72,72 | 0 |
| 86 | ZN | Q3 | 501 | 1/1 | 0.97 | 0.12 | -0.92 | 108,108,108,108 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 84 | MG | 1 | 3562 | 1/1 | 0.99 | 0.10 | -0.94 | 80,80,80,80 | 0 |
| 84 | MG | 5 | 3733 | 1/1 | 0.97 | 0.14 | -0.94 | 65,65,65,65 | 0 |
| 84 | MG | 5 | 3607 | 1/1 | 0.94 | 0.21 | -0.96 | 83,83,83,83 | 0 |
| 84 | MG | 7 | 209 | 1/1 | 0.89 | 0.12 | -1.02 | 64,64,64,64 | 0 |
| 86 | ZN | D6 | 500 | 1/1 | 0.99 | 0.13 | -1.02 | 101,101,101,101 | 0 |
| 84 | MG | N8 | 201 | 1/1 | 0.93 | 0.23 | -1.08 | 75,75,75,75 | 0 |
| 84 | MG | 5 | 3655 | 1/1 | 0.98 | 0.17 | -1.08 | 78,78,78,78 | 0 |
| 86 | ZN | d9 | 101 | 1/1 | 0.99 | 0.12 | -1.09 | 89,89,89,89 | 0 |
| 84 | MG | 1 | 3629 | 1/1 | 0.83 | 0.14 | -1.10 | 136,136,136,136 | 0 |
| 84 | MG | N3 | 203 | 1/1 | 0.88 | 0.25 | -1.10 | 75,75,75,75 | 0 |
| 84 | MG | 5 | 3952 | 1/1 | 0.97 | 0.19 | -1.12 | 58,58,58,58 | 0 |
| 84 | MG | 6 | 2044 | 1/1 | 0.97 | 0.15 | -1.12 | 71,71,71,71 | 0 |
| 84 | MG | 1 | 3594 | 1/1 | 0.91 | 0.18 | -1.14 | 53,53,53,53 | 0 |
| 84 | MG | M3 | 202 | 1/1 | 0.88 | 0.20 | -1.18 | 80,80,80,80 | 0 |
| 84 | MG | l9 | 208 | 1/1 | 0.77 | 0.18 | -1.19 | 54,54,54,54 | 0 |
| 84 | MG | 5 | 4054 | 1/1 | 0.92 | 0.12 | -1.19 | 97,97,97,97 | 0 |
| 84 | MG | 2 | 2030 | 1/1 | 0.93 | 0.09 | -1.19 | 122,122,122,122 | 0 |
| 84 | MG | d5 | 201 | 1/1 | 0.94 | 0.17 | -1.22 | 90,90,90,90 | 0 |
| 84 | MG | 5 | 3474 | 1/1 | 0.88 | 0.18 | -1.23 | 67,67,67,67 | 0 |
| 86 | ZN | D9 | 101 | 1/1 | 0.98 | 0.11 | -1.26 | 121,121,121,121 | 0 |
| 86 | ZN | d7 | 101 | 1/1 | 0.82 | 0.15 | -1.28 | 272,272,272,272 | 0 |
| 84 | MG | n8 | 202 | 1/1 | 0.89 | 0.20 | -1.28 | 73,73,73,73 | 0 |
| 84 | MG | 5 | 3960 | 1/1 | 0.78 | 0.18 | -1.28 | 74,74,74,74 | 0 |
| 84 | MG | q2 | 508 | 1/1 | 0.91 | 0.18 | -1.29 | 62,62,62,62 | 0 |
| 84 | MG | 2 | 1958 | 1/1 | 0.89 | 0.15 | -1.29 | 108,108,108,108 | 0 |
| 86 | ZN | e1 | 501 | 1/1 | 0.92 | 0.10 | -1.29 | 150,150,150,150 | 0 |
| 84 | MG | 1 | 3731 | 1/1 | 0.97 | 0.15 | -1.30 | 80,80,80,80 | 0 |
| 84 | MG | 1 | 3814 | 1/1 | 0.93 | 0.15 | -1.32 | 103,103,103,103 | 0 |
| 84 | MG | O4 | 502 | 1/1 | 0.97 | 0.10 | -1.34 | 106,106,106,106 | 0 |
| 84 | MG | 6 | 1955 | 1/1 | 0.97 | 0.16 | -1.34 | 77,77,77,77 | 0 |
| 86 | ZN | O4 | 501 | 1/1 | 0.97 | 0.08 | -1.36 | 141,141,141,141 | 0 |
| 84 | MG | 5 | 3724 | 1/1 | 0.97 | 0.17 | -1.39 | 60,60,60,60 | 1 |
| 86 | ZN | q0 | 201 | 1/1 | 1.00 | 0.15 | -1.43 | 52,52,52,52 | 0 |
| 86 | ZN | E1 | 501 | 1/1 | 0.96 | 0.09 | -1.43 | 182,182,182,182 | 0 |
| 84 | MG | 5 | 3521 | 1/1 | 0.99 | 0.19 | -1.43 | 50,50,50,50 | 0 |
| 84 | MG | M0 | 304 | 1/1 | 0.97 | 0.13 | -1.46 | 62,62,62,62 | 0 |
| 86 | ZN | O7 | 101 | 1/1 | 1.00 | 0.14 | -1.46 | 77,77,77,77 | 0 |
| 84 | MG | 5 | 3712 | 1/1 | 0.92 | 0.13 | -1.49 | 75,75,75,75 | 0 |
| 84 | MG | c8 | 203 | 1/1 | 0.93 | 0.11 | -1.50 | 74,74,74,74 | 0 |
| 84 | MG | d1 | 102 | 1/1 | 0.95 | 0.10 | -1.56 | 106,106,106,106 | 0 |
| 84 | MG | m5 | 303 | 1/1 | 0.79 | 0.17 | -1.57 | 79,79,79,79 | 0 |
| 84 | MG | 5 | 3476 | 1/1 | 0.91 | 0.19 | -1.57 | 53,53,53,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 84 | MG | 5 | 3682 | 1/1 | 0.96 | 0.17 | -1.58 | 73,73,73,73 | 0 |
| 86 | ZN | Q2 | 501 | 1/1 | 0.98 | 0.08 | -1.62 | 102,102,102,102 | 0 |
| 84 | MG | 1 | 3567 | 1/1 | 0.98 | 0.16 | -1.65 | 66,66,66,66 | 0 |
| 84 | MG | 2 | 1989 | 1/1 | 0.86 | 0.10 | -1.68 | 114,114,114,114 | 0 |
| 84 | MG | 6 | 2045 | 1/1 | 0.96 | 0.12 | -1.68 | 68,68,68,68 | 0 |
| 84 | MG | 19 | 204 | 1/1 | 0.89 | 0.21 | -1.71 | 57,57,57,57 | 0 |
| 84 | MG | 2 | 1986 | 1/1 | 0.92 | 0.13 | -1.75 | 117,117,117,117 | 0 |
| 84 | MG | 5 | 4066 | 1/1 | 0.94 | 0.12 | -1.77 | 84,84,84,84 | 0 |
| 84 | MG | 2 | 2024 | 1/1 | 0.79 | 0.07 | -1.80 | 130,130,130,130 | 0 |
| 84 | MG | 1 | 3724 | 1/1 | 0.90 | 0.15 | -1.85 | 63,63,63,63 | 0 |
| 84 | MG | 5 | 3816 | 1/1 | 0.99 | 0.17 | -1.85 | 43,43,43,43 | 0 |
| 84 | MG | 1 | 3420 | 1/1 | 0.97 | 0.18 | -1.86 | 53,53,53,53 | 0 |
| 84 | MG | 2 | 1998 | 1/1 | 0.94 | 0.10 | -1.86 | 154,154,154,154 | 0 |
| 84 | MG | 5 | 4011 | 1/1 | 0.96 | 0.16 | -1.91 | 45,45,45,45 | 0 |
| 84 | MG | C8 | 201 | 1/1 | 0.94 | 0.05 | -1.93 | 138,138,138,138 | 0 |
| 84 | MG | 2 | 2019 | 1/1 | 0.86 | 0.09 | -1.98 | 127,127,127,127 | 0 |
| 84 | MG | 2 | 2032 | 1/1 | 0.94 | 0.09 | -2.01 | 111,111,111,111 | 0 |
| 84 | MG | 1 | 3523 | 1/1 | 0.98 | 0.18 | -2.03 | 70,70,70,70 | 0 |
| 86 | ZN | q2 | 501 | 1/1 | 0.99 | 0.10 | -2.03 | 94,94,94,94 | 0 |
| 84 | MG | 1 | 3713 | 1/1 | 0.87 | 0.12 | -2.07 | 81,81,81,81 | 0 |
| 84 | MG | 1 | 3940 | 1/1 | 0.96 | 0.13 | -2.07 | 64,64,64,64 | 0 |
| 84 | MG | 5 | 3482 | 1/1 | 0.93 | 0.19 | -2.11 | 46,46,46,46 | 0 |
| 84 | MG | 5 | 3646 | 1/1 | 0.94 | 0.17 | -2.12 | 65,65,65,65 | 0 |
| 84 | MG | 5 | 3938 | 1/1 | 0.87 | 0.16 | -2.17 | 66,66,66,66 | 0 |
| 84 | MG | 7 | 211 | 1/1 | 0.96 | 0.14 | -2.19 | 67,67,67,67 | 0 |
| 84 | MG | 5 | 3425 | 1/1 | 0.95 | 0.17 | -2.30 | 46,46,46,46 | 0 |
| 84 | MG | 6 | 2047 | 1/1 | 0.95 | 0.12 | -2.31 | 79,79,79,79 | 0 |
| 84 | MG | 5 | 4050 | 1/1 | 0.99 | 0.10 | -2.31 | 80,80,80,80 | 0 |
| 84 | MG | 1 | 3845 | 1/1 | 0.92 | 0.17 | -2.41 | 53,53,53,53 | 0 |
| 84 | MG | 5 | 3457 | 1/1 | 0.96 | 0.13 | -2.51 | 51,51,51,51 | 0 |
| 84 | MG | 5 | 3770 | 1/1 | 0.96 | 0.12 | -2.61 | 79,79,79,79 | 0 |
| 84 | MG | d3 | 203 | 1/1 | 0.98 | 0.11 | -2.63 | 68,68,68,68 | 0 |
| 84 | MG | 5 | 4068 | 1/1 | 0.91 | 0.12 | -2.87 | 112,112,112,112 | 0 |
| 84 | MG | 5 | 3409 | 1/1 | 0.92 | 0.18 | -2.87 | 45,45,45,45 | 0 |
| 84 | MG | 5 | 3605 | 1/1 | 0.87 | 0.12 | -2.96 | 76,76,76,76 | 0 |
| 84 | MG | 5 | 4113 | 1/1 | 0.92 | 0.18 | -2.98 | 72,72,72,72 | 0 |
| 84 | MG | 5 | 3578 | 1/1 | 0.98 | 0.17 | -3.01 | 48,48,48,48 | 1 |
| 84 | MG | 5 | 3720 | 1/1 | 0.97 | 0.09 | -3.13 | 71,71,71,71 | 0 |
| 84 | MG | 5 | 3452 | 1/1 | 0.98 | 0.16 | -3.20 | 48,48,48,48 | 0 |
| 84 | MG | 5 | 3603 | 1/1 | 0.91 | 0.15 | -3.27 | 80,80,80,80 | 0 |
| 84 | MG | 5 | 4069 | 1/1 | 0.86 | 0.12 | -3.30 | 110,110,110,110 | 0 |
| 84 | MG | 6 | 2109 | 1/1 | 0.92 | 0.11 | -3.46 | 91,91,91,91 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 84 | MG | 5 | 3468 | 1/1 | 0.92 | 0.14 | -3.48 | 55,55,55,55 | 0 |
| 84 | MG | 6 | 2066 | 1/1 | 0.80 | 0.10 | -3.67 | 121,121,121,121 | 0 |
| 84 | MG | 1 | 3809 | 1/1 | 0.94 | 0.14 | -3.70 | 59,59,59,59 | 0 |
| 84 | MG | 5 | 3887 | 1/1 | 0.87 | 0.12 | -3.70 | 84,84,84,84 | 0 |
| 84 | MG | 6 | 2071 | 1/1 | 0.93 | 0.14 | -4.00 | 76,76,76,76 | 1 |
| 84 | MG | 6 | 2046 | 1/1 | 0.91 | 0.11 | -4.07 | 72,72,72,72 | 0 |
| 84 | MG | 1 | 3982 | 1/1 | 0.94 | 0.12 | -4.62 | 90,90,90,90 | 0 |
| 84 | MG | 1 | 3728 | 1/1 | 0.95 | 0.13 | -4.73 | 83,83,83,83 | 0 |
| 84 | MG | 6 | 2155 | 1/1 | 0.93 | 0.11 | -4.83 | 84,84,84,84 | 0 |
| 84 | MG | 5 | 4028 | 1/1 | 0.94 | 0.10 | -5.57 | 59,59,59,59 | 0 |
| 84 | MG | 1 | 3682 | 1/1 | 0.99 | 0.09 | -5.79 | 65,65,65,65 | 0 |
| 84 | MG | 1 | 3968 | 1/1 | 0.92 | 0.11 | -5.90 | 74,74,74,74 | 0 |
| 84 | MG | 1 | 3647 | 1/1 | 0.97 | 0.13 | -6.22 | 55,55,55,55 | 0 |
| 84 | MG | 1 | 3451 | 1/1 | 0.89 | 0.11 | -6.85 | 69,69,69,69 | 0 |
| 84 | MG | 1 | 3918 | 1/1 | 0.96 | 0.16 | -7.66 | 59,59,59,59 | 0 |
| 84 | MG | 5 | 3559 | 1/1 | 0.99 | 0.11 | -7.86 | 56,56,56,56 | 1 |
| 84 | MG | 5 | 3666 | 1/1 | 0.97 | 0.14 | -7.98 | 55,55,55,55 | 0 |
| 84 | MG | 5 | 3830 | 1/1 | 0.97 | 0.07 | -8.79 | 49,49,49,49 | 1 |
| 84 | MG | 2 | 2041 | 1/1 | 0.95 | 0.08 | -9.78 | 94,94,94,94 | 0 |
| 84 | MG | 5 | 3576 | 1/1 | 0.86 | 0.33 | - | 52,52,52,52 | 0 |
| 84 | MG | 1 | 3848 | 1/1 | 0.97 | 0.15 | - | 57,57,57,57 | 0 |
| 84 | MG | 5 | 3859 | 1/1 | 0.80 | 0.56 | - | 71,71,71,71 | 0 |
| 84 | MG | 6 | 2010 | 1/1 | 0.87 | 0.33 | - | 68,68,68,68 | 0 |
| 84 | MG | l5 | 304 | 1/1 | 0.93 | 0.07 | - | 80,80,80,80 | 0 |
| 84 | MG | 1 | 3916 | 1/1 | 0.90 | 0.15 | - | 70,70,70,70 | 0 |
| 84 | MG | 5 | 3950 | 1/1 | 0.86 | 0.66 | - | 61,61,61,61 | 0 |
| 84 | MG | 5 | 3759 | 1/1 | 0.94 | 0.32 | - | 67,67,67,67 | 0 |
| 84 | MG | 5 | 4038 | 1/1 | 0.97 | 0.10 | - | 79,79,79,79 | 0 |
| 84 | MG | m4 | 202 | 1/1 | 0.98 | 0.19 | - | 52,52,52,52 | 0 |
| 84 | MG | L4 | 402 | 1/1 | 0.98 | 0.08 | - | 65,65,65,65 | 0 |
| 84 | MG | 5 | 3511 | 1/1 | 0.98 | 0.18 | - | 47,47,47,47 | 0 |
| 84 | MG | 1 | 3626 | 1/1 | 0.86 | 0.26 | - | 63,63,63,63 | 0 |
| 84 | MG | 1 | 3927 | 1/1 | 0.60 | 0.17 | - | 77,77,77,77 | 1 |
| 84 | MG | 5 | 3944 | 1/1 | 0.83 | 0.67 | - | 61,61,61,61 | 0 |
| 84 | MG | 5 | 3822 | 1/1 | 0.85 | 0.16 | - | 60,60,60,60 | 0 |
| 84 | MG | 1 | 3898 | 1/1 | 0.89 | 0.09 | - | 99,99,99,99 | 0 |
| 84 | MG | 1 | 3409 | 1/1 | 0.81 | 0.40 | - | 49,49,49,49 | 0 |
| 84 | MG | 2 | 1940 | 1/1 | 0.51 | 0.65 | - | 82,82,82,82 | 0 |
| 84 | MG | 1 | 3821 | 1/1 | 0.84 | 0.75 | - | 68,68,68,68 | 0 |
| 84 | MG | 6 | 1957 | 1/1 | 0.95 | 0.17 | - | 66,66,66,66 | 0 |
| 84 | MG | 1 | 3772 | 1/1 | 0.96 | 0.23 | - | 59,59,59,59 | 1 |
| 84 | MG | 5 | 4142 | 1/1 | 0.95 | 0.33 | - | 69,69,69,69 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 5 | 3910 | 1/1 | 0.88 | 0.27 | - | 52,52,52,52 | 0 |
| 84 | MG | 5 | 3806 | 1/1 | 0.86 | 0.39 | - | 73,73,73,73 | 0 |
| 84 | MG | 2 | 1969 | 1/1 | 0.93 | 0.22 | - | 100,100,100,100 | 0 |
| 84 | MG | 5 | 4006 | 1/1 | 0.87 | 0.44 | - | 64,64,64,64 | 0 |
| 84 | MG | 2 | 1996 | 1/1 | 0.92 | 0.15 | - | 111,111,111,111 | 0 |
| 84 | MG | 1 | 3836 | 1/1 | 0.94 | 0.21 | - | 58,58,58,58 | 0 |
| 84 | MG | 1 | 3542 | 1/1 | 0.98 | 0.26 | - | 52,52,52,52 | 0 |
| 84 | MG | 6 | 1939 | 1/1 | 0.92 | 0.40 | - | 58,58,58,58 | 0 |
| 84 | MG | 1 | 3479 | 1/1 | 0.95 | 0.41 | - | 59,59,59,59 | 0 |
| 84 | MG | 5 | 3899 | 1/1 | 0.80 | 0.80 | - | 59,59,59,59 | 0 |
| 84 | MG | 5 | 3926 | 1/1 | 0.94 | 0.21 | - | 55,55,55,55 | 1 |
| 84 | MG | 1 | 3503 | 1/1 | 0.88 | 0.31 | - | 61,61,61,61 | 0 |
| 84 | MG | 4 | 214 | 1/1 | 0.93 | 0.36 | - | 63,63,63,63 | 0 |
| 84 | MG | 1 | 3843 | 1/1 | 0.95 | 0.28 | - | 58,58,58,58 | 0 |
| 84 | MG | 1 | 3491 | 1/1 | 0.98 | 0.34 | - | 79,79,79,79 | 0 |
| 84 | MG | 5 | 4057 | 1/1 | 0.53 | 0.15 | - | 99,99,99,99 | 1 |
| 84 | MG | 1 | 3985 | 1/1 | 0.64 | 0.40 | - | 77,77,77,77 | 0 |
| 84 | MG | 2 | 1979 | 1/1 | 0.70 | 0.84 | - | 68,68,68,68 | 0 |
| 84 | MG | 6 | 2159 | 1/1 | 0.97 | 0.15 | - | 81,81,81,81 | 0 |
| 84 | MG | 1 | 3734 | 1/1 | 0.97 | 0.17 | - | 77,77,77,77 | 0 |
| 84 | MG | 5 | 3498 | 1/1 | 0.94 | 0.15 | - | 52,52,52,52 | 0 |
| 84 | MG | 6 | 2085 | 1/1 | 0.78 | 0.15 | - | 88,88,88,88 | 0 |
| 84 | MG | 5 | 4084 | 1/1 | 0.86 | 0.19 | - | 96,96,96,96 | 0 |
| 84 | MG | 5 | 3440 | 1/1 | 0.95 | 0.16 | - | 56,56,56,56 | 0 |
| 84 | MG | 5 | 3506 | 1/1 | 0.93 | 0.32 | - | 49,49,49,49 | 0 |
| 84 | MG | 6 | 2042 | 1/1 | 0.91 | 0.15 | - | 77,77,77,77 | 0 |
| 84 | MG | 1 | 3551 | 1/1 | 0.90 | 0.22 | - | 68,68,68,68 | 0 |
| 84 | MG | 2 | 1920 | 1/1 | 0.92 | 0.28 | - | 88,88,88,88 | 0 |
| 84 | MG | 5 | 3812 | 1/1 | 0.82 | 0.53 | - | 46,46,46,46 | 0 |
| 84 | MG | 5 | 3456 | 1/1 | 0.88 | 0.23 | - | 53,53,53,53 | 0 |
| 84 | MG | 1 | 3448 | 1/1 | 0.93 | 0.52 | - | 68,68,68,68 | 0 |
| 84 | MG | 5 | 3557 | 1/1 | 0.86 | 0.24 | - | 62,62,62,62 | 1 |
| 84 | MG | 6 | 2130 | 1/1 | 0.83 | 0.15 | - | 95,95,95,95 | 0 |
| 84 | MG | 1 | 3666 | 1/1 | 0.84 | 0.27 | - | 72,72,72,72 | 0 |
| 84 | MG | 6 | 2087 | 1/1 | 0.95 | 0.22 | - | 82,82,82,82 | 0 |
| 84 | MG | 5 | 3965 | 1/1 | 0.79 | 0.57 | - | 65,65,65,65 | 0 |
| 84 | MG | 1 | 3692 | 1/1 | 0.88 | 0.39 | - | 64,64,64,64 | 0 |
| 84 | MG | M5 | 301 | 1/1 | 0.82 | 0.35 | - | 69,69,69,69 | 0 |
| 84 | MG | 1 | 3655 | 1/1 | 0.96 | 0.31 | - | 50,50,50,50 | 0 |
| 84 | MG | L9 | 201 | 1/1 | 0.84 | 0.27 | - | 59,59,59,59 | 0 |
| 84 | MG | 1 | 3714 | 1/1 | 0.90 | 0.16 | - | 90,90,90,90 | 0 |
| 84 | MG | 1 | 3860 | 1/1 | 0.93 | 0.19 | - | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 1 | 3414 | 1/1 | 0.95 | 0.21 | - | 56,56,56,56 | 0 |
| 84 | MG | 6 | 2078 | 1/1 | 0.96 | 0.28 | - | 65,65,65,65 | 0 |
| 84 | MG | 6 | 2134 | 1/1 | 0.67 | 0.14 | - | 99,99,99,99 | 0 |
| 84 | MG | 5 | 3502 | 1/1 | 0.94 | 0.18 | - | 50,50,50,50 | 0 |
| 84 | MG | 1 | 3459 | 1/1 | 0.87 | 0.47 | - | 61,61,61,61 | 0 |
| 84 | MG | M0 | 302 | 1/1 | 0.81 | 0.83 | - | 64,64,64,64 | 0 |
| 84 | MG | 6 | 1938 | 1/1 | 0.86 | 0.35 | - | 59,59,59,59 | 0 |
| 84 | MG | 1 | 3677 | 1/1 | 0.89 | 0.54 | - | 66,66,66,66 | 0 |
| 84 | MG | 1 | 3530 | 1/1 | 0.95 | 0.28 | - | 67,67,67,67 | 0 |
| 84 | MG | 2 | 1950 | 1/1 | 0.92 | 0.34 | - | 94,94,94,94 | 0 |
| 84 | MG | 5 | 4032 | 1/1 | 0.93 | 0.06 | - | 69,69,69,69 | 1 |
| 84 | MG | 1 | 3488 | 1/1 | 0.87 | 0.26 | - | 73,73,73,73 | 0 |
| 84 | MG | 6 | 2059 | 1/1 | 0.69 | 0.18 | - | 76,76,76,76 | 0 |
| 84 | MG | 5 | 3424 | 1/1 | 0.88 | 0.32 | - | 54,54,54,54 | 0 |
| 84 | MG | 5 | 3597 | 1/1 | 0.84 | 0.35 | - | 70,70,70,70 | 0 |
| 84 | MG | 2 | 1928 | 1/1 | 0.97 | 0.47 | - | 67,67,67,67 | 0 |
| 84 | MG | 3 | 219 | 1/1 | 0.85 | 0.30 | - | 79,79,79,79 | 0 |
| 84 | MG | 1 | 3416 | 1/1 | 0.98 | 0.17 | - | 56,56,56,56 | 0 |
| 84 | MG | 2 | 1942 | 1/1 | 0.86 | 0.45 | - | 84,84,84,84 | 0 |
| 84 | MG | 5 | 3645 | 1/1 | 0.57 | 0.55 | - | 59,59,59,59 | 0 |
| 84 | MG | 5 | 3864 | 1/1 | 0.97 | 0.34 | - | 68,68,68,68 | 0 |
| 84 | MG | 5 | 3543 | 1/1 | 0.84 | 0.32 | - | 52,52,52,52 | 1 |
| 84 | MG | q2 | 504 | 1/1 | 0.85 | 0.56 | - | 60,60,60,60 | 0 |
| 84 | MG | 6 | 2160 | 1/1 | 0.87 | 0.28 | - | 88,88,88,88 | 0 |
| 84 | MG | 6 | 2018 | 1/1 | 0.72 | 0.31 | - | 81,81,81,81 | 0 |
| 84 | MG | 1 | 3980 | 1/1 | 0.60 | 0.14 | - | 91,91,91,91 | 0 |
| 84 | MG | 1 | 3638 | 1/1 | 0.97 | 0.17 | - | 90,90,90,90 | 0 |
| 84 | MG | 2 | 2031 | 1/1 | 0.84 | 0.35 | - | 105,105,105,105 | 0 |
| 84 | MG | 5 | 3571 | 1/1 | 0.84 | 0.18 | - | 77,77,77,77 | 0 |
| 84 | MG | 1 | 3694 | 1/1 | 0.74 | 0.38 | - | 62,62,62,62 | 0 |
| 84 | MG | 1 | 3533 | 1/1 | 0.95 | 0.56 | - | 75,75,75,75 | 0 |
| 84 | MG | 2 | 1937 | 1/1 | 0.94 | 0.23 | - | 80,80,80,80 | 0 |
| 84 | MG | 5 | 3464 | 1/1 | 0.97 | 0.29 | - | 52,52,52,52 | 0 |
| 84 | MG | 1 | 3565 | 1/1 | 0.74 | 0.20 | - | 71,71,71,71 | 0 |
| 84 | MG | 2 | 1982 | 1/1 | 0.99 | 0.14 | - | 97,97,97,97 | 0 |
| 84 | MG | 1 | 3723 | 1/1 | 0.72 | 0.32 | - | 47,47,47,47 | 0 |
| 84 | MG | 1 | 3461 | 1/1 | 0.69 | 0.44 | - | 59,59,59,59 | 0 |
| 84 | MG | 1 | 3755 | 1/1 | 0.91 | 0.73 | - | 60,60,60,60 | 0 |
| 84 | MG | 6 | 2105 | 1/1 | 0.94 | 0.25 | - | 67,67,67,67 | 0 |
| 84 | MG | 1 | 3812 | 1/1 | 0.88 | 0.19 | - | 82,82,82,82 | 0 |
| 84 | MG | l5 | 301 | 1/1 | 0.97 | 0.15 | - | 56,56,56,56 | 0 |
| 84 | MG | 1 | 3802 | 1/1 | 0.95 | 0.20 | - | 98,98,98,98 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | M0 | 301 | 1/1 | 0.94 | 0.23 | - | 51,51,51,51 | 0 |
| 84 | MG | 5 | 3661 | 1/1 | 0.93 | 0.34 | - | 61,61,61,61 | 0 |
| 84 | MG | 6 | 1986 | 1/1 | 0.92 | 0.28 | - | 82,82,82,82 | 0 |
| 84 | MG | 6 | 2144 | 1/1 | 0.84 | 0.15 | - | 76,76,76,76 | 0 |
| 84 | MG | 5 | 3890 | 1/1 | 0.97 | 0.19 | - | 62,62,62,62 | 0 |
| 84 | MG | m6 | 202 | 1/1 | 0.76 | 0.29 | - | 47,47,47,47 | 0 |
| 84 | MG | 6 | 2103 | 1/1 | 0.91 | 0.13 | - | 94,94,94,94 | 0 |
| 84 | MG | 5 | 3608 | 1/1 | 0.87 | 0.13 | - | 95,95,95,95 | 0 |
| 84 | MG | 6 | 1998 | 1/1 | 0.82 | 0.26 | - | 78,78,78,78 | 0 |
| 84 | MG | 5 | 3863 | 1/1 | 0.66 | 0.53 | - | 76,76,76,76 | 0 |
| 84 | MG | 1 | 3630 | 1/1 | 0.62 | 0.12 | - | 106,106,106,106 | 0 |
| 84 | MG | 5 | 4100 | 1/1 | 0.94 | 0.45 | - | 90,90,90,90 | 0 |
| 84 | MG | 5 | 3888 | 1/1 | 0.89 | 0.32 | - | 62,62,62,62 | 0 |
| 84 | MG | 1 | 3828 | 1/1 | 0.86 | 0.58 | - | 67,67,67,67 | 0 |
| 84 | MG | 5 | 4089 | 1/1 | 0.91 | 0.70 | - | 62,62,62,62 | 0 |
| 84 | MG | 6 | 2069 | 1/1 | 0.92 | 0.11 | - | 86,86,86,86 | 0 |
| 84 | MG | 7 | 201 | 1/1 | 0.98 | 0.27 | - | 45,45,45,45 | 0 |
| 84 | MG | 6 | 2037 | 1/1 | 0.81 | 0.16 | - | 87,87,87,87 | 0 |
| 84 | MG | 1 | 3527 | 1/1 | 0.92 | 0.45 | - | 70,70,70,70 | 0 |
| 84 | MG | 1 | 3841 | 1/1 | 0.86 | 0.45 | - | 92,92,92,92 | 0 |
| 84 | MG | 2 | 1902 | 1/1 | 0.95 | 0.09 | - | 95,95,95,95 | 0 |
| 84 | MG | m7 | 207 | 1/1 | 0.74 | 0.53 | - | 66,66,66,66 | 0 |
| 84 | MG | O4 | 504 | 1/1 | 0.82 | 0.48 | - | 76,76,76,76 | 0 |
| 84 | MG | 1 | 3633 | 1/1 | 0.91 | 0.29 | - | 79,79,79,79 | 0 |
| 84 | MG | 5 | 3751 | 1/1 | 0.56 | 0.59 | - | 61,61,61,61 | 0 |
| 84 | MG | 2 | 2008 | 1/1 | 0.92 | 0.16 | - | 117,117,117,117 | 0 |
| 84 | MG | 5 | 4139 | 1/1 | 0.93 | 0.29 | - | 66,66,66,66 | 0 |
| 84 | MG | 5 | 3992 | 1/1 | 0.81 | 0.42 | - | 49,49,49,49 | 0 |
| 84 | MG | 6 | 2138 | 1/1 | 0.96 | 0.13 | - | 84,84,84,84 | 0 |
| 84 | MG | 1 | 3919 | 1/1 | 0.95 | 0.25 | - | 69,69,69,69 | 0 |
| 84 | MG | 3 | 208 | 1/1 | 0.73 | 0.46 | - | 64,64,64,64 | 0 |
| 84 | MG | 6 | 2129 | 1/1 | 0.56 | 0.35 | - | 88,88,88,88 | 0 |
| 84 | MG | 2 | 2014 | 1/1 | 0.94 | 0.24 | - | 88,88,88,88 | 0 |
| 84 | MG | 1 | 3637 | 1/1 | 0.42 | 0.37 | - | 91,91,91,91 | 0 |
| 84 | MG | 6 | 1951 | 1/1 | 0.69 | 0.21 | - | 74,74,74,74 | 0 |
| 84 | MG | 5 | 3619 | 1/1 | 0.90 | 0.18 | - | 86,86,86,86 | 0 |
| 84 | MG | 1 | 3738 | 1/1 | 0.74 | 0.73 | - | 75,75,75,75 | 0 |
| 84 | MG | 4 | 220 | 1/1 | 0.91 | 0.25 | - | 71,71,71,71 | 0 |
| 84 | MG | 5 | 3487 | 1/1 | 0.95 | 0.16 | - | 61,61,61,61 | 0 |
| 84 | MG | 6 | 2074 | 1/1 | 0.93 | 0.15 | - | 64,64,64,64 | 0 |
| 84 | MG | 5 | 3439 | 1/1 | 0.95 | 0.25 | - | 54,54,54,54 | 0 |
| 84 | MG | 5 | 3526 | 1/1 | 0.76 | 0.62 | - | 61,61,61,61 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 6 | 1976 | 1/1 | 0.82 | 0.22 | - | 84,84,84,84 | 0 |
| 84 | MG | 1 | 3950 | 1/1 | 0.03 | 0.55 | - | 85,85,85,85 | 0 |
| 84 | MG | 5 | 3711 | 1/1 | 0.66 | 0.34 | - | 70,70,70,70 | 0 |
| 84 | MG | 2 | 1911 | 1/1 | 0.89 | 0.16 | - | 91,91,91,91 | 0 |
| 84 | MG | 1 | 3849 | 1/1 | 0.91 | 0.22 | - | 58,58,58,58 | 0 |
| 84 | MG | N8 | 202 | 1/1 | 0.90 | 0.72 | - | 73,73,73,73 | 0 |
| 84 | MG | 1 | 3803 | 1/1 | 0.61 | 0.45 | - | 76,76,76,76 | 0 |
| 84 | MG | 5 | 3685 | 1/1 | 0.92 | 0.32 | - | 66,66,66,66 | 0 |
| 84 | MG | 2 | 2007 | 1/1 | 0.65 | 0.24 | - | 88,88,88,88 | 0 |
| 84 | MG | 1 | 3440 | 1/1 | 0.88 | 0.23 | - | 82,82,82,82 | 0 |
| 84 | MG | 5 | 3423 | 1/1 | 0.83 | 0.30 | - | 54,54,54,54 | 1 |
| 84 | MG | 1 | 3904 | 1/1 | 0.70 | 0.27 | - | 76,76,76,76 | 0 |
| 84 | MG | 1 | 3823 | 1/1 | 0.71 | 0.69 | - | 89,89,89,89 | 0 |
| 84 | MG | 1 | 3978 | 1/1 | 0.85 | 0.31 | - | 89,89,89,89 | 0 |
| 84 | MG | 7 | 210 | 1/1 | 0.93 | 0.14 | - | 67,67,67,67 | 0 |
| 84 | MG | 5 | 3630 | 1/1 | 0.97 | 0.20 | - | 50,50,50,50 | 0 |
| 84 | MG | 5 | 4099 | 1/1 | 0.85 | 0.27 | - | 105,105,105,105 | 0 |
| 84 | MG | 2 | 1963 | 1/1 | 0.92 | 0.14 | - | 117,117,117,117 | 0 |
| 84 | MG | 6 | 2014 | 1/1 | 0.80 | 0.21 | - | 74,74,74,74 | 0 |
| 84 | MG | 6 | 1924 | 1/1 | 0.52 | 0.29 | - | 70,70,70,70 | 0 |
| 84 | MG | m4 | 206 | 1/1 | 0.75 | 0.35 | - | 58,58,58,58 | 0 |
| 84 | MG | 1 | 3784 | 1/1 | 0.87 | 0.51 | - | 72,72,72,72 | 0 |
| 84 | MG | 1 | 3575 | 1/1 | 0.82 | 0.18 | - | 61,61,61,61 | 0 |
| 84 | MG | 1 | 3888 | 1/1 | 0.62 | 0.38 | - | 68,68,68,68 | 0 |
| 84 | MG | 1 | 3672 | 1/1 | 0.90 | 0.31 | - | 52,52,52,52 | 0 |
| 84 | MG | 5 | 3753 | 1/1 | 0.91 | 0.47 | - | 85,85,85,85 | 0 |
| 84 | MG | M0 | 303 | 1/1 | 0.80 | 0.33 | - | 66,66,66,66 | 0 |
| 84 | MG | 2 | 2004 | 1/1 | 0.76 | 0.72 | - | 81,81,81,81 | 0 |
| 84 | MG | 5 | 4092 | 1/1 | 0.92 | 0.43 | - | 71,71,71,71 | 0 |
| 84 | MG | 5 | 4115 | 1/1 | 0.87 | 0.44 | - | 59,59,59,59 | 0 |
| 84 | MG | 6 | 2108 | 1/1 | 0.70 | 0.33 | - | 79,79,79,79 | 0 |
| 84 | MG | 1 | 3652 | 1/1 | 0.81 | 0.23 | - | 59,59,59,59 | 0 |
| 84 | MG | 7 | 222 | 1/1 | 0.84 | 0.13 | - | 66,66,66,66 | 0 |
| 84 | MG | 1 | 3708 | 1/1 | 0.90 | 0.38 | - | 66,66,66,66 | 0 |
| 84 | MG | 6 | 1993 | 1/1 | 0.67 | 0.72 | - | 71,71,71,71 | 0 |
| 84 | MG | 5 | 4044 | 1/1 | 0.98 | 0.40 | - | 72,72,72,72 | 0 |
| 84 | MG | 5 | 3843 | 1/1 | 0.95 | 0.11 | - | 50,50,50,50 | 0 |
| 84 | MG | 1 | 3869 | 1/1 | 0.87 | 0.39 | - | 62,62,62,62 | 0 |
| 84 | MG | 5 | 3882 | 1/1 | 0.92 | 0.28 | - | 67,67,67,67 | 0 |
| 84 | MG | 6 | 2072 | 1/1 | 0.43 | 0.26 | - | 77,77,77,77 | 0 |
| 84 | MG | q2 | 506 | 1/1 | 0.59 | 0.33 | - | 68,68,68,68 | 0 |
| 84 | MG | 6 | 1994 | 1/1 | 0.81 | 0.59 | - | 69,69,69,69 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 5 | 3879 | 1/1 | 0.92 | 0.31 | - | 64,64,64,64 | 0 |
| 84 | MG | 6 | 1933 | 1/1 | 0.64 | 0.57 | - | 74,74,74,74 | 0 |
| 84 | MG | 1 | 3926 | 1/1 | 0.91 | 0.33 | - | 54,54,54,54 | 0 |
| 84 | MG | 6 | 1960 | 1/1 | 0.74 | 0.41 | - | 62,62,62,62 | 0 |
| 84 | MG | 5 | 3647 | 1/1 | 0.90 | 0.36 | - | 58,58,58,58 | 0 |
| 84 | MG | 6 | 2003 | 1/1 | 0.95 | 0.16 | - | 64,64,64,64 | 0 |
| 84 | MG | 5 | 3555 | 1/1 | 0.95 | 0.21 | - | 62,62,62,62 | 1 |
| 84 | MG | 5 | 3517 | 1/1 | 0.94 | 0.60 | - | 49,49,49,49 | 0 |
| 84 | MG | 5 | 4148 | 1/1 | 0.85 | 0.47 | - | 54,54,54,54 | 0 |
| 84 | MG | 5 | 4024 | 1/1 | 0.79 | 0.39 | - | 68,68,68,68 | 0 |
| 84 | MG | 5 | 3515 | 1/1 | 0.96 | 0.21 | - | 43,43,43,43 | 0 |
| 84 | MG | 5 | 3988 | 1/1 | 0.97 | 0.36 | - | 45,45,45,45 | 0 |
| 84 | MG | 5 | 3730 | 1/1 | 0.89 | 0.29 | - | 74,74,74,74 | 0 |
| 84 | MG | 6 | 1975 | 1/1 | 0.85 | 0.23 | - | 83,83,83,83 | 0 |
| 84 | MG | 5 | 3570 | 1/1 | 0.93 | 0.24 | - | 67,67,67,67 | 0 |
| 84 | MG | 6 | 2021 | 1/1 | 0.82 | 0.09 | - | 86,86,86,86 | 0 |
| 84 | MG | 1 | 3632 | 1/1 | 0.89 | 0.10 | - | 72,72,72,72 | 0 |
| 84 | MG | 4 | 211 | 1/1 | 0.68 | 0.27 | - | 86,86,86,86 | 0 |
| 84 | MG | 5 | 3486 | 1/1 | 0.89 | 0.31 | - | 52,52,52,52 | 0 |
| 84 | MG | 1 | 3667 | 1/1 | 0.55 | 0.53 | - | 73,73,73,73 | 0 |
| 84 | MG | 5 | 4065 | 1/1 | 0.88 | 0.36 | - | 58,58,58,58 | 0 |
| 84 | MG | o1 | 201 | 1/1 | 0.92 | 0.18 | - | 79,79,79,79 | 0 |
| 84 | MG | 2 | 1910 | 1/1 | 0.91 | 0.79 | - | 80,80,80,80 | 0 |
| 84 | MG | 2 | 1990 | 1/1 | 0.81 | 0.21 | - | 116,116,116,116 | 0 |
| 84 | MG | 6 | 1963 | 1/1 | 0.99 | 0.32 | - | 68,68,68,68 | 0 |
| 84 | MG | L4 | 405 | 1/1 | 0.80 | 0.42 | - | 63,63,63,63 | 0 |
| 84 | MG | 1 | 3524 | 1/1 | 0.89 | 0.40 | - | 71,71,71,71 | 0 |
| 84 | MG | 6 | 2024 | 1/1 | 0.62 | 0.23 | - | 80,80,80,80 | 0 |
| 84 | MG | 6 | 2073 | 1/1 | 0.86 | 0.27 | - | 80,80,80,80 | 0 |
| 84 | MG | L3 | 401 | 1/1 | 0.88 | 0.17 | - | 76,76,76,76 | 0 |
| 84 | MG | 5 | 3934 | 1/1 | 0.74 | 0.46 | - | 48,48,48,48 | 1 |
| 84 | MG | 4 | 205 | 1/1 | 0.91 | 0.20 | - | 87,87,87,87 | 0 |
| 84 | MG | 1 | 3742 | 1/1 | 0.78 | 0.51 | - | 78,78,78,78 | 0 |
| 84 | MG | 2 | 1961 | 1/1 | 0.43 | 0.17 | - | 109,109,109,109 | 0 |
| 84 | MG | 5 | 3800 | 1/1 | 0.85 | 0.21 | - | 69,69,69,69 | 0 |
| 84 | MG | 5 | 3702 | 1/1 | 0.97 | 0.11 | - | 85,85,85,85 | 0 |
| 84 | MG | O6 | 201 | 1/1 | 0.54 | 0.25 | - | 78,78,78,78 | 0 |
| 84 | MG | 6 | 2121 | 1/1 | 0.54 | 0.61 | - | 97,97,97,97 | 0 |
| 84 | MG | 8 | 208 | 1/1 | 0.75 | 0.21 | - | 79,79,79,79 | 0 |
| 84 | MG | 4 | 217 | 1/1 | 0.93 | 0.25 | - | 79,79,79,79 | 0 |
| 84 | MG | 6 | 2061 | 1/1 | 0.84 | 0.20 | - | 80,80,80,80 | 0 |
| 84 | MG | 5 | 3679 | 1/1 | 0.97 | 0.23 | - | 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 | MG | 1 | 3792 | 1/1 | 0.79 | 0.23 | - | 94,94,94,94 | 0 |
| 84 | MG | 6 | 2009 | 1/1 | 0.97 | 0.12 | - | 73,73,73,73 | 0 |
| 84 | MG | 1 | 3817 | 1/1 | 0.81 | 0.66 | - | 72,72,72,72 | 0 |
| 84 | MG | 5 | 3810 | 1/1 | 0.93 | 0.33 | - | 59,59,59,59 | 0 |
| 84 | MG | 2 | 1977 | 1/1 | 0.71 | 1.32 | - | 77,77,77,77 | 0 |
| 84 | MG | 1 | 3580 | 1/1 | 0.74 | 0.24 | - | 75,75,75,75 | 0 |
| 84 | MG | 5 | 4063 | 1/1 | 0.77 | 0.17 | - | 94,94,94,94 | 0 |
| 84 | MG | 5 | 4120 | 1/1 | 0.75 | 0.10 | - | 90,90,90,90 | 0 |
| 84 | MG | 6 | 1949 | 1/1 | 0.88 | 0.18 | - | 74,74,74,74 | 0 |
| 84 | MG | c3 | 206 | 1/1 | 0.91 | 0.24 | - | 80,80,80,80 | 0 |
| 84 | MG | 5 | 3929 | 1/1 | 0.92 | 0.27 | - | 43,43,43,43 | 0 |
| 84 | MG | N0 | 204 | 1/1 | 0.97 | 0.13 | - | 68,68,68,68 | 0 |
| 84 | MG | 5 | 3777 | 1/1 | 0.92 | 0.35 | - | 70,70,70,70 | 0 |
| 84 | MG | 5 | 3970 | 1/1 | 0.49 | 0.72 | - | 75,75,75,75 | 0 |
| 84 | MG | 6 | 2002 | 1/1 | 0.97 | 0.12 | - | 68,68,68,68 | 0 |
| 84 | MG | 1 | 3882 | 1/1 | 0.95 | 0.24 | - | 71,71,71,71 | 0 |
| 84 | MG | 6 | 2141 | 1/1 | 0.52 | 0.32 | - | 99,99,99,99 | 0 |
| 84 | MG | M7 | 203 | 1/1 | 0.89 | 0.22 | - | 59,59,59,59 | 0 |
| 84 | MG | 5 | 4070 | 1/1 | 0.93 | 0.11 | - | 99,99,99,99 | 0 |
| 84 | MG | 5 | 3962 | 1/1 | 0.86 | 0.52 | - | 95,95,95,95 | 0 |
| 84 | MG | 6 | 1990 | 1/1 | 0.86 | 0.26 | - | 73,73,73,73 | 0 |
| 84 | MG | 5 | 4088 | 1/1 | 0.95 | 0.22 | - | 69,69,69,69 | 0 |
| 84 | MG | 2 | 2033 | 1/1 | 0.82 | 0.23 | - | 108,108,108,108 | 0 |
| 84 | MG | 1 | 3676 | 1/1 | 0.93 | 0.52 | - | 53,53,53,53 | 0 |
| 84 | MG | 1 | 3942 | 1/1 | 0.96 | 0.27 | - | 49,49,49,49 | 0 |
| 84 | MG | 3 | 218 | 1/1 | 0.94 | 0.13 | - | 97,97,97,97 | 0 |
| 84 | MG | 5 | 3937 | 1/1 | 0.65 | 0.35 | - | 60,60,60,60 | 0 |
| 84 | MG | 1 | 3595 | 1/1 | 0.98 | 0.27 | - | 54,54,54,54 | 0 |
| 84 | MG | 5 | 3998 | 1/1 | 0.92 | 0.23 | - | 54,54,54,54 | 0 |
| 84 | MG | 5 | 3444 | 1/1 | 0.99 | 0.24 | - | 45,45,45,45 | 0 |
| 84 | MG | 6 | 2091 | 1/1 | 0.87 | 0.49 | - | 68,68,68,68 | 0 |
| 84 | MG | 5 | 3731 | 1/1 | 0.93 | 0.11 | - | 69,69,69,69 | 0 |
| 84 | MG | 5 | 3914 | 1/1 | 0.93 | 0.24 | - | 56,56,56,56 | 0 |
| 84 | MG | 7 | 214 | 1/1 | 0.86 | 0.33 | - | 80,80,80,80 | 0 |
| 84 | MG | d6 | 103 | 1/1 | 0.90 | 0.24 | - | 77,77,77,77 | 0 |
| 84 | MG | 5 | 3566 | 1/1 | 0.83 | 0.27 | - | 60,60,60,60 | 0 |
| 84 | MG | 1 | 3768 | 1/1 | 0.90 | 0.45 | - | 67,67,67,67 | 0 |
| 84 | MG | 7 | 216 | 1/1 | 0.83 | 0.09 | - | 74,74,74,74 | 1 |
| 84 | MG | 5 | 3550 | 1/1 | 0.86 | 0.39 | - | 59,59,59,59 | 0 |
| 84 | MG | 5 | 3896 | 1/1 | 0.65 | 0.83 | - | 71,71,71,71 | 0 |
| 84 | MG | 6 | 1916 | 1/1 | 0.86 | 0.22 | - | 94,94,94,94 | 0 |
| 84 | MG | 5 | 3886 | 1/1 | 0.60 | 0.36 | - | 77,77,77,77 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 5 | 3406 | 1/1 | 0.99 | 0.27 | - | 44,44,44,44 | 0 |
| 84 | MG | 5 | 3507 | 1/1 | 0.96 | 0.20 | - | 55,55,55,55 | 0 |
| 84 | MG | 5 | 3533 | 1/1 | 0.98 | 0.27 | - | 45,45,45,45 | 0 |
| 84 | MG | 5 | 3707 | 1/1 | 0.95 | 0.18 | - | 73,73,73,73 | 0 |
| 84 | MG | 5 | 3919 | 1/1 | 0.85 | 0.30 | - | 51,51,51,51 | 0 |
| 84 | MG | 5 | 3404 | 1/1 | 0.95 | 0.22 | - | 55,55,55,55 | 0 |
| 84 | MG | 1 | 3653 | 1/1 | 0.89 | 0.26 | - | 59,59,59,59 | 0 |
| 84 | MG | 5 | 3966 | 1/1 | 0.61 | 0.63 | - | 95,95,95,95 | 0 |
| 84 | MG | 1 | 3815 | 1/1 | 0.72 | 0.74 | - | 77,77,77,77 | 0 |
| 84 | MG | 5 | 4013 | 1/1 | 0.90 | 0.32 | - | 58,58,58,58 | 0 |
| 84 | MG | 5 | 3776 | 1/1 | 0.96 | 0.12 | - | 65,65,65,65 | 0 |
| 84 | MG | 5 | 3828 | 1/1 | 0.77 | 0.31 | - | 46,46,46,46 | 0 |
| 84 | MG | 5 | 3534 | 1/1 | 0.92 | 0.39 | - | 50,50,50,50 | 0 |
| 84 | MG | s5 | 303 | 1/1 | 0.97 | 0.33 | - | 77,77,77,77 | 0 |
| 84 | MG | 5 | 4004 | 1/1 | 0.85 | 0.32 | - | 80,80,80,80 | 0 |
| 84 | MG | 1 | 3743 | 1/1 | 0.94 | 0.63 | - | 72,72,72,72 | 0 |
| 84 | MG | M5 | 304 | 1/1 | 0.95 | 0.26 | - | 67,67,67,67 | 0 |
| 84 | MG | 1 | 3949 | 1/1 | 0.79 | 0.14 | - | 79,79,79,79 | 0 |
| 84 | MG | l4 | 1101 | 1/1 | 0.90 | 0.29 | - | 65,65,65,65 | 0 |
| 84 | MG | 5 | 3752 | 1/1 | 0.82 | 0.36 | - | 59,59,59,59 | 0 |
| 84 | MG | 1 | 3583 | 1/1 | 0.93 | 0.19 | - | 63,63,63,63 | 0 |
| 84 | MG | n1 | 201 | 1/1 | 0.81 | 0.14 | - | 61,61,61,61 | 0 |
| 84 | MG | 1 | 3876 | 1/1 | 0.53 | 0.67 | - | 76,76,76,76 | 0 |
| 84 | MG | 5 | 3516 | 1/1 | 0.95 | 0.18 | - | 49,49,49,49 | 0 |
| 84 | MG | 6 | 2032 | 1/1 | 0.92 | 0.06 | - | 77,77,77,77 | 0 |
| 84 | MG | 5 | 3795 | 1/1 | 0.69 | 0.22 | - | 74,74,74,74 | 0 |
| 84 | MG | 1 | 3696 | 1/1 | 0.80 | 0.50 | - | 55,55,55,55 | 0 |
| 84 | MG | 6 | 2139 | 1/1 | 0.73 | 0.19 | - | 82,82,82,82 | 0 |
| 84 | MG | 1 | 3907 | 1/1 | 0.95 | 0.31 | - | 62,62,62,62 | 0 |
| 84 | MG | 5 | 4150 | 1/1 | 0.86 | 0.19 | - | 81,81,81,81 | 0 |
| 84 | MG | 1 | 3482 | 1/1 | 0.95 | 0.25 | - | 72,72,72,72 | 0 |
| 84 | MG | l5 | 303 | 1/1 | 0.91 | 0.19 | - | 74,74,74,74 | 0 |
| 84 | MG | 1 | 3615 | 1/1 | 0.85 | 0.26 | - | 59,59,59,59 | 0 |
| 84 | MG | 1 | 3470 | 1/1 | 0.94 | 0.38 | - | 56,56,56,56 | 0 |
| 84 | MG | 5 | 3703 | 1/1 | 0.91 | 0.20 | - | 70,70,70,70 | 0 |
| 84 | MG | 4 | 203 | 1/1 | 0.83 | 0.27 | - | 61,61,61,61 | 0 |
| 84 | MG | 2 | 1964 | 1/1 | 0.92 | 0.20 | - | 90,90,90,90 | 0 |
| 84 | MG | 2 | 1930 | 1/1 | 0.84 | 0.71 | - | 81,81,81,81 | 0 |
| 84 | MG | 5 | 3827 | 1/1 | 0.92 | 0.16 | - | 51,51,51,51 | 1 |
| 84 | MG | 1 | 3556 | 1/1 | 0.81 | 0.35 | - | 73,73,73,73 | 0 |
| 84 | MG | 1 | 3593 | 1/1 | 0.85 | 0.47 | - | 63,63,63,63 | 0 |
| 84 | MG | 1 | 3958 | 1/1 | 0.69 | 0.19 | - | 88,88,88,88 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 1 | 3617 | 1/1 | 0.93 | 0.60 | - | 70,70,70,70 | 0 |
| 84 | MG | 1 | 3685 | 1/1 | 0.92 | 0.40 | - | 56,56,56,56 | 0 |
| 84 | MG | 1 | 3966 | 1/1 | 0.94 | 0.17 | - | 68,68,68,68 | 0 |
| 84 | MG | 5 | 3701 | 1/1 | 0.93 | 0.18 | - | 66,66,66,66 | 0 |
| 84 | MG | 5 | 3913 | 1/1 | 0.93 | 0.31 | - | 57,57,57,57 | 0 |
| 84 | MG | 5 | 3999 | 1/1 | 0.68 | 0.31 | - | 52,52,52,52 | 0 |
| 84 | MG | 5 | 3815 | 1/1 | 0.92 | 0.35 | - | 55,55,55,55 | 0 |
| 84 | MG | 5 | 4108 | 1/1 | 0.94 | 0.19 | - | 59,59,59,59 | 0 |
| 84 | MG | 2 | 2003 | 1/1 | 0.84 | 0.28 | - | 118,118,118,118 | 0 |
| 84 | MG | 5 | 3958 | 1/1 | 0.80 | 0.62 | - | 66,66,66,66 | 0 |
| 84 | MG | 1 | 3445 | 1/1 | 0.83 | 0.41 | - | 64,64,64,64 | 0 |
| 84 | MG | 1 | 3764 | 1/1 | 0.75 | 0.57 | - | 69,69,69,69 | 0 |
| 84 | MG | 1 | 3981 | 1/1 | 0.96 | 0.39 | - | 63,63,63,63 | 0 |
| 84 | MG | 5 | 3624 | 1/1 | 0.75 | 0.57 | - | 65,65,65,65 | 0 |
| 84 | MG | 2 | 2034 | 1/1 | 0.80 | 0.19 | - | 92,92,92,92 | 0 |
| 84 | MG | l3 | 410 | 1/1 | 0.75 | 0.17 | - | 73,73,73,73 | 0 |
| 84 | MG | 1 | 3835 | 1/1 | 0.86 | 0.24 | - | 58,58,58,58 | 0 |
| 84 | MG | 1 | 3670 | 1/1 | 0.80 | 0.31 | - | 76,76,76,76 | 0 |
| 84 | MG | l9 | 203 | 1/1 | 0.90 | 0.24 | - | 49,49,49,49 | 0 |
| 84 | MG | 6 | 1936 | 1/1 | 0.89 | 0.79 | - | 65,65,65,65 | 0 |
| 84 | MG | s2 | 301 | 1/1 | 0.92 | 0.34 | - | 69,69,69,69 | 0 |
| 84 | MG | 1 | 3557 | 1/1 | 0.96 | 0.18 | - | 71,71,71,71 | 0 |
| 84 | MG | 1 | 3730 | 1/1 | 0.84 | 0.38 | - | 65,65,65,65 | 0 |
| 84 | MG | 1 | 3986 | 1/1 | 0.95 | 0.41 | - | 68,68,68,68 | 0 |
| 84 | MG | 5 | 3579 | 1/1 | 0.97 | 0.45 | - | 45,45,45,45 | 0 |
| 84 | MG | 5 | 3813 | 1/1 | 0.64 | 0.55 | - | 58,58,58,58 | 0 |
| 84 | MG | q2 | 503 | 1/1 | 0.82 | 0.35 | - | 52,52,52,52 | 0 |
| 84 | MG | 5 | 3818 | 1/1 | 0.95 | 0.18 | - | 54,54,54,54 | 0 |
| 84 | MG | O2 | 201 | 1/1 | 0.99 | 0.11 | - | 60,60,60,60 | 0 |
| 84 | MG | 6 | 1991 | 1/1 | 0.55 | 0.54 | - | 71,71,71,71 | 0 |
| 84 | MG | 2 | 2013 | 1/1 | 0.78 | 0.12 | - | 120,120,120,120 | 0 |
| 84 | MG | 5 | 4131 | 1/1 | 0.95 | 0.31 | - | 70,70,70,70 | 0 |
| 84 | MG | 5 | 4097 | 1/1 | 0.49 | 0.48 | - | 68,68,68,68 | 0 |
| 84 | MG | 5 | 3573 | 1/1 | 0.98 | 0.31 | - | 61,61,61,61 | 0 |
| 84 | MG | 5 | 4119 | 1/1 | 0.88 | 0.09 | - | 142,142,142,142 | 0 |
| 84 | MG | 5 | 3790 | 1/1 | 0.95 | 0.31 | - | 47,47,47,47 | 0 |
| 84 | MG | 1 | 3460 | 1/1 | 0.99 | 0.27 | - | 58,58,58,58 | 0 |
| 84 | MG | 6 | 2081 | 1/1 | 0.97 | 0.20 | - | 69,69,69,69 | 0 |
| 84 | MG | m8 | 203 | 1/1 | 0.65 | 0.39 | - | 69,69,69,69 | 0 |
| 84 | MG | 5 | 4043 | 1/1 | 0.87 | 0.33 | - | 51,51,51,51 | 0 |
| 84 | MG | 6 | 2135 | 1/1 | 0.93 | 0.25 | - | 77,77,77,77 | 0 |
| 84 | MG | 1 | 3793 | 1/1 | 0.95 | 0.17 | - | 85,85,85,85 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 5 | 3658 | 1/1 | 0.95 | 0.17 | - | 71,71,71,71 | 0 |
| 84 | MG | 1 | 3748 | 1/1 | 0.93 | 0.37 | - | 61,61,61,61 | 0 |
| 84 | MG | 6 | 1952 | 1/1 | 0.93 | 0.14 | - | 68,68,68,68 | 0 |
| 84 | MG | 5 | 3787 | 1/1 | 0.91 | 0.24 | - | 48,48,48,48 | 1 |
| 84 | MG | 1 | 3710 | 1/1 | 0.88 | 0.28 | - | 90,90,90,90 | 0 |
| 84 | MG | 2 | 1984 | 1/1 | 0.74 | 0.43 | - | 113,113,113,113 | 0 |
| 84 | MG | Q2 | 503 | 1/1 | 0.95 | 0.27 | - | 67,67,67,67 | 0 |
| 84 | MG | 1 | 3865 | 1/1 | 0.69 | 0.55 | - | 81,81,81,81 | 0 |
| 84 | MG | 1 | 3963 | 1/1 | 0.81 | 0.33 | - | 76,76,76,76 | 0 |
| 84 | MG | 1 | 3915 | 1/1 | 0.89 | 0.16 | - | 78,78,78,78 | 0 |
| 84 | MG | 5 | 4126 | 1/1 | 0.88 | 0.48 | - | 60,60,60,60 | 0 |
| 84 | MG | 1 | 3709 | 1/1 | 0.90 | 0.27 | - | 60,60,60,60 | 0 |
| 84 | MG | 1 | 3485 | 1/1 | 0.98 | 0.21 | - | 70,70,70,70 | 0 |
| 84 | MG | 2 | 1947 | 1/1 | 0.84 | 0.48 | - | 92,92,92,92 | 0 |
| 84 | MG | 6 | 1915 | 1/1 | 0.88 | 0.13 | - | 74,74,74,74 | 0 |
| 84 | MG | 6 | 1909 | 1/1 | 0.91 | 0.28 | - | 67,67,67,67 | 0 |
| 84 | MG | 5 | 3963 | 1/1 | 0.96 | 0.12 | - | 102,102,102,102 | 0 |
| 84 | MG | 1 | 3900 | 1/1 | 0.73 | 0.11 | - | 85,85,85,85 | 0 |
| 84 | MG | 5 | 3766 | 1/1 | 0.77 | 0.49 | - | 57,57,57,57 | 0 |
| 84 | MG | 5 | 4026 | 1/1 | 0.93 | 0.26 | - | 66,66,66,66 | 0 |
| 84 | MG | 2 | 1935 | 1/1 | 0.88 | 0.44 | - | 66,66,66,66 | 0 |
| 84 | MG | 1 | 3758 | 1/1 | 0.62 | 0.59 | - | 74,74,74,74 | 0 |
| 84 | MG | 6 | 2163 | 1/1 | 0.87 | 0.43 | - | 66,66,66,66 | 1 |
| 84 | MG | 1 | 3571 | 1/1 | 0.72 | 0.27 | - | 71,71,71,71 | 0 |
| 84 | MG | 1 | 3878 | 1/1 | 0.85 | 0.44 | - | 60,60,60,60 | 0 |
| 84 | MG | 5 | 3562 | 1/1 | 0.94 | 0.41 | - | 57,57,57,57 | 0 |
| 84 | MG | 5 | 4104 | 1/1 | 0.81 | 0.30 | - | 56,56,56,56 | 0 |
| 84 | MG | 5 | 3461 | 1/1 | 0.96 | 0.24 | - | 50,50,50,50 | 0 |
| 84 | MG | 19 | 205 | 1/1 | 0.93 | 0.13 | - | 72,72,72,72 | 0 |
| 84 | MG | 5 | 3876 | 1/1 | 0.90 | 0.14 | - | 66,66,66,66 | 0 |
| 84 | MG | 1 | 3489 | 1/1 | 0.89 | 0.24 | - | 79,79,79,79 | 0 |
| 84 | MG | 5 | 3726 | 1/1 | 0.94 | 0.45 | - | 52,52,52,52 | 0 |
| 84 | MG | O4 | 503 | 1/1 | 0.67 | 0.13 | - | 127,127,127,127 | 0 |
| 84 | MG | 6 | 1945 | 1/1 | 0.69 | 0.49 | - | 70,70,70,70 | 0 |
| 84 | MG | 6 | 1973 | 1/1 | 0.91 | 0.38 | - | 65,65,65,65 | 0 |
| 84 | MG | 1 | 3476 | 1/1 | 0.86 | 0.49 | - | 54,54,54,54 | 0 |
| 84 | MG | 1 | 3501 | 1/1 | 0.79 | 0.24 | - | 64,64,64,64 | 0 |
| 84 | MG | 5 | 4134 | 1/1 | 0.70 | 0.30 | - | 73,73,73,73 | 0 |
| 84 | MG | 5 | 4001 | 1/1 | 0.88 | 0.25 | - | 59,59,59,59 | 0 |
| 84 | MG | 1 | 3961 | 1/1 | 0.86 | 0.18 | - | 80,80,80,80 | 0 |
| 84 | MG | d3 | 201 | 1/1 | 0.78 | 0.48 | - | 65,65,65,65 | 0 |
| 84 | MG | 5 | 3524 | 1/1 | 0.77 | 0.47 | - | 53,53,53,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 1 | 3609 | 1/1 | 0.86 | 0.36 | - | 52,52,52,52 | 0 |
| 84 | MG | 6 | 2048 | 1/1 | 0.91 | 0.40 | - | 68,68,68,68 | 0 |
| 84 | MG | 1 | 3776 | 1/1 | 0.94 | 0.27 | - | 68,68,68,68 | 1 |
| 84 | MG | 5 | 3825 | 1/1 | 0.67 | 0.35 | - | 58,58,58,58 | 0 |
| 84 | MG | q2 | 507 | 1/1 | 0.76 | 0.20 | - | 51,51,51,51 | 0 |
| 84 | MG | 5 | 3403 | 1/1 | 0.86 | 0.37 | - | 54,54,54,54 | 0 |
| 84 | MG | 2 | 1955 | 1/1 | 0.65 | 0.33 | - | 86,86,86,86 | 0 |
| 84 | MG | q3 | 504 | 1/1 | 0.98 | 0.23 | - | 74,74,74,74 | 0 |
| 84 | MG | 5 | 3623 | 1/1 | 0.96 | 0.30 | - | 62,62,62,62 | 0 |
| 84 | MG | m3 | 203 | 1/1 | 0.83 | 0.48 | - | 81,81,81,81 | 0 |
| 84 | MG | 2 | 1907 | 1/1 | 0.90 | 0.17 | - | 95,95,95,95 | 0 |
| 84 | MG | 1 | 3691 | 1/1 | 0.87 | 0.26 | - | 59,59,59,59 | 0 |
| 84 | MG | 5 | 4129 | 1/1 | 0.68 | 0.57 | - | 90,90,90,90 | 0 |
| 84 | MG | 1 | 3620 | 1/1 | 0.87 | 0.66 | - | 65,65,65,65 | 0 |
| 84 | MG | s3 | 301 | 1/1 | 0.83 | 0.29 | - | 84,84,84,84 | 0 |
| 84 | MG | 1 | 3495 | 1/1 | 0.73 | 0.62 | - | 75,75,75,75 | 0 |
| 84 | MG | 1 | 3912 | 1/1 | 0.91 | 0.17 | - | 58,58,58,58 | 0 |
| 84 | MG | 4 | 208 | 1/1 | 0.67 | 0.40 | - | 60,60,60,60 | 0 |
| 84 | MG | 1 | 3736 | 1/1 | 0.96 | 0.15 | - | 82,82,82,82 | 0 |
| 84 | MG | q1 | 102 | 1/1 | 0.86 | 0.34 | - | 64,64,64,64 | 0 |
| 84 | MG | 5 | 3941 | 1/1 | 0.88 | 0.62 | - | 78,78,78,78 | 0 |
| 84 | MG | 1 | 3773 | 1/1 | 0.91 | 0.33 | - | 62,62,62,62 | 0 |
| 84 | MG | 5 | 3467 | 1/1 | 0.90 | 0.25 | - | 48,48,48,48 | 0 |
| 84 | MG | 1 | 3868 | 1/1 | 0.95 | 0.21 | - | 61,61,61,61 | 0 |
| 84 | MG | 1 | 3749 | 1/1 | 0.91 | 0.37 | - | 60,60,60,60 | 0 |
| 84 | MG | 1 | 3555 | 1/1 | 0.75 | 0.16 | - | 92,92,92,92 | 0 |
| 84 | MG | m9 | 202 | 1/1 | 0.88 | 0.62 | - | 90,90,90,90 | 0 |
| 84 | MG | 6 | 2070 | 1/1 | 0.72 | 0.17 | - | 128,128,128,128 | 0 |
| 84 | MG | 5 | 3621 | 1/1 | 0.89 | 0.15 | - | 77,77,77,77 | 0 |
| 84 | MG | 6 | 1937 | 1/1 | 0.81 | 0.93 | - | 62,62,62,62 | 0 |
| 84 | MG | 5 | 3410 | 1/1 | 0.94 | 0.52 | - | 46,46,46,46 | 0 |
| 84 | MG | 1 | 3480 | 1/1 | 0.97 | 0.31 | - | 62,62,62,62 | 0 |
| 84 | MG | o2 | 202 | 1/1 | 0.92 | 0.42 | - | 55,55,55,55 | 0 |
| 84 | MG | 5 | 3492 | 1/1 | 0.77 | 0.42 | - | 74,74,74,74 | 0 |
| 84 | MG | 2 | 1912 | 1/1 | 0.88 | 0.55 | - | 86,86,86,86 | 0 |
| 84 | MG | 5 | 3491 | 1/1 | 0.87 | 0.14 | - | 62,62,62,62 | 0 |
| 84 | MG | 1 | 3486 | 1/1 | 0.93 | 0.33 | - | 62,62,62,62 | 0 |
| 84 | MG | l3 | 407 | 1/1 | 0.85 | 0.33 | - | 55,55,55,55 | 0 |
| 84 | MG | 5 | 3451 | 1/1 | 0.93 | 0.44 | - | 45,45,45,45 | 0 |
| 84 | MG | 1 | 3689 | 1/1 | 0.96 | 0.26 | - | 58,58,58,58 | 0 |
| 84 | MG | 1 | 3837 | 1/1 | 0.83 | 0.48 | - | 58,58,58,58 | 0 |
| 84 | MG | 5 | 4021 | 1/1 | 0.83 | 0.28 | - | 60,60,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 5 | 3748 | 1/1 | 0.89 | 0.33 | - | 46,46,46,46 | 0 |
| 84 | MG | 5 | 3438 | 1/1 | 0.93 | 0.16 | - | 64,64,64,64 | 1 |
| 84 | MG | 1 | 3902 | 1/1 | 0.52 | 0.19 | - | 77,77,77,77 | 0 |
| 84 | MG | 8 | 212 | 1/1 | 0.82 | 0.34 | - | 66,66,66,66 | 0 |
| 84 | MG | 1 | 3786 | 1/1 | 0.88 | 0.78 | - | 70,70,70,70 | 0 |
| 84 | MG | 5 | 3897 | 1/1 | 0.83 | 0.42 | - | 76,76,76,76 | 0 |
| 84 | MG | l6 | 202 | 1/1 | 0.77 | 0.39 | - | 66,66,66,66 | 0 |
| 84 | MG | 5 | 3536 | 1/1 | 0.98 | 0.43 | - | 56,56,56,56 | 0 |
| 84 | MG | 1 | 3955 | 1/1 | 0.65 | 0.47 | - | 69,69,69,69 | 0 |
| 84 | MG | 5 | 3784 | 1/1 | 0.95 | 0.37 | - | 44,44,44,44 | 0 |
| 84 | MG | 5 | 3532 | 1/1 | 0.93 | 0.18 | - | 43,43,43,43 | 0 |
| 84 | MG | n5 | 202 | 1/1 | 0.66 | 0.32 | - | 78,78,78,78 | 0 |
| 84 | MG | 1 | 3867 | 1/1 | 0.89 | 0.34 | - | 59,59,59,59 | 0 |
| 84 | MG | 5 | 3656 | 1/1 | 0.98 | 0.19 | - | 78,78,78,78 | 0 |
| 84 | MG | 1 | 3603 | 1/1 | 0.95 | 0.35 | - | 45,45,45,45 | 0 |
| 84 | MG | 5 | 3942 | 1/1 | 0.72 | 0.39 | - | 79,79,79,79 | 0 |
| 84 | MG | 1 | 3422 | 1/1 | 0.98 | 0.25 | - | 50,50,50,50 | 0 |
| 84 | MG | 5 | 3689 | 1/1 | 0.96 | 0.14 | - | 78,78,78,78 | 0 |
| 84 | MG | d3 | 205 | 1/1 | 0.92 | 0.29 | - | 98,98,98,98 | 0 |
| 84 | MG | 1 | 3933 | 1/1 | 0.91 | 0.71 | - | 84,84,84,84 | 0 |
| 84 | MG | 1 | 3846 | 1/1 | 0.97 | 0.26 | - | 53,53,53,53 | 0 |
| 84 | MG | 5 | 3567 | 1/1 | 0.89 | 0.19 | - | 62,62,62,62 | 0 |
| 84 | MG | 5 | 3697 | 1/1 | 0.80 | 0.44 | - | 65,65,65,65 | 0 |
| 84 | MG | D3 | 204 | 1/1 | 0.73 | 0.51 | - | 94,94,94,94 | 0 |
| 84 | MG | 5 | 3715 | 1/1 | 0.99 | 0.15 | - | 54,54,54,54 | 0 |
| 84 | MG | o2 | 203 | 1/1 | 0.87 | 0.27 | - | 51,51,51,51 | 0 |
| 84 | MG | 5 | 4056 | 1/1 | 0.80 | 0.16 | - | 95,95,95,95 | 0 |
| 84 | MG | 5 | 3495 | 1/1 | 0.89 | 0.26 | - | 58,58,58,58 | 0 |
| 84 | MG | 5 | 3705 | 1/1 | 0.93 | 0.32 | - | 81,81,81,81 | 0 |
| 84 | MG | 5 | 3908 | 1/1 | 0.98 | 0.33 | - | 48,48,48,48 | 0 |
| 84 | MG | 5 | 3769 | 1/1 | 0.89 | 0.23 | - | 79,79,79,79 | 0 |
| 84 | MG | 5 | 3528 | 1/1 | 0.86 | 0.89 | - | 56,56,56,56 | 0 |
| 84 | MG | 5 | 4008 | 1/1 | 0.81 | 0.36 | - | 56,56,56,56 | 0 |
| 84 | MG | 1 | 3763 | 1/1 | 0.73 | 0.42 | - | 66,66,66,66 | 0 |
| 84 | MG | 1 | 3577 | 1/1 | 0.78 | 0.23 | - | 81,81,81,81 | 0 |
| 84 | MG | 6 | 2065 | 1/1 | 0.83 | 0.20 | - | 104,104,104,104 | 0 |
| 84 | MG | d3 | 202 | 1/1 | 0.83 | 0.35 | - | 69,69,69,69 | 0 |
| 84 | MG | 5 | 3820 | 1/1 | 0.97 | 0.13 | - | 52,52,52,52 | 0 |
| 84 | MG | 6 | 2090 | 1/1 | 0.50 | 0.40 | - | 91,91,91,91 | 0 |
| 84 | MG | 5 | 3837 | 1/1 | 0.85 | 0.30 | - | 72,72,72,72 | 0 |
| 84 | MG | 1 | 3581 | 1/1 | 0.94 | 0.15 | - | 64,64,64,64 | 0 |
| 84 | MG | 6 | 2132 | 1/1 | 0.91 | 0.13 | - | 83,83,83,83 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 5 | 3637 | 1/1 | 0.95 | 0.30 | - | 48,48,48,48 | 0 |
| 84 | MG | 6 | 1972 | 1/1 | 0.94 | 0.42 | - | 70,70,70,70 | 0 |
| 84 | MG | 5 | 3510 | 1/1 | 0.88 | 0.27 | - | 62,62,62,62 | 0 |
| 84 | MG | 5 | 3782 | 1/1 | 0.96 | 0.16 | - | 67,67,67,67 | 0 |
| 84 | MG | 1 | 3720 | 1/1 | 0.95 | 0.47 | - | 59,59,59,59 | 0 |
| 84 | MG | 1 | 3504 | 1/1 | 0.93 | 0.28 | - | 66,66,66,66 | 0 |
| 84 | MG | 7 | 227 | 1/1 | 0.80 | 0.28 | - | 76,76,76,76 | 0 |
| 84 | MG | 5 | 4094 | 1/1 | 0.94 | 0.14 | - | 63,63,63,63 | 0 |
| 84 | MG | 5 | 3979 | 1/1 | 0.97 | 0.37 | - | 46,46,46,46 | 0 |
| 84 | MG | s4 | 301 | 1/1 | 0.90 | 0.23 | - | 103,103,103,103 | 0 |
| 84 | MG | 5 | 3686 | 1/1 | 0.83 | 0.30 | - | 68,68,68,68 | 0 |
| 84 | MG | 2 | 1960 | 1/1 | 0.83 | 0.20 | - | 94,94,94,94 | 0 |
| 84 | MG | 5 | 4149 | 1/1 | 0.78 | 0.32 | - | 74,74,74,74 | 0 |
| 84 | MG | 1 | 3614 | 1/1 | 0.88 | 0.32 | - | 58,58,58,58 | 0 |
| 84 | MG | 5 | 3490 | 1/1 | 0.95 | 0.24 | - | 58,58,58,58 | 0 |
| 84 | MG | m6 | 201 | 1/1 | 0.89 | 0.25 | - | 52,52,52,52 | 0 |
| 84 | MG | 1 | 3439 | 1/1 | 0.96 | 0.26 | - | 49,49,49,49 | 0 |
| 84 | MG | L2 | 304 | 1/1 | 0.94 | 0.32 | - | 73,73,73,73 | 0 |
| 84 | MG | 6 | 2140 | 1/1 | 0.91 | 0.33 | - | 65,65,65,65 | 0 |
| 84 | MG | 5 | 3900 | 1/1 | 0.99 | 0.41 | - | 51,51,51,51 | 0 |
| 84 | MG | 1 | 3722 | 1/1 | 0.92 | 0.10 | - | 68,68,68,68 | 0 |
| 84 | MG | 6 | 2063 | 1/1 | 0.80 | 0.13 | - | 117,117,117,117 | 0 |
| 84 | MG | 6 | 2131 | 1/1 | 0.87 | 0.16 | - | 89,89,89,89 | 0 |
| 84 | MG | 5 | 3912 | 1/1 | 0.92 | 0.28 | - | 45,45,45,45 | 0 |
| 84 | MG | 1 | 3785 | 1/1 | 0.85 | 0.26 | - | 73,73,73,73 | 0 |
| 84 | MG | 6 | 2054 | 1/1 | 0.96 | 0.14 | - | 76,76,76,76 | 0 |
| 84 | MG | 2 | 1970 | 1/1 | 0.98 | 0.18 | - | 105,105,105,105 | 0 |
| 84 | MG | 5 | 3758 | 1/1 | 0.98 | 0.25 | - | 65,65,65,65 | 0 |
| 84 | MG | 3 | 216 | 1/1 | 0.95 | 0.08 | - | 74,74,74,74 | 0 |
| 84 | MG | 6 | 2137 | 1/1 | 0.94 | 0.29 | - | 76,76,76,76 | 0 |
| 84 | MG | 1 | 3913 | 1/1 | 0.87 | 0.29 | - | 59,59,59,59 | 0 |
| 84 | MG | 8 | 210 | 1/1 | 0.94 | 0.18 | - | 96,96,96,96 | 0 |
| 84 | MG | 1 | 3707 | 1/1 | 0.79 | 0.37 | - | 59,59,59,59 | 0 |
| 84 | MG | 5 | 3861 | 1/1 | 0.83 | 0.34 | - | 63,63,63,63 | 0 |
| 84 | MG | 2 | 1954 | 1/1 | 0.71 | 0.29 | - | 106,106,106,106 | 0 |
| 84 | MG | 1 | 3481 | 1/1 | 0.69 | 0.79 | - | 73,73,73,73 | 0 |
| 84 | MG | 5 | 3935 | 1/1 | 0.85 | 0.28 | - | 52,52,52,52 | 0 |
| 84 | MG | 8 | 216 | 1/1 | 0.75 | 0.68 | - | 67,67,67,67 | 0 |
| 84 | MG | 2 | 1938 | 1/1 | 0.91 | 0.51 | - | 76,76,76,76 | 0 |
| 84 | MG | 6 | 2142 | 1/1 | 0.74 | 0.24 | - | 89,89,89,89 | 0 |
| 84 | MG | 5 | 4018 | 1/1 | 0.81 | 0.51 | - | 66,66,66,66 | 0 |
| 84 | MG | 1 | 3896 | 1/1 | 0.84 | 0.19 | - | 73,73,73,73 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 2 | 2028 | 1/1 | 0.87 | 0.21 | - | 117,117,117,117 | 0 |
| 84 | MG | 2 | 1936 | 1/1 | 0.94 | 0.35 | - | 86,86,86,86 | 0 |
| 84 | MG | 1 | 3717 | 1/1 | 0.99 | 0.64 | - | 56,56,56,56 | 0 |
| 84 | MG | 1 | 3450 | 1/1 | 0.96 | 0.35 | - | 62,62,62,62 | 0 |
| 84 | MG | 1 | 3608 | 1/1 | 0.95 | 0.19 | - | 57,57,57,57 | 0 |
| 84 | MG | 6 | 2150 | 1/1 | 0.83 | 0.21 | - | 81,81,81,81 | 0 |
| 84 | MG | 7 | 205 | 1/1 | 0.88 | 0.38 | - | 55,55,55,55 | 0 |
| 84 | MG | 1 | 3787 | 1/1 | 0.96 | 0.85 | - | 67,67,67,67 | 0 |
| 84 | MG | 5 | 4080 | 1/1 | 0.60 | 0.16 | - | 67,67,67,67 | 0 |
| 84 | MG | 5 | 3732 | 1/1 | 0.85 | 0.31 | - | 70,70,70,70 | 0 |
| 84 | MG | 1 | 3547 | 1/1 | 0.86 | 0.30 | - | 65,65,65,65 | 0 |
| 84 | MG | 1 | 3425 | 1/1 | 0.96 | 0.26 | - | 57,57,57,57 | 0 |
| 84 | MG | 5 | 4095 | 1/1 | 0.98 | 0.12 | - | 68,68,68,68 | 0 |
| 84 | MG | 1 | 3975 | 1/1 | 0.80 | 0.28 | - | 63,63,63,63 | 0 |
| 84 | MG | 8 | 206 | 1/1 | 0.81 | 0.25 | - | 81,81,81,81 | 0 |
| 84 | MG | 1 | 3636 | 1/1 | 0.51 | 0.22 | - | 104,104,104,104 | 0 |
| 84 | MG | 1 | 3956 | 1/1 | 0.91 | 0.25 | - | 71,71,71,71 | 0 |
| 84 | MG | 6 | 2082 | 1/1 | 0.95 | 0.26 | - | 67,67,67,67 | 0 |
| 84 | MG | 5 | 3558 | 1/1 | 0.70 | 0.46 | - | 60,60,60,60 | 0 |
| 84 | MG | 5 | 3834 | 1/1 | 0.89 | 0.32 | - | 60,60,60,60 | 0 |
| 84 | MG | n1 | 202 | 1/1 | 0.90 | 0.26 | - | 61,61,61,61 | 0 |
| 84 | MG | c3 | 204 | 1/1 | 0.64 | 0.14 | - | 107,107,107,107 | 0 |
| 84 | MG | 1 | 3643 | 1/1 | 0.91 | 0.17 | - | 67,67,67,67 | 0 |
| 84 | MG | 5 | 3419 | 1/1 | 0.81 | 0.37 | - | 49,49,49,49 | 0 |
| 84 | MG | N0 | 203 | 1/1 | 0.83 | 0.09 | - | 80,80,80,80 | 0 |
| 84 | MG | 6 | 2025 | 1/1 | 0.91 | 0.17 | - | 81,81,81,81 | 1 |
| 84 | MG | 1 | 3552 | 1/1 | 0.90 | 0.14 | - | 84,84,84,84 | 0 |
| 84 | MG | 1 | 3901 | 1/1 | 0.89 | 0.20 | - | 74,74,74,74 | 0 |
| 84 | MG | 1 | 3854 | 1/1 | 0.72 | 0.31 | - | 60,60,60,60 | 0 |
| 84 | MG | 5 | 3472 | 1/1 | 0.98 | 0.17 | - | 57,57,57,57 | 0 |
| 84 | MG | 1 | 3515 | 1/1 | 0.78 | 1.16 | - | 64,64,64,64 | 0 |
| 84 | MG | 6 | 2076 | 1/1 | 0.97 | 0.21 | - | 64,64,64,64 | 0 |
| 84 | MG | 5 | 3839 | 1/1 | 0.83 | 0.25 | - | 68,68,68,68 | 0 |
| 84 | MG | 5 | 3780 | 1/1 | 0.75 | 0.30 | - | 64,64,64,64 | 0 |
| 84 | MG | 5 | 3512 | 1/1 | 0.84 | 0.36 | - | 56,56,56,56 | 0 |
| 84 | MG | 2 | 1909 | 1/1 | 0.95 | 0.45 | - | 94,94,94,94 | 0 |
| 84 | MG | 1 | 3984 | 1/1 | 0.84 | 0.32 | - | 65,65,65,65 | 0 |
| 84 | MG | 1 | 3829 | 1/1 | 0.79 | 0.53 | - | 71,71,71,71 | 0 |
| 84 | MG | 2 | 1945 | 1/1 | 0.97 | 0.31 | - | 87,87,87,87 | 0 |
| 84 | MG | l3 | 409 | 1/1 | 0.90 | 0.22 | - | 70,70,70,70 | 0 |
| 84 | MG | 6 | 2106 | 1/1 | 0.57 | 0.58 | - | 91,91,91,91 | 0 |
| 84 | MG | 1 | 3648 | 1/1 | 0.92 | 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 | MG | 6 | 1947 | 1/1 | 0.86 | 0.42 | - | 64,64,64,64 | 0 |
| 84 | MG | 5 | 4046 | 1/1 | 0.75 | 0.43 | - | 67,67,67,67 | 0 |
| 84 | MG | 1 | 3702 | 1/1 | 0.90 | 0.63 | - | 64,64,64,64 | 0 |
| 84 | MG | 5 | 3757 | 1/1 | 0.95 | 0.09 | - | 64,64,64,64 | 0 |
| 84 | MG | 5 | 3609 | 1/1 | 0.84 | 0.20 | - | 87,87,87,87 | 0 |
| 84 | MG | 5 | 3522 | 1/1 | 0.98 | 0.22 | - | 42,42,42,42 | 0 |
| 84 | MG | 6 | 1942 | 1/1 | 0.70 | 0.40 | - | 60,60,60,60 | 0 |
| 84 | MG | 1 | 3855 | 1/1 | 0.93 | 0.28 | - | 55,55,55,55 | 1 |
| 84 | MG | 1 | 3751 | 1/1 | 0.91 | 0.80 | - | 72,72,72,72 | 0 |
| 84 | MG | 5 | 3680 | 1/1 | 0.94 | 0.15 | - | 73,73,73,73 | 0 |
| 84 | MG | 5 | 3798 | 1/1 | 0.95 | 0.40 | - | 58,58,58,58 | 0 |
| 84 | MG | 1 | 3641 | 1/1 | 0.86 | 0.29 | - | 104,104,104,104 | 0 |
| 84 | MG | 5 | 4007 | 1/1 | 0.69 | 0.47 | - | 63,63,63,63 | 0 |
| 84 | MG | 2 | 1905 | 1/1 | 0.68 | 0.09 | - | 127,127,127,127 | 0 |
| 84 | MG | 2 | 2039 | 1/1 | 0.97 | 0.20 | - | 95,95,95,95 | 0 |
| 84 | MG | 1 | 3572 | 1/1 | 0.90 | 0.17 | - | 70,70,70,70 | 0 |
| 84 | MG | 5 | 4093 | 1/1 | 0.97 | 0.15 | - | 73,73,73,73 | 0 |
| 84 | MG | 5 | 3414 | 1/1 | 0.84 | 0.51 | - | 54,54,54,54 | 0 |
| 84 | MG | 1 | 3753 | 1/1 | 0.89 | 0.46 | - | 64,64,64,64 | 0 |
| 84 | MG | 6 | 2089 | 1/1 | 0.84 | 0.25 | - | 71,71,71,71 | 0 |
| 84 | MG | 5 | 4023 | 1/1 | 0.84 | 0.17 | - | 58,58,58,58 | 1 |
| 84 | MG | N0 | 202 | 1/1 | 0.98 | 0.12 | - | 49,49,49,49 | 0 |
| 84 | MG | 6 | 2049 | 1/1 | 0.80 | 0.14 | - | 78,78,78,78 | 0 |
| 84 | MG | 5 | 3866 | 1/1 | 0.92 | 0.27 | - | 51,51,51,51 | 1 |
| 84 | MG | 1 | 3939 | 1/1 | 0.90 | 0.30 | - | 61,61,61,61 | 0 |
| 84 | MG | 1 | 3654 | 1/1 | 0.88 | 0.34 | - | 53,53,53,53 | 0 |
| 84 | MG | 1 | 3447 | 1/1 | 0.68 | 0.45 | - | 58,58,58,58 | 0 |
| 84 | MG | 1 | 3592 | 1/1 | 0.86 | 0.35 | - | 62,62,62,62 | 1 |
| 84 | MG | 7 | 228 | 1/1 | 0.87 | 0.27 | - | 73,73,73,73 | 0 |
| 84 | MG | l3 | 404 | 1/1 | 0.99 | 0.27 | - | 42,42,42,42 | 0 |
| 84 | MG | 6 | 2126 | 1/1 | 0.91 | 0.33 | - | 92,92,92,92 | 0 |
| 84 | MG | 6 | 2123 | 1/1 | 0.84 | 0.59 | - | 142,142,142,142 | 0 |
| 84 | MG | 1 | 3483 | 1/1 | 0.56 | 0.59 | - | 68,68,68,68 | 0 |
| 84 | MG | 1 | 3778 | 1/1 | 0.96 | 0.39 | - | 61,61,61,61 | 0 |
| 84 | MG | 5 | 3841 | 1/1 | 0.83 | 0.25 | - | 61,61,61,61 | 0 |
| 84 | MG | 4 | 213 | 1/1 | 0.90 | 0.42 | - | 80,80,80,80 | 0 |
| 84 | MG | 6 | 2060 | 1/1 | 0.93 | 0.13 | - | 86,86,86,86 | 0 |
| 84 | MG | 5 | 3664 | 1/1 | 0.68 | 0.41 | - | 56,56,56,56 | 0 |
| 84 | MG | 1 | 3467 | 1/1 | 0.73 | 0.38 | - | 58,58,58,58 | 0 |
| 84 | MG | 5 | 3860 | 1/1 | 0.92 | 0.18 | - | 56,56,56,56 | 0 |
| 84 | MG | 6 | 1992 | 1/1 | 0.78 | 0.47 | - | 78,78,78,78 | 0 |
| 84 | MG | 5 | 3744 | 1/1 | 0.87 | 0.40 | - | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 1 | 3534 | 1/1 | 0.97 | 0.46 | - | 63,63,63,63 | 0 |
| 84 | MG | 2 | 1924 | 1/1 | 0.88 | 0.24 | - | 90,90,90,90 | 0 |
| 84 | MG | 5 | 3493 | 1/1 | 0.96 | 0.18 | - | 57,57,57,57 | 0 |
| 84 | MG | 5 | 3509 | 1/1 | 0.84 | 0.48 | - | 65,65,65,65 | 0 |
| 84 | MG | 1 | 3727 | 1/1 | 0.87 | 0.48 | - | 55,55,55,55 | 0 |
| 84 | MG | 1 | 3959 | 1/1 | 0.94 | 0.34 | - | 61,61,61,61 | 0 |
| 84 | MG | 1 | 3970 | 1/1 | 0.88 | 0.42 | - | 50,50,50,50 | 0 |
| 84 | MG | 6 | 1926 | 1/1 | 0.95 | 0.24 | - | 75,75,75,75 | 0 |
| 84 | MG | 1 | 3861 | 1/1 | 0.94 | 0.30 | - | 58,58,58,58 | 0 |
| 84 | MG | 5 | 3735 | 1/1 | 0.93 | 0.13 | - | 64,64,64,64 | 0 |
| 84 | MG | 4 | 204 | 1/1 | 0.87 | 0.30 | - | 69,69,69,69 | 0 |
| 84 | MG | n5 | 203 | 1/1 | 0.97 | 0.06 | - | 89,89,89,89 | 0 |
| 84 | MG | 2 | 1992 | 1/1 | 0.78 | 0.14 | - | 98,98,98,98 | 0 |
| 84 | MG | 5 | 3877 | 1/1 | 0.97 | 0.17 | - | 89,89,89,89 | 0 |
| 84 | MG | 5 | 3428 | 1/1 | 0.97 | 0.14 | - | 47,47,47,47 | 0 |
| 84 | MG | 5 | 4109 | 1/1 | 0.99 | 0.23 | - | 42,42,42,42 | 0 |
| 84 | MG | 7 | 202 | 1/1 | 0.97 | 0.23 | - | 52,52,52,52 | 0 |
| 84 | MG | M5 | 302 | 1/1 | 0.84 | 0.32 | - | 58,58,58,58 | 0 |
| 84 | MG | 5 | 3875 | 1/1 | 0.90 | 0.39 | - | 80,80,80,80 | 0 |
| 84 | MG | 1 | 3746 | 1/1 | 0.77 | 0.39 | - | 69,69,69,69 | 0 |
| 84 | MG | 1 | 3718 | 1/1 | 0.84 | 0.26 | - | 60,60,60,60 | 0 |
| 84 | MG | 5 | 3442 | 1/1 | 0.79 | 0.45 | - | 53,53,53,53 | 0 |
| 84 | MG | 1 | 3908 | 1/1 | 0.84 | 0.36 | - | 60,60,60,60 | 0 |
| 84 | MG | 1 | 3733 | 1/1 | 0.91 | 0.61 | - | 80,80,80,80 | 0 |
| 84 | MG | 7 | 218 | 1/1 | 0.94 | 0.09 | - | 68,68,68,68 | 0 |
| 84 | MG | 4 | 206 | 1/1 | 0.60 | 0.53 | - | 60,60,60,60 | 0 |
| 84 | MG | m3 | 204 | 1/1 | 0.89 | 0.35 | - | 59,59,59,59 | 0 |
| 84 | MG | 5 | 3620 | 1/1 | 0.89 | 0.13 | - | 65,65,65,65 | 0 |
| 84 | MG | 7 | 217 | 1/1 | 0.93 | 0.13 | - | 63,63,63,63 | 0 |
| 84 | MG | 5 | 3596 | 1/1 | 0.87 | 0.34 | - | 82,82,82,82 | 0 |
| 84 | MG | 5 | 3660 | 1/1 | 0.84 | 0.17 | - | 96,96,96,96 | 0 |
| 84 | MG | 1 | 3510 | 1/1 | 0.50 | 0.51 | - | 57,57,57,57 | 0 |
| 84 | MG | 5 | 3840 | 1/1 | 0.66 | 0.30 | - | 61,61,61,61 | 0 |
| 84 | MG | 5 | 3739 | 1/1 | 0.95 | 0.33 | - | 52,52,52,52 | 0 |
| 84 | MG | 8 | 218 | 1/1 | 0.90 | 0.32 | - | 84,84,84,84 | 0 |
| 84 | MG | 5 | 4060 | 1/1 | 0.82 | 0.32 | - | 68,68,68,68 | 0 |
| 84 | MG | 5 | 4141 | 1/1 | 0.84 | 0.29 | - | 62,62,62,62 | 0 |
| 84 | MG | 5 | 4067 | 1/1 | 0.86 | 0.24 | - | 76,76,76,76 | 0 |
| 84 | MG | 5 | 3563 | 1/1 | 0.76 | 0.46 | - | 55,55,55,55 | 0 |
| 84 | MG | 5 | 4090 | 1/1 | 0.95 | 0.39 | - | 60,60,60,60 | 0 |
| 84 | MG | 5 | 3821 | 1/1 | 0.89 | 0.26 | - | 53,53,53,53 | 0 |
| 84 | MG | o3 | 202 | 1/1 | 0.92 | 0.22 | - | 70,70,70,70 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 6 | 2006 | 1/1 | 0.92 | 0.39 | - | 63,63,63,63 | 0 |
| 84 | MG | 1 | 3834 | 1/1 | 0.84 | 0.71 | - | 70,70,70,70 | 0 |
| 84 | MG | 1 | 3947 | 1/1 | 0.98 | 0.48 | - | 79,79,79,79 | 0 |
| 84 | MG | 1 | 3716 | 1/1 | 0.99 | 0.32 | - | 66,66,66,66 | 0 |
| 84 | MG | 5 | 3978 | 1/1 | 0.90 | 0.37 | - | 51,51,51,51 | 0 |
| 84 | MG | N1 | 202 | 1/1 | 0.71 | 0.34 | - | 98,98,98,98 | 0 |
| 84 | MG | m6 | 205 | 1/1 | 0.83 | 0.27 | - | 51,51,51,51 | 1 |
| 84 | MG | 3 | 210 | 1/1 | 0.81 | 0.22 | - | 65,65,65,65 | 0 |
| 84 | MG | 5 | 3648 | 1/1 | 0.93 | 0.17 | - | 65,65,65,65 | 0 |
| 84 | MG | 5 | 3525 | 1/1 | 0.90 | 0.17 | - | 51,51,51,51 | 1 |
| 84 | MG | 5 | 3796 | 1/1 | 0.92 | 0.10 | - | 67,67,67,67 | 0 |
| 84 | MG | 5 | 3593 | 1/1 | 0.76 | 0.50 | - | 68,68,68,68 | 0 |
| 84 | MG | 6 | 2115 | 1/1 | 0.82 | 0.12 | - | 93,93,93,93 | 0 |
| 84 | MG | 1 | 3872 | 1/1 | 0.91 | 0.31 | - | 73,73,73,73 | 0 |
| 84 | MG | 1 | 3455 | 1/1 | 0.88 | 0.42 | - | 70,70,70,70 | 0 |
| 84 | MG | 1 | 3935 | 1/1 | 0.83 | 0.27 | - | 68,68,68,68 | 0 |
| 84 | MG | 5 | 3431 | 1/1 | 0.89 | 0.33 | - | 53,53,53,53 | 0 |
| 84 | MG | 1 | 3747 | 1/1 | 0.86 | 0.23 | - | 71,71,71,71 | 0 |
| 84 | MG | 5 | 3771 | 1/1 | 0.96 | 0.14 | - | 77,77,77,77 | 0 |
| 84 | MG | 2 | 1956 | 1/1 | 0.84 | 0.38 | - | 72,72,72,72 | 0 |
| 84 | MG | 1 | 3661 | 1/1 | 0.89 | 0.26 | - | 78,78,78,78 | 0 |
| 84 | MG | l9 | 201 | 1/1 | 0.93 | 0.18 | - | 53,53,53,53 | 0 |
| 84 | MG | 1 | 3475 | 1/1 | 0.98 | 0.30 | - | 60,60,60,60 | 0 |
| 84 | MG | 6 | 2101 | 1/1 | 0.87 | 0.34 | - | 82,82,82,82 | 0 |
| 84 | MG | m6 | 208 | 1/1 | 0.66 | 0.50 | - | 56,56,56,56 | 0 |
| 84 | MG | l5 | 305 | 1/1 | 0.77 | 0.08 | - | 77,77,77,77 | 0 |
| 84 | MG | 8 | 204 | 1/1 | 0.89 | 0.30 | - | 70,70,70,70 | 0 |
| 84 | MG | 5 | 3453 | 1/1 | 0.86 | 0.36 | - | 56,56,56,56 | 0 |
| 84 | MG | 5 | 3985 | 1/1 | 0.94 | 0.25 | - | 56,56,56,56 | 0 |
| 84 | MG | 5 | 3443 | 1/1 | 0.92 | 0.33 | - | 49,49,49,49 | 0 |
| 84 | MG | 5 | 3471 | 1/1 | 0.97 | 0.40 | - | 56,56,56,56 | 0 |
| 84 | MG | 5 | 3459 | 1/1 | 0.97 | 0.14 | - | 52,52,52,52 | 1 |
| 84 | MG | 6 | 2027 | 1/1 | 0.84 | 0.19 | - | 61,61,61,61 | 0 |
| 84 | MG | 5 | 3676 | 1/1 | 0.98 | 0.10 | - | 65,65,65,65 | 0 |
| 84 | MG | O2 | 203 | 1/1 | 0.80 | 0.35 | - | 57,57,57,57 | 0 |
| 84 | MG | 6 | 1944 | 1/1 | 0.53 | 0.86 | - | 71,71,71,71 | 0 |
| 84 | MG | 8 | 219 | 1/1 | 0.79 | 0.38 | - | 90,90,90,90 | 0 |
| 84 | MG | 5 | 3564 | 1/1 | 0.78 | 0.47 | - | 59,59,59,59 | 0 |
| 84 | MG | 1 | 3750 | 1/1 | 0.94 | 0.57 | - | 70,70,70,70 | 0 |
| 84 | MG | 5 | 3851 | 1/1 | 0.98 | 0.20 | - | 54,54,54,54 | 0 |
| 84 | MG | 6 | 2156 | 1/1 | 0.92 | 0.43 | - | 77,77,77,77 | 0 |
| 84 | MG | 6 | 2143 | 1/1 | 0.94 | 0.26 | - | 104,104,104,104 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 1 | 3798 | 1/1 | 0.90 | 0.36 | - | 60,60,60,60 | 0 |
| 84 | MG | 5 | 4037 | 1/1 | 0.92 | 0.17 | - | 77,77,77,77 | 0 |
| 84 | MG | 5 | 4146 | 1/1 | 0.86 | 0.22 | - | 63,63,63,63 | 0 |
| 84 | MG | 1 | 3418 | 1/1 | 0.82 | 0.57 | - | 65,65,65,65 | 0 |
| 84 | MG | 5 | 4019 | 1/1 | 0.81 | 0.63 | - | 66,66,66,66 | 0 |
| 84 | MG | 1 | 3800 | 1/1 | 0.81 | 0.52 | - | 67,67,67,67 | 0 |
| 84 | MG | 1 | 3813 | 1/1 | 0.86 | 0.29 | - | 80,80,80,80 | 0 |
| 84 | MG | 5 | 3948 | 1/1 | 0.71 | 0.65 | - | 58,58,58,58 | 0 |
| 84 | MG | 6 | 2064 | 1/1 | 0.76 | 0.15 | - | 126,126,126,126 | 0 |
| 84 | MG | 1 | 3863 | 1/1 | 0.85 | 0.29 | - | 74,74,74,74 | 0 |
| 84 | MG | 3 | 204 | 1/1 | 0.94 | 0.15 | - | 85,85,85,85 | 0 |
| 84 | MG | 6 | 1903 | 1/1 | 0.68 | 0.77 | - | 67,67,67,67 | 0 |
| 84 | MG | 8 | 201 | 1/1 | 0.75 | 0.42 | - | 81,81,81,81 | 0 |
| 84 | MG | 1 | 3934 | 1/1 | 0.70 | 0.48 | - | 65,65,65,65 | 0 |
| 84 | MG | 5 | 3717 | 1/1 | 0.97 | 0.32 | - | 52,52,52,52 | 0 |
| 84 | MG | o3 | 201 | 1/1 | 0.87 | 0.23 | - | 56,56,56,56 | 0 |
| 84 | MG | 2 | 2009 | 1/1 | 0.85 | 0.19 | - | 117,117,117,117 | 0 |
| 84 | MG | D3 | 201 | 1/1 | 0.79 | 0.32 | - | 72,72,72,72 | 0 |
| 84 | MG | 5 | 3814 | 1/1 | 0.95 | 0.13 | - | 48,48,48,48 | 0 |
| 84 | MG | 1 | 3932 | 1/1 | 0.79 | 0.69 | - | 71,71,71,71 | 0 |
| 84 | MG | 2 | 2015 | 1/1 | 0.64 | 0.59 | - | 84,84,84,84 | 0 |
| 84 | MG | 5 | 3760 | 1/1 | 0.92 | 0.29 | - | 59,59,59,59 | 0 |
| 84 | MG | 1 | 3538 | 1/1 | 0.90 | 0.35 | - | 64,64,64,64 | 0 |
| 84 | MG | 5 | 4025 | 1/1 | 0.93 | 0.18 | - | 55,55,55,55 | 0 |
| 84 | MG | 5 | 3552 | 1/1 | 0.81 | 0.52 | - | 68,68,68,68 | 0 |
| 84 | MG | 6 | 2104 | 1/1 | 0.96 | 0.11 | - | 89,89,89,89 | 0 |
| 84 | MG | 5 | 4087 | 1/1 | 0.92 | 0.28 | - | 52,52,52,52 | 0 |
| 84 | MG | 5 | 3650 | 1/1 | 0.85 | 0.51 | - | 80,80,80,80 | 0 |
| 84 | MG | 5 | 3736 | 1/1 | 0.89 | 0.43 | - | 59,59,59,59 | 0 |
| 84 | MG | 1 | 3857 | 1/1 | 0.97 | 0.44 | - | 47,47,47,47 | 0 |
| 84 | MG | m7 | 206 | 1/1 | 0.94 | 0.36 | - | 55,55,55,55 | 0 |
| 84 | MG | 1 | 3890 | 1/1 | 0.92 | 0.39 | - | 50,50,50,50 | 0 |
| 84 | MG | 2 | 1917 | 1/1 | 0.87 | 0.22 | - | 88,88,88,88 | 0 |
| 84 | MG | 1 | 3410 | 1/1 | 0.94 | 0.55 | - | 56,56,56,56 | 0 |
| 84 | MG | n0 | 206 | 1/1 | 0.85 | 0.44 | - | 48,48,48,48 | 0 |
| 84 | MG | 1 | 3681 | 1/1 | 0.75 | 0.36 | - | 62,62,62,62 | 0 |
| 84 | MG | 5 | 3779 | 1/1 | 0.90 | 0.38 | - | 67,67,67,67 | 0 |
| 84 | MG | 6 | 2102 | 1/1 | 0.89 | 0.29 | - | 80,80,80,80 | 0 |
| 84 | MG | 5 | 4014 | 1/1 | 0.88 | 0.32 | - | 62,62,62,62 | 0 |
| 84 | MG | 5 | 3809 | 1/1 | 0.87 | 0.20 | - | 60,60,60,60 | 0 |
| 84 | MG | 1 | 3847 | 1/1 | 0.79 | 0.51 | - | 53,53,53,53 | 0 |
| 84 | MG | 6 | 2161 | 1/1 | 0.73 | 0.27 | - | 75,75,75,75 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 5 | 3716 | 1/1 | 0.95 | 0.57 | - | 62,62,62,62 | 0 |
| 84 | MG | 5 | 3523 | 1/1 | 0.87 | 0.34 | - | 55,55,55,55 | 0 |
| 84 | MG | 6 | 2145 | 1/1 | 0.85 | 0.20 | - | 77,77,77,77 | 0 |
| 84 | MG | 5 | 3549 | 1/1 | 0.92 | 0.41 | - | 63,63,63,63 | 0 |
| 84 | MG | 6 | 2111 | 1/1 | 0.80 | 0.19 | - | 113,113,113,113 | 0 |
| 84 | MG | 1 | 3462 | 1/1 | 0.89 | 0.21 | - | 54,54,54,54 | 1 |
| 84 | MG | 6 | 1983 | 1/1 | 0.70 | 0.18 | - | 100,100,100,100 | 0 |
| 84 | MG | 1 | 3719 | 1/1 | 0.95 | 0.25 | - | 55,55,55,55 | 0 |
| 84 | MG | 5 | 3786 | 1/1 | 0.82 | 0.38 | - | 43,43,43,43 | 0 |
| 84 | MG | 5 | 3422 | 1/1 | 0.98 | 0.27 | - | 49,49,49,49 | 0 |
| 84 | MG | 5 | 3636 | 1/1 | 0.94 | 0.41 | - | 53,53,53,53 | 0 |
| 84 | MG | 6 | 2148 | 1/1 | 0.69 | 0.26 | - | 78,78,78,78 | 0 |
| 84 | MG | 1 | 3881 | 1/1 | 0.80 | 0.18 | - | 78,78,78,78 | 0 |
| 84 | MG | N0 | 201 | 1/1 | 0.69 | 0.35 | - | 67,67,67,67 | 0 |
| 84 | MG | 7 | 230 | 1/1 | 0.82 | 0.45 | - | 75,75,75,75 | 0 |
| 84 | MG | 6 | 1968 | 1/1 | 0.66 | 0.54 | - | 65,65,65,65 | 0 |
| 84 | MG | 6 | 1920 | 1/1 | 0.75 | 0.23 | - | 81,81,81,81 | 0 |
| 84 | MG | 5 | 3674 | 1/1 | 0.86 | 0.45 | - | 65,65,65,65 | 0 |
| 84 | MG | S3 | 301 | 1/1 | 0.97 | 0.14 | - | 100,100,100,100 | 0 |
| 84 | MG | 1 | 3816 | 1/1 | 0.63 | 0.46 | - | 78,78,78,78 | 0 |
| 84 | MG | 5 | 3627 | 1/1 | 0.86 | 0.32 | - | 53,53,53,53 | 1 |
| 84 | MG | 5 | 4116 | 1/1 | 0.85 | 0.13 | - | 82,82,82,82 | 0 |
| 84 | MG | S4 | 301 | 1/1 | 0.66 | 0.20 | - | 120,120,120,120 | 0 |
| 84 | MG | 1 | 3519 | 1/1 | 0.95 | 0.35 | - | 70,70,70,70 | 0 |
| 84 | MG | 4 | 221 | 1/1 | 0.52 | 0.45 | - | 75,75,75,75 | 0 |
| 84 | MG | 1 | 3911 | 1/1 | 0.90 | 0.41 | - | 56,56,56,56 | 0 |
| 84 | MG | 1 | 3880 | 1/1 | 0.79 | 0.45 | - | 73,73,73,73 | 0 |
| 84 | MG | 5 | 3972 | 1/1 | 0.86 | 0.45 | - | 60,60,60,60 | 0 |
| 84 | MG | 5 | 4072 | 1/1 | 0.83 | 0.09 | - | 109,109,109,109 | 0 |
| 84 | MG | 5 | 3432 | 1/1 | 0.95 | 0.19 | - | 54,54,54,54 | 0 |
| 84 | MG | 5 | 3723 | 1/1 | 0.88 | 0.25 | - | 74,74,74,74 | 0 |
| 84 | MG | 5 | 4061 | 1/1 | 0.96 | 0.38 | - | 68,68,68,68 | 0 |
| 84 | MG | L4 | 403 | 1/1 | 0.92 | 0.22 | - | 55,55,55,55 | 0 |
| 84 | MG | 5 | 3755 | 1/1 | 0.76 | 0.44 | - | 59,59,59,59 | 0 |
| 84 | MG | 1 | 3426 | 1/1 | 0.75 | 0.32 | - | 45,45,45,45 | 0 |
| 84 | MG | L4 | 404 | 1/1 | 0.90 | 0.59 | - | 59,59,59,59 | 0 |
| 84 | MG | 1 | 3693 | 1/1 | 0.94 | 0.27 | - | 64,64,64,64 | 0 |
| 84 | MG | 1 | 3973 | 1/1 | 0.88 | 0.35 | - | 64,64,64,64 | 0 |
| 84 | MG | 1 | 3877 | 1/1 | 0.89 | 0.31 | - | 68,68,68,68 | 0 |
| 84 | MG | M8 | 201 | 1/1 | 0.72 | 0.23 | - | 67,67,67,67 | 0 |
| 84 | MG | 5 | 3651 | 1/1 | 0.75 | 0.38 | - | 77,77,77,77 | 0 |
| 84 | MG | l8 | 301 | 1/1 | 0.66 | 0.45 | - | 99,99,99,99 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 6 | 2122 | 1/1 | 0.98 | 0.30 | - | 96,96,96,96 | 0 |
| 84 | MG | 2 | 1966 | 1/1 | 0.64 | 0.28 | - | 106,106,106,106 | 0 |
| 84 | MG | 5 | 3936 | 1/1 | 0.71 | 0.45 | - | 55,55,55,55 | 0 |
| 84 | MG | 5 | 4114 | 1/1 | 0.80 | 0.20 | - | 83,83,83,83 | 0 |
| 84 | MG | Q2 | 504 | 1/1 | 0.75 | 0.37 | - | 59,59,59,59 | 0 |
| 84 | MG | 1 | 3765 | 1/1 | 0.96 | 0.29 | - | 61,61,61,61 | 0 |
| 84 | MG | 5 | 3665 | 1/1 | 0.94 | 0.54 | - | 56,56,56,56 | 0 |
| 84 | MG | 5 | 3925 | 1/1 | 0.87 | 0.31 | - | 53,53,53,53 | 0 |
| 84 | MG | 1 | 3494 | 1/1 | 0.82 | 0.40 | - | 81,81,81,81 | 0 |
| 84 | MG | 6 | 1918 | 1/1 | 0.68 | 0.22 | - | 84,84,84,84 | 0 |
| 84 | MG | 1 | 3810 | 1/1 | 0.81 | 0.27 | - | 70,70,70,70 | 0 |
| 84 | MG | 5 | 3652 | 1/1 | 0.95 | 0.19 | - | 76,76,76,76 | 0 |
| 84 | MG | 6 | 2094 | 1/1 | 0.84 | 0.30 | - | 69,69,69,69 | 0 |
| 84 | MG | 5 | 4027 | 1/1 | 0.83 | 0.54 | - | 50,50,50,50 | 0 |
| 84 | MG | 2 | 1933 | 1/1 | 0.94 | 0.16 | - | 88,88,88,88 | 0 |
| 84 | MG | 3 | 201 | 1/1 | 0.98 | 0.13 | - | 81,81,81,81 | 0 |
| 84 | MG | 5 | 3898 | 1/1 | 0.98 | 0.20 | - | 56,56,56,56 | 0 |
| 84 | MG | 1 | 3568 | 1/1 | 0.92 | 0.14 | - | 83,83,83,83 | 0 |
| 84 | MG | 5 | 3672 | 1/1 | 0.93 | 0.46 | - | 67,67,67,67 | 0 |
| 84 | MG | 1 | 3404 | 1/1 | 0.97 | 0.34 | - | 53,53,53,53 | 0 |
| 84 | MG | 5 | 3983 | 1/1 | 0.93 | 0.21 | - | 50,50,50,50 | 0 |
| 84 | MG | 5 | 3481 | 1/1 | 0.98 | 0.32 | - | 49,49,49,49 | 0 |
| 84 | MG | 5 | 3595 | 1/1 | 0.93 | 0.17 | - | 74,74,74,74 | 0 |
| 84 | MG | 6 | 2041 | 1/1 | 0.91 | 0.16 | - | 73,73,73,73 | 0 |
| 84 | MG | 2 | 1978 | 1/1 | 0.77 | 0.50 | - | 64,64,64,64 | 0 |
| 84 | MG | N8 | 203 | 1/1 | 0.81 | 0.44 | - | 63,63,63,63 | 0 |
| 84 | MG | S1 | 301 | 1/1 | 0.87 | 0.27 | - | 94,94,94,94 | 0 |
| 84 | MG | 1 | 3625 | 1/1 | 0.87 | 0.17 | - | 71,71,71,71 | 0 |
| 84 | MG | 1 | 3805 | 1/1 | 0.78 | 0.32 | - | 74,74,74,74 | 0 |
| 84 | MG | c8 | 202 | 1/1 | 0.90 | 0.19 | - | 75,75,75,75 | 0 |
| 84 | MG | 1 | 3639 | 1/1 | 0.64 | 0.30 | - | 96,96,96,96 | 0 |
| 84 | MG | 7 | 206 | 1/1 | 0.97 | 0.12 | - | 62,62,62,62 | 0 |
| 84 | MG | 1 | 3546 | 1/1 | 0.88 | 0.27 | - | 63,63,63,63 | 0 |
| 84 | MG | 1 | 3726 | 1/1 | 0.61 | 0.47 | - | 69,69,69,69 | 0 |
| 84 | MG | 5 | 3734 | 1/1 | 0.92 | 0.17 | - | 67,67,67,67 | 0 |
| 84 | MG | 1 | 3775 | 1/1 | 0.87 | 0.36 | - | 62,62,62,62 | 0 |
| 84 | MG | 1 | 3700 | 1/1 | 0.85 | 0.91 | - | 52,52,52,52 | 0 |
| 84 | MG | 5 | 4041 | 1/1 | 0.77 | 0.30 | - | 79,79,79,79 | 0 |
| 84 | MG | 5 | 3489 | 1/1 | 0.98 | 0.16 | - | 55,55,55,55 | 0 |
| 84 | MG | n9 | 101 | 1/1 | 0.84 | 0.44 | - | 49,49,49,49 | 0 |
| 84 | MG | 6 | 2036 | 1/1 | 0.93 | 0.09 | - | 83,83,83,83 | 0 |
| 84 | MG | 5 | 4091 | 1/1 | 0.96 | 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 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 1 | 3582 | 1/1 | 0.87 | 0.28 | - | 65,65,65,65 | 0 |
| 84 | MG | 2 | 1973 | 1/1 | 0.95 | 0.20 | - | 96,96,96,96 | 0 |
| 84 | MG | 1 | 3492 | 1/1 | 0.83 | 0.38 | - | 80,80,80,80 | 0 |
| 84 | MG | 5 | 3654 | 1/1 | 0.50 | 0.39 | - | 79,79,79,79 | 0 |
| 84 | MG | 6 | 2068 | 1/1 | 0.88 | 0.14 | - | 83,83,83,83 | 0 |
| 84 | MG | 5 | 3924 | 1/1 | 0.85 | 0.30 | - | 56,56,56,56 | 0 |
| 84 | MG | 5 | 3484 | 1/1 | 0.87 | 0.47 | - | 74,74,74,74 | 0 |
| 84 | MG | 5 | 3640 | 1/1 | 0.97 | 0.42 | - | 41,41,41,41 | 0 |
| 84 | MG | N4 | 201 | 1/1 | 0.78 | 0.40 | - | 70,70,70,70 | 0 |
| 84 | MG | 1 | 3618 | 1/1 | 0.90 | 0.61 | - | 58,58,58,58 | 1 |
| 84 | MG | 1 | 3623 | 1/1 | 0.84 | 0.35 | - | 68,68,68,68 | 0 |
| 84 | MG | 5 | 3747 | 1/1 | 0.90 | 0.24 | - | 46,46,46,46 | 0 |
| 84 | MG | 5 | 3704 | 1/1 | 0.70 | 0.38 | - | 77,77,77,77 | 0 |
| 84 | MG | 6 | 1970 | 1/1 | 0.93 | 0.35 | - | 63,63,63,63 | 0 |
| 84 | MG | 1 | 3413 | 1/1 | 0.85 | 0.21 | - | 55,55,55,55 | 1 |
| 84 | MG | 6 | 1982 | 1/1 | 0.92 | 0.21 | - | 104,104,104,104 | 0 |
| 84 | MG | l5 | 306 | 1/1 | 0.87 | 0.13 | - | 70,70,70,70 | 0 |
| 84 | MG | 5 | 4049 | 1/1 | 0.64 | 0.20 | - | 79,79,79,79 | 0 |
| 84 | MG | 6 | 1931 | 1/1 | 0.98 | 0.31 | - | 67,67,67,67 | 0 |
| 84 | MG | q3 | 502 | 1/1 | 0.92 | 0.39 | - | 68,68,68,68 | 0 |
| 84 | MG | 1 | 3635 | 1/1 | 0.94 | 0.09 | - | 117,117,117,117 | 0 |
| 84 | MG | 4 | 207 | 1/1 | 0.96 | 0.24 | - | 59,59,59,59 | 0 |
| 84 | MG | 5 | 3629 | 1/1 | 0.88 | 0.33 | - | 60,60,60,60 | 0 |
| 84 | MG | 1 | 3807 | 1/1 | 0.83 | 0.46 | - | 77,77,77,77 | 0 |
| 84 | MG | 5 | 3984 | 1/1 | 0.63 | 0.49 | - | 62,62,62,62 | 0 |
| 84 | MG | 2 | 2018 | 1/1 | 0.83 | 0.10 | - | 135,135,135,135 | 0 |
| 84 | MG | 1 | 3658 | 1/1 | 0.66 | 0.37 | - | 70,70,70,70 | 0 |
| 84 | MG | 8 | 209 | 1/1 | 0.68 | 0.23 | - | 80,80,80,80 | 0 |
| 84 | MG | 2 | 1999 | 1/1 | 0.92 | 0.63 | - | 73,73,73,73 | 0 |
| 84 | MG | 5 | 3588 | 1/1 | 0.79 | 0.94 | - | 62,62,62,62 | 0 |
| 84 | MG | 1 | 3569 | 1/1 | 0.86 | 0.16 | - | 75,75,75,75 | 0 |
| 84 | MG | 5 | 3433 | 1/1 | 0.90 | 0.38 | - | 48,48,48,48 | 0 |
| 84 | MG | 6 | 2112 | 1/1 | 0.91 | 0.26 | - | 81,81,81,81 | 0 |
| 84 | MG | 5 | 3721 | 1/1 | 0.94 | 0.21 | - | 65,65,65,65 | 0 |
| 84 | MG | 6 | 1985 | 1/1 | 0.93 | 0.14 | - | 92,92,92,92 | 0 |
| 84 | MG | 5 | 3539 | 1/1 | 0.94 | 0.49 | - | 54,54,54,54 | 0 |
| 84 | MG | 1 | 3729 | 1/1 | 0.97 | 0.21 | - | 72,72,72,72 | 0 |
| 84 | MG | 6 | 2154 | 1/1 | 0.84 | 0.15 | - | 78,78,78,78 | 0 |
| 84 | MG | 1 | 3870 | 1/1 | 0.97 | 0.21 | - | 58,58,58,58 | 0 |
| 84 | MG | 2 | 1962 | 1/1 | 0.90 | 0.19 | - | 100,100,100,100 | 0 |
| 84 | MG | 5 | 4033 | 1/1 | 0.76 | 0.13 | - | 74,74,74,74 | 0 |
| 84 | MG | 5 | 3687 | 1/1 | 0.93 | 0.40 | - | 69,69,69,69 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | L2 | 302 | 1/1 | 0.93 | 0.46 | - | 43,43,43,43 | 0 |
| 84 | MG | 5 | 3475 | 1/1 | 0.95 | 0.17 | - | 64,64,64,64 | 0 |
| 84 | MG | 7 | 204 | 1/1 | 0.97 | 0.28 | - | 54,54,54,54 | 0 |
| 84 | MG | 5 | 3867 | 1/1 | 0.72 | 0.39 | - | 55,55,55,55 | 0 |
| 84 | MG | 5 | 4085 | 1/1 | 0.81 | 0.16 | - | 79,79,79,79 | 0 |
| 84 | MG | 5 | 3583 | 1/1 | 0.80 | 0.59 | - | 59,59,59,59 | 0 |
| 84 | MG | 5 | 3789 | 1/1 | 0.96 | 0.35 | - | 48,48,48,48 | 0 |
| 84 | MG | 2 | 1965 | 1/1 | 0.62 | 0.32 | - | 91,91,91,91 | 0 |
| 84 | MG | 5 | 3829 | 1/1 | 0.89 | 0.20 | - | 57,57,57,57 | 0 |
| 84 | MG | 5 | 3477 | 1/1 | 0.85 | 0.42 | - | 60,60,60,60 | 0 |
| 84 | MG | 5 | 3989 | 1/1 | 0.97 | 0.28 | - | 47,47,47,47 | 0 |
| 84 | MG | 6 | 1907 | 1/1 | 0.94 | 0.21 | - | 69,69,69,69 | 0 |
| 84 | MG | 1 | 3791 | 1/1 | 0.86 | 0.18 | - | 83,83,83,83 | 0 |
| 84 | MG | l9 | 206 | 1/1 | 0.81 | 0.32 | - | 68,68,68,68 | 0 |
| 84 | MG | Q1 | 101 | 1/1 | 0.97 | 0.25 | - | 83,83,83,83 | 0 |
| 84 | MG | O7 | 102 | 1/1 | 0.76 | 0.39 | - | 61,61,61,61 | 0 |
| 84 | MG | 1 | 3628 | 1/1 | 0.42 | 0.69 | - | 80,80,80,80 | 0 |
| 84 | MG | 1 | 3497 | 1/1 | 0.94 | 0.22 | - | 73,73,73,73 | 0 |
| 84 | MG | 6 | 1978 | 1/1 | 0.91 | 0.13 | - | 93,93,93,93 | 0 |
| 84 | MG | 3 | 209 | 1/1 | 0.86 | 0.18 | - | 70,70,70,70 | 0 |
| 84 | MG | 2 | 2005 | 1/1 | 0.87 | 0.16 | - | 83,83,83,83 | 0 |
| 84 | MG | 1 | 3490 | 1/1 | 0.60 | 0.16 | - | 80,80,80,80 | 0 |
| 84 | MG | 6 | 1912 | 1/1 | 0.84 | 0.13 | - | 95,95,95,95 | 0 |
| 84 | MG | 5 | 3976 | 1/1 | 0.92 | 0.20 | - | 68,68,68,68 | 0 |
| 84 | MG | 6 | 1995 | 1/1 | 0.92 | 0.11 | - | 117,117,117,117 | 0 |
| 84 | MG | 1 | 3910 | 1/1 | 0.88 | 0.64 | - | 56,56,56,56 | 0 |
| 84 | MG | 2 | 1944 | 1/1 | 0.91 | 0.72 | - | 87,87,87,87 | 0 |
| 84 | MG | 1 | 3988 | 1/1 | 0.89 | 0.23 | - | 53,53,53,53 | 0 |
| 84 | MG | 5 | 4111 | 1/1 | 0.91 | 0.43 | - | 46,46,46,46 | 0 |
| 84 | MG | 1 | 3953 | 1/1 | 0.79 | 0.30 | - | 72,72,72,72 | 0 |
| 84 | MG | 1 | 3703 | 1/1 | 0.86 | 0.47 | - | 65,65,65,65 | 0 |
| 84 | MG | 5 | 3873 | 1/1 | 0.88 | 0.27 | - | 71,71,71,71 | 0 |
| 84 | MG | 1 | 3781 | 1/1 | 0.91 | 0.33 | - | 69,69,69,69 | 1 |
| 84 | MG | 5 | 4002 | 1/1 | 0.87 | 0.22 | - | 64,64,64,64 | 0 |
| 84 | MG | 6 | 2125 | 1/1 | 0.84 | 0.23 | - | 71,71,71,71 | 0 |
| 84 | MG | 4 | 210 | 1/1 | 0.75 | 0.15 | - | 90,90,90,90 | 0 |
| 84 | MG | m4 | 201 | 1/1 | 0.69 | 0.21 | - | 69,69,69,69 | 1 |
| 84 | MG | q2 | 502 | 1/1 | 0.76 | 0.27 | - | 63,63,63,63 | 0 |
| 84 | MG | 7 | 225 | 1/1 | 0.78 | 0.20 | - | 71,71,71,71 | 0 |
| 84 | MG | 5 | 4020 | 1/1 | 0.85 | 0.34 | - | 72,72,72,72 | 0 |
| 84 | MG | 1 | 3782 | 1/1 | 0.73 | 0.74 | - | 69,69,69,69 | 0 |
| 84 | MG | 1 | 3706 | 1/1 | 0.93 | 0.26 | - | 51,51,51,51 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 2 | 1951 | 1/1 | 0.87 | 0.70 | - | 95,95,95,95 | 0 |
| 84 | MG | 5 | 3554 | 1/1 | 0.90 | 0.22 | - | 60,60,60,60 | 0 |
| 84 | MG | 5 | 3975 | 1/1 | 0.65 | 0.57 | - | 71,71,71,71 | 0 |
| 84 | MG | 5 | 4124 | 1/1 | 0.99 | 0.22 | - | 50,50,50,50 | 0 |
| 84 | MG | s0 | 301 | 1/1 | 0.83 | 0.16 | - | 103,103,103,103 | 0 |
| 84 | MG | 1 | 3554 | 1/1 | 0.84 | 0.21 | - | 67,67,67,67 | 0 |
| 84 | MG | 1 | 3892 | 1/1 | 0.95 | 0.23 | - | 64,64,64,64 | 0 |
| 84 | MG | 1 | 3543 | 1/1 | 0.84 | 0.64 | - | 51,51,51,51 | 0 |
| 84 | MG | 5 | 3421 | 1/1 | 0.93 | 0.20 | - | 51,51,51,51 | 0 |
| 84 | MG | 5 | 4030 | 1/1 | 0.60 | 0.50 | - | 99,99,99,99 | 0 |
| 84 | MG | 2 | 2026 | 1/1 | 0.79 | 0.22 | - | 126,126,126,126 | 0 |
| 84 | MG | 1 | 3679 | 1/1 | 0.98 | 0.18 | - | 68,68,68,68 | 0 |
| 84 | MG | 5 | 3931 | 1/1 | 0.94 | 0.51 | - | 44,44,44,44 | 0 |
| 84 | MG | 5 | 3804 | 1/1 | 0.90 | 0.06 | - | 73,73,73,73 | 1 |
| 84 | MG | 1 | 3884 | 1/1 | 0.84 | 0.22 | - | 80,80,80,80 | 0 |
| 84 | MG | 7 | 229 | 1/1 | 0.85 | 0.27 | - | 72,72,72,72 | 0 |
| 84 | MG | 1 | 3578 | 1/1 | 0.76 | 0.21 | - | 78,78,78,78 | 0 |
| 84 | MG | 6 | 2100 | 1/1 | 0.72 | 0.28 | - | 84,84,84,84 | 0 |
| 84 | MG | 5 | 3642 | 1/1 | 0.90 | 0.47 | - | 52,52,52,52 | 0 |
| 84 | MG | 5 | 3946 | 1/1 | 0.81 | 0.69 | - | 64,64,64,64 | 0 |
| 84 | MG | 5 | 3586 | 1/1 | 0.92 | 0.42 | - | 55,55,55,55 | 0 |
| 84 | MG | 2 | 2029 | 1/1 | 0.87 | 0.18 | - | 110,110,110,110 | 0 |
| 84 | MG | 5 | 3514 | 1/1 | 0.95 | 0.26 | - | 65,65,65,65 | 0 |
| 84 | MG | 6 | 1977 | 1/1 | 0.74 | 0.27 | - | 103,103,103,103 | 0 |
| 84 | MG | d1 | 101 | 1/1 | 0.66 | 0.40 | - | 93,93,93,93 | 0 |
| 84 | MG | 5 | 4078 | 1/1 | 0.81 | 0.25 | - | 67,67,67,67 | 0 |
| 84 | MG | 2 | 1953 | 1/1 | 0.75 | 0.33 | - | 96,96,96,96 | 0 |
| 84 | MG | 1 | 3468 | 1/1 | 0.86 | 0.45 | - | 61,61,61,61 | 0 |
| 84 | MG | 1 | 3725 | 1/1 | 0.98 | 0.26 | - | 62,62,62,62 | 0 |
| 84 | MG | 3 | 212 | 1/1 | 0.83 | 0.33 | - | 64,64,64,64 | 0 |
| 84 | MG | 1 | 3757 | 1/1 | 0.90 | 0.56 | - | 62,62,62,62 | 0 |
| 84 | MG | 2 | 2042 | 1/1 | 0.84 | 0.17 | - | 101,101,101,101 | 0 |
| 84 | MG | 2 | 1946 | 1/1 | 0.88 | 0.56 | - | 80,80,80,80 | 0 |
| 84 | MG | 5 | 3878 | 1/1 | 0.79 | 0.47 | - | 79,79,79,79 | 0 |
| 84 | MG | N1 | 201 | 1/1 | 0.82 | 0.29 | - | 68,68,68,68 | 0 |
| 84 | MG | M3 | 201 | 1/1 | 0.95 | 0.16 | - | 65,65,65,65 | 0 |
| 84 | MG | 1 | 3477 | 1/1 | 0.82 | 0.38 | - | 51,51,51,51 | 0 |
| 84 | MG | 1 | 3541 | 1/1 | 0.79 | 0.32 | - | 58,58,58,58 | 0 |
| 84 | MG | 5 | 4107 | 1/1 | 0.91 | 0.27 | - | 59,59,59,59 | 0 |
| 84 | MG | 1 | 3741 | 1/1 | 0.77 | 0.34 | - | 80,80,80,80 | 0 |
| 84 | MG | 1 | 3777 | 1/1 | 0.93 | 0.61 | - | 62,62,62,62 | 0 |
| 84 | MG | 5 | 3542 | 1/1 | 0.78 | 0.42 | - | 54,54,54,54 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 5 | 4125 | 1/1 | 0.85 | 0.44 | - | 55,55,55,55 | 0 |
| 84 | MG | 1 | 3903 | 1/1 | 0.86 | 0.23 | - | 80,80,80,80 | 0 |
| 84 | MG | 5 | 3644 | 1/1 | 0.92 | 0.26 | - | 64,64,64,64 | 0 |
| 84 | MG | 5 | 3754 | 1/1 | 0.83 | 0.46 | - | 69,69,69,69 | 0 |
| 84 | MG | 6 | 2157 | 1/1 | 0.92 | 0.24 | - | 63,63,63,63 | 0 |
| 84 | MG | 1 | 3705 | 1/1 | 0.92 | 0.25 | - | 59,59,59,59 | 0 |
| 84 | MG | 6 | 2093 | 1/1 | 0.88 | 0.26 | - | 75,75,75,75 | 0 |
| 84 | MG | 6 | 1969 | 1/1 | 0.94 | 0.15 | - | 69,69,69,69 | 1 |
| 84 | MG | 5 | 3598 | 1/1 | 0.84 | 0.56 | - | 84,84,84,84 | 0 |
| 84 | MG | 5 | 3538 | 1/1 | 0.95 | 0.27 | - | 52,52,52,52 | 0 |
| 84 | MG | 5 | 3436 | 1/1 | 0.94 | 0.22 | - | 66,66,66,66 | 0 |
| 84 | MG | q2 | 505 | 1/1 | 0.92 | 0.26 | - | 63,63,63,63 | 0 |
| 84 | MG | n0 | 204 | 1/1 | 0.69 | 0.28 | - | 57,57,57,57 | 0 |
| 84 | MG | 1 | 3640 | 1/1 | 0.94 | 0.19 | - | 100,100,100,100 | 0 |
| 84 | MG | 1 | 3563 | 1/1 | 0.90 | 0.14 | - | 76,76,76,76 | 0 |
| 84 | MG | 1 | 3665 | 1/1 | 0.78 | 0.22 | - | 67,67,67,67 | 0 |
| 84 | MG | 5 | 3670 | 1/1 | 0.98 | 0.30 | - | 63,63,63,63 | 0 |
| 84 | MG | 5 | 3741 | 1/1 | 0.87 | 0.45 | - | 58,58,58,58 | 0 |
| 84 | MG | 2 | 2037 | 1/1 | 0.74 | 0.35 | - | 99,99,99,99 | 0 |
| 84 | MG | 5 | 4081 | 1/1 | 0.93 | 0.08 | - | 79,79,79,79 | 0 |
| 84 | MG | 5 | 3649 | 1/1 | 0.86 | 0.14 | - | 63,63,63,63 | 1 |
| 84 | MG | 6 | 1902 | 1/1 | 0.90 | 0.34 | - | 51,51,51,51 | 0 |
| 84 | MG | 1 | 3788 | 1/1 | 0.68 | 0.19 | - | 76,76,76,76 | 1 |
| 84 | MG | 5 | 3853 | 1/1 | 0.95 | 0.15 | - | 58,58,58,58 | 0 |
| 84 | MG | n3 | 202 | 1/1 | 0.95 | 0.51 | - | 62,62,62,62 | 1 |
| 84 | MG | 5 | 3494 | 1/1 | 0.86 | 0.23 | - | 59,59,59,59 | 0 |
| 84 | MG | 6 | 1910 | 1/1 | 0.92 | 0.29 | - | 60,60,60,60 | 0 |
| 84 | MG | 5 | 3548 | 1/1 | 0.98 | 0.33 | - | 60,60,60,60 | 0 |
| 84 | MG | 5 | 3991 | 1/1 | 0.91 | 0.59 | - | 57,57,57,57 | 0 |
| 84 | MG | 1 | 3936 | 1/1 | 0.82 | 0.38 | - | 67,67,67,67 | 0 |
| 84 | MG | 1 | 3808 | 1/1 | 0.89 | 0.24 | - | 71,71,71,71 | 0 |
| 84 | MG | 6 | 2016 | 1/1 | 0.91 | 0.17 | - | 79,79,79,79 | 0 |
| 84 | MG | 5 | 3749 | 1/1 | 0.87 | 0.39 | - | 77,77,77,77 | 0 |
| 84 | MG | 1 | 3818 | 1/1 | 0.65 | 0.54 | - | 88,88,88,88 | 0 |
| 84 | MG | 5 | 3824 | 1/1 | 0.97 | 0.15 | - | 58,58,58,58 | 0 |
| 84 | MG | m7 | 203 | 1/1 | 0.86 | 0.38 | - | 63,63,63,63 | 0 |
| 84 | MG | 7 | 220 | 1/1 | 0.93 | 0.21 | - | 66,66,66,66 | 0 |
| 84 | MG | 5 | 3961 | 1/1 | 0.91 | 0.33 | - | 53,53,53,53 | 0 |
| 84 | MG | 5 | 3616 | 1/1 | 0.83 | 0.17 | - | 82,82,82,82 | 0 |
| 84 | MG | 1 | 3830 | 1/1 | 0.93 | 0.51 | - | 72,72,72,72 | 0 |
| 84 | MG | 6 | 2007 | 1/1 | 0.93 | 0.35 | - | 61,61,61,61 | 0 |
| 84 | MG | L8 | 301 | 1/1 | 0.82 | 0.18 | - | 103,103,103,103 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 6 | 2075 | 1/1 | 0.91 | 0.28 | - | 61,61,61,61 | 0 |
| 84 | MG | 1 | 3796 | 1/1 | 0.97 | 0.18 | - | 60,60,60,60 | 0 |
| 84 | MG | 1 | 3759 | 1/1 | 0.43 | 0.82 | - | 73,73,73,73 | 0 |
| 84 | MG | 7 | 226 | 1/1 | 0.90 | 0.14 | - | 72,72,72,72 | 0 |
| 84 | MG | 1 | 3711 | 1/1 | 0.78 | 0.19 | - | 84,84,84,84 | 0 |
| 84 | MG | 1 | 3893 | 1/1 | 0.75 | 0.30 | - | 57,57,57,57 | 0 |
| 84 | MG | 1 | 3511 | 1/1 | 0.98 | 0.40 | - | 59,59,59,59 | 0 |
| 84 | MG | 5 | 4039 | 1/1 | 0.92 | 0.22 | - | 77,77,77,77 | 0 |
| 84 | MG | 5 | 3844 | 1/1 | 0.90 | 0.28 | - | 52,52,52,52 | 0 |
| 84 | MG | 6 | 2052 | 1/1 | 0.95 | 0.11 | - | 73,73,73,73 | 0 |
| 84 | MG | 5 | 3728 | 1/1 | 0.82 | 0.21 | - | 51,51,51,51 | 0 |
| 84 | MG | 6 | 1967 | 1/1 | 0.57 | 0.85 | - | 74,74,74,74 | 0 |
| 84 | MG | 2 | 1934 | 1/1 | 0.94 | 0.29 | - | 87,87,87,87 | 0 |
| 84 | MG | 12 | 303 | 1/1 | 0.76 | 0.36 | - | 72,72,72,72 | 0 |
| 84 | MG | 6 | 2147 | 1/1 | 0.88 | 0.18 | - | 78,78,78,78 | 0 |
| 84 | MG | 2 | 1906 | 1/1 | 0.67 | 0.40 | - | 86,86,86,86 | 0 |
| 84 | MG | c3 | 202 | 1/1 | 0.86 | 0.29 | - | 87,87,87,87 | 0 |
| 84 | MG | 2 | 1941 | 1/1 | 0.87 | 0.37 | - | 60,60,60,60 | 0 |
| 84 | MG | 5 | 3527 | 1/1 | 0.90 | 0.59 | - | 53,53,53,53 | 0 |
| 84 | MG | 2 | 2021 | 1/1 | 0.96 | 0.40 | - | 90,90,90,90 | 0 |
| 84 | MG | 5 | 3529 | 1/1 | 0.91 | 0.35 | - | 47,47,47,47 | 0 |
| 84 | MG | 1 | 3683 | 1/1 | 0.88 | 0.29 | - | 64,64,64,64 | 0 |
| 84 | MG | 5 | 4000 | 1/1 | 0.95 | 0.27 | - | 45,45,45,45 | 0 |
| 84 | MG | 2 | 2020 | 1/1 | 0.84 | 0.21 | - | 111,111,111,111 | 0 |
| 84 | MG | 8 | 202 | 1/1 | 0.74 | 0.19 | - | 90,90,90,90 | 0 |
| 84 | MG | c3 | 205 | 1/1 | 0.89 | 0.28 | - | 84,84,84,84 | 0 |
| 84 | MG | 5 | 3967 | 1/1 | 0.80 | 0.62 | - | 71,71,71,71 | 0 |
| 84 | MG | 1 | 3463 | 1/1 | 0.93 | 0.28 | - | 52,52,52,52 | 0 |
| 84 | MG | 3 | 217 | 1/1 | 0.88 | 0.13 | - | 100,100,100,100 | 0 |
| 84 | MG | 5 | 4122 | 1/1 | 0.95 | 0.17 | - | 89,89,89,89 | 0 |
| 84 | MG | 6 | 2001 | 1/1 | 0.92 | 0.36 | - | 79,79,79,79 | 0 |
| 84 | MG | 5 | 3614 | 1/1 | 0.91 | 0.21 | - | 81,81,81,81 | 0 |
| 84 | MG | 1 | 3822 | 1/1 | 0.84 | 0.30 | - | 86,86,86,86 | 0 |
| 84 | MG | 1 | 3646 | 1/1 | 0.99 | 0.22 | - | 52,52,52,52 | 0 |
| 84 | MG | 5 | 3997 | 1/1 | 0.96 | 0.16 | - | 50,50,50,50 | 0 |
| 84 | MG | 6 | 1971 | 1/1 | 0.84 | 0.36 | - | 73,73,73,73 | 0 |
| 84 | MG | 1 | 3591 | 1/1 | 0.98 | 0.41 | - | 46,46,46,46 | 0 |
| 84 | MG | 6 | 1956 | 1/1 | 0.96 | 0.33 | - | 69,69,69,69 | 0 |
| 84 | MG | 1 | 3948 | 1/1 | 0.75 | 0.51 | - | 82,82,82,82 | 0 |
| 84 | MG | 5 | 3581 | 1/1 | 0.87 | 0.44 | - | 53,53,53,53 | 0 |
| 84 | MG | 5 | 4010 | 1/1 | 0.91 | 0.33 | - | 53,53,53,53 | 0 |
| 84 | MG | 5 | 4071 | 1/1 | 0.68 | 0.13 | - | 103,103,103,103 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 5 | 4118 | 1/1 | 0.84 | 0.17 | - | 87,87,87,87 | 0 |
| 84 | MG | 1 | 3453 | 1/1 | 0.96 | 0.09 | - | 70,70,70,70 | 0 |
| 84 | MG | M3 | 204 | 1/1 | 0.84 | 0.29 | - | 69,69,69,69 | 0 |
| 84 | MG | 6 | 2092 | 1/1 | 0.91 | 0.21 | - | 66,66,66,66 | 0 |
| 84 | MG | m8 | 201 | 1/1 | 0.85 | 0.28 | - | 55,55,55,55 | 0 |
| 84 | MG | 6 | 2011 | 1/1 | 0.91 | 0.29 | - | 68,68,68,68 | 0 |
| 84 | MG | 1 | 3979 | 1/1 | 0.86 | 0.19 | - | 69,69,69,69 | 0 |
| 84 | MG | l3 | 406 | 1/1 | 0.79 | 0.44 | - | 63,63,63,63 | 0 |
| 84 | MG | 6 | 1932 | 1/1 | 0.97 | 0.34 | - | 62,62,62,62 | 0 |
| 84 | MG | 5 | 3870 | 1/1 | 0.92 | 0.37 | - | 54,54,54,54 | 0 |
| 84 | MG | 5 | 3883 | 1/1 | 0.93 | 0.23 | - | 67,67,67,67 | 0 |
| 84 | MG | 5 | 4140 | 1/1 | 0.85 | 0.34 | - | 57,57,57,57 | 0 |
| 84 | MG | 7 | 213 | 1/1 | 0.94 | 0.17 | - | 71,71,71,71 | 0 |
| 84 | MG | 5 | 3669 | 1/1 | 0.98 | 0.23 | - | 63,63,63,63 | 0 |
| 84 | MG | 2 | 1904 | 1/1 | 0.91 | 0.27 | - | 91,91,91,91 | 0 |
| 84 | MG | 5 | 3761 | 1/1 | 0.98 | 0.34 | - | 69,69,69,69 | 0 |
| 84 | MG | 5 | 3626 | 1/1 | 0.97 | 0.28 | - | 52,52,52,52 | 0 |
| 84 | MG | 6 | 2107 | 1/1 | 0.62 | 0.46 | - | 90,90,90,90 | 0 |
| 84 | MG | S2 | 301 | 1/1 | 0.44 | 0.55 | - | 107,107,107,107 | 0 |
| 84 | MG | 5 | 3504 | 1/1 | 0.92 | 0.18 | - | 54,54,54,54 | 0 |
| 84 | MG | 5 | 3894 | 1/1 | 0.86 | 0.51 | - | 72,72,72,72 | 0 |
| 84 | MG | 5 | 3684 | 1/1 | 0.94 | 0.12 | - | 79,79,79,79 | 0 |
| 84 | MG | 5 | 3823 | 1/1 | 0.84 | 0.20 | - | 57,57,57,57 | 1 |
| 84 | MG | 5 | 3556 | 1/1 | 0.95 | 0.49 | - | 57,57,57,57 | 0 |
| 84 | MG | 1 | 3431 | 1/1 | 0.86 | 0.35 | - | 56,56,56,56 | 0 |
| 84 | MG | 5 | 4074 | 1/1 | 0.83 | 0.08 | - | 105,105,105,105 | 0 |
| 84 | MG | 5 | 3805 | 1/1 | 0.78 | 0.15 | - | 75,75,75,75 | 0 |
| 84 | MG | 2 | 2035 | 1/1 | 0.82 | 0.27 | - | 101,101,101,101 | 0 |
| 84 | MG | 5 | 3846 | 1/1 | 0.89 | 0.21 | - | 55,55,55,55 | 0 |
| 84 | MG | 6 | 2088 | 1/1 | 0.93 | 0.38 | - | 83,83,83,83 | 0 |
| 84 | MG | 5 | 3553 | 1/1 | 0.91 | 0.39 | - | 59,59,59,59 | 0 |
| 84 | MG | 1 | 3550 | 1/1 | 0.90 | 0.24 | - | 69,69,69,69 | 0 |
| 84 | MG | 1 | 3972 | 1/1 | 0.83 | 0.20 | - | 65,65,65,65 | 0 |
| 84 | MG | 5 | 3785 | 1/1 | 0.91 | 0.38 | - | 51,51,51,51 | 0 |
| 84 | MG | 1 | 3642 | 1/1 | 0.90 | 0.25 | - | 71,71,71,71 | 0 |
| 84 | MG | 1 | 3797 | 1/1 | 0.95 | 0.54 | - | 56,56,56,56 | 0 |
| 84 | MG | 2 | 1929 | 1/1 | 0.59 | 0.60 | - | 88,88,88,88 | 0 |
| 84 | MG | 5 | 3519 | 1/1 | 0.93 | 0.33 | - | 42,42,42,42 | 0 |
| 84 | MG | 5 | 3791 | 1/1 | 0.93 | 0.33 | - | 54,54,54,54 | 0 |
| 84 | MG | 1 | 3976 | 1/1 | 0.82 | 0.23 | - | 71,71,71,71 | 0 |
| 84 | MG | 7 | 212 | 1/1 | 0.89 | 0.26 | - | 65,65,65,65 | 0 |
| 84 | MG | 5 | 4103 | 1/1 | 0.93 | 0.20 | - | 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 | MG | 5 | 3499 | 1/1 | 0.99 | 0.15 | - | 53,53,53,53 | 0 |
| 84 | MG | 1 | 3627 | 1/1 | 0.70 | 0.44 | - | 81,81,81,81 | 0 |
| 84 | MG | 5 | 3675 | 1/1 | 0.76 | 0.25 | - | 67,67,67,67 | 0 |
| 84 | MG | s6 | 301 | 1/1 | 0.82 | 0.28 | - | 78,78,78,78 | 0 |
| 84 | MG | 5 | 3772 | 1/1 | 0.81 | 0.32 | - | 128,128,128,128 | 0 |
| 84 | MG | 5 | 3885 | 1/1 | 0.98 | 0.20 | - | 65,65,65,65 | 0 |
| 84 | MG | 5 | 3990 | 1/1 | 0.89 | 0.34 | - | 47,47,47,47 | 0 |
| 84 | MG | 5 | 3775 | 1/1 | 0.76 | 0.45 | - | 120,120,120,120 | 0 |
| 84 | MG | 1 | 3895 | 1/1 | 0.97 | 0.18 | - | 66,66,66,66 | 0 |
| 84 | MG | 7 | 221 | 1/1 | 0.93 | 0.09 | - | 75,75,75,75 | 0 |
| 84 | MG | 1 | 3971 | 1/1 | 0.93 | 0.40 | - | 56,56,56,56 | 0 |
| 84 | MG | 5 | 3847 | 1/1 | 0.97 | 0.31 | - | 45,45,45,45 | 0 |
| 84 | MG | 1 | 3871 | 1/1 | 0.94 | 0.14 | - | 73,73,73,73 | 0 |
| 84 | MG | 7 | 208 | 1/1 | 0.95 | 0.11 | - | 65,65,65,65 | 0 |
| 84 | MG | 5 | 3892 | 1/1 | 0.91 | 0.80 | - | 68,68,68,68 | 0 |
| 84 | MG | 5 | 3458 | 1/1 | 0.80 | 0.29 | - | 57,57,57,57 | 0 |
| 84 | MG | n8 | 203 | 1/1 | 0.90 | 0.20 | - | 70,70,70,70 | 0 |
| 84 | MG | 6 | 1974 | 1/1 | 0.75 | 0.17 | - | 90,90,90,90 | 0 |
| 84 | MG | 1 | 3589 | 1/1 | 0.96 | 0.09 | - | 55,55,55,55 | 0 |
| 84 | MG | 5 | 4005 | 1/1 | 0.97 | 0.21 | - | 58,58,58,58 | 0 |
| 84 | MG | l2 | 304 | 1/1 | 0.72 | 0.39 | - | 76,76,76,76 | 0 |
| 84 | MG | 5 | 3838 | 1/1 | 0.78 | 0.31 | - | 57,57,57,57 | 0 |
| 84 | MG | n0 | 201 | 1/1 | 0.87 | 0.16 | - | 68,68,68,68 | 0 |
| 84 | MG | 2 | 1914 | 1/1 | 0.84 | 0.51 | - | 83,83,83,83 | 0 |
| 84 | MG | 6 | 1946 | 1/1 | 0.91 | 0.14 | - | 70,70,70,70 | 0 |
| 84 | MG | 6 | 1913 | 1/1 | 0.79 | 0.15 | - | 107,107,107,107 | 0 |
| 84 | MG | 5 | 3612 | 1/1 | 0.94 | 0.20 | - | 80,80,80,80 | 0 |
| 84 | MG | 5 | 3600 | 1/1 | 0.93 | 0.21 | - | 92,92,92,92 | 0 |
| 84 | MG | 5 | 4077 | 1/1 | 0.84 | 0.26 | - | 70,70,70,70 | 0 |
| 84 | MG | 2 | 1967 | 1/1 | 0.82 | 0.35 | - | 90,90,90,90 | 0 |
| 84 | MG | 5 | 3971 | 1/1 | 0.89 | 0.84 | - | 72,72,72,72 | 0 |
| 84 | MG | 1 | 3570 | 1/1 | 0.88 | 0.34 | - | 71,71,71,71 | 0 |
| 84 | MG | 2 | 2038 | 1/1 | 0.86 | 0.12 | - | 117,117,117,117 | 0 |
| 84 | MG | L2 | 303 | 1/1 | 0.68 | 0.27 | - | 88,88,88,88 | 0 |
| 84 | MG | d7 | 102 | 1/1 | 0.64 | 0.40 | - | 78,78,78,78 | 0 |
| 84 | MG | 5 | 3933 | 1/1 | 0.90 | 0.34 | - | 55,55,55,55 | 0 |
| 84 | MG | 2 | 1991 | 1/1 | 0.83 | 0.15 | - | 103,103,103,103 | 0 |
| 84 | MG | 5 | 3713 | 1/1 | 0.96 | 0.21 | - | 78,78,78,78 | 0 |
| 84 | MG | 5 | 3671 | 1/1 | 0.95 | 0.37 | - | 63,63,63,63 | 0 |
| 84 | MG | 2 | 2017 | 1/1 | 0.71 | 0.57 | - | 86,86,86,86 | 0 |
| 84 | MG | 5 | 4137 | 1/1 | 0.91 | 0.31 | - | 58,58,58,58 | 0 |
| 84 | MG | 6 | 2083 | 1/1 | 0.85 | 0.29 | - | 78,78,78,78 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 5 | 3801 | 1/1 | 0.90 | 0.17 | - | 61,61,61,61 | 0 |
| 84 | MG | 6 | 1996 | 1/1 | 0.76 | 0.32 | - | 74,74,74,74 | 0 |
| 84 | MG | 5 | 3469 | 1/1 | 0.76 | 0.46 | - | 54,54,54,54 | 0 |
| 84 | MG | 2 | 1959 | 1/1 | 0.97 | 0.15 | - | 110,110,110,110 | 0 |
| 84 | MG | 1 | 3906 | 1/1 | 0.91 | 0.19 | - | 67,67,67,67 | 0 |
| 84 | MG | 1 | 3574 | 1/1 | 0.95 | 0.12 | - | 67,67,67,67 | 0 |
| 84 | MG | 6 | 2008 | 1/1 | 0.90 | 0.25 | - | 67,67,67,67 | 0 |
| 84 | MG | m6 | 203 | 1/1 | 0.78 | 0.34 | - | 55,55,55,55 | 0 |
| 84 | MG | 3 | 214 | 1/1 | 0.94 | 0.07 | - | 86,86,86,86 | 0 |
| 84 | MG | 1 | 3657 | 1/1 | 0.93 | 0.26 | - | 50,50,50,50 | 0 |
| 84 | MG | 2 | 1957 | 1/1 | 0.95 | 0.13 | - | 95,95,95,95 | 0 |
| 84 | MG | 1 | 3866 | 1/1 | 0.97 | 0.28 | - | 55,55,55,55 | 0 |
| 84 | MG | 1 | 3602 | 1/1 | 0.94 | 0.43 | - | 49,49,49,49 | 0 |
| 84 | MG | 5 | 3496 | 1/1 | 0.89 | 0.24 | - | 56,56,56,56 | 0 |
| 84 | MG | 1 | 3745 | 1/1 | 0.97 | 0.11 | - | 73,73,73,73 | 0 |
| 84 | MG | 5 | 3973 | 1/1 | 0.94 | 0.33 | - | 69,69,69,69 | 0 |
| 84 | MG | 5 | 3617 | 1/1 | 0.76 | 0.29 | - | 75,75,75,75 | 0 |
| 84 | MG | 1 | 3507 | 1/1 | 0.98 | 0.35 | - | 60,60,60,60 | 0 |
| 84 | MG | 5 | 3696 | 1/1 | 0.81 | 0.39 | - | 94,94,94,94 | 0 |
| 84 | MG | 1 | 3883 | 1/1 | 0.94 | 0.11 | - | 75,75,75,75 | 0 |
| 84 | MG | 1 | 3456 | 1/1 | 0.73 | 0.36 | - | 67,67,67,67 | 0 |
| 84 | MG | 5 | 3455 | 1/1 | 0.88 | 0.34 | - | 55,55,55,55 | 0 |
| 84 | MG | 5 | 3902 | 1/1 | 0.99 | 0.42 | - | 55,55,55,55 | 0 |
| 84 | MG | 1 | 3573 | 1/1 | 0.86 | 0.13 | - | 65,65,65,65 | 0 |
| 84 | MG | 5 | 4086 | 1/1 | 0.70 | 0.17 | - | 96,96,96,96 | 0 |
| 84 | MG | 5 | 3657 | 1/1 | 0.89 | 0.27 | - | 73,73,73,73 | 0 |
| 84 | MG | 5 | 4031 | 1/1 | 0.56 | 0.37 | - | 65,65,65,65 | 0 |
| 84 | MG | 5 | 4034 | 1/1 | 0.86 | 0.24 | - | 68,68,68,68 | 0 |
| 84 | MG | 1 | 3945 | 1/1 | 0.92 | 0.28 | - | 54,54,54,54 | 0 |
| 84 | MG | o4 | 503 | 1/1 | 0.93 | 0.11 | - | 94,94,94,94 | 0 |
| 84 | MG | 2 | 1974 | 1/1 | 0.93 | 0.27 | - | 96,96,96,96 | 0 |
| 84 | MG | 1 | 3952 | 1/1 | 0.64 | 1.00 | - | 88,88,88,88 | 0 |
| 84 | MG | m8 | 204 | 1/1 | 0.96 | 0.49 | - | 63,63,63,63 | 0 |
| 84 | MG | 5 | 3628 | 1/1 | 0.89 | 0.40 | - | 60,60,60,60 | 0 |
| 84 | MG | 7 | 223 | 1/1 | 0.73 | 0.23 | - | 75,75,75,75 | 0 |
| 84 | MG | 5 | 3729 | 1/1 | 0.89 | 0.36 | - | 57,57,57,57 | 0 |
| 84 | MG | 6 | 1961 | 1/1 | 0.88 | 0.29 | - | 75,75,75,75 | 0 |
| 84 | MG | 5 | 3865 | 1/1 | 0.93 | 0.37 | - | 56,56,56,56 | 0 |
| 84 | MG | 5 | 3426 | 1/1 | 0.99 | 0.21 | - | 48,48,48,48 | 0 |
| 84 | MG | 1 | 3576 | 1/1 | 0.84 | 0.26 | - | 72,72,72,72 | 0 |
| 84 | MG | 5 | 3632 | 1/1 | 0.88 | 0.38 | - | 49,49,49,49 | 0 |
| 84 | MG | 3 | 207 | 1/1 | 0.87 | 0.21 | - | 58,58,58,58 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 5 | 3792 | 1/1 | 0.81 | 0.26 | - | 63,63,63,63 | 1 |
| 84 | MG | 6 | 2116 | 1/1 | 0.94 | 0.24 | - | 71,71,71,71 | 0 |
| 84 | MG | 5 | 3903 | 1/1 | 0.96 | 1.06 | - | 61,61,61,61 | 0 |
| 84 | MG | 5 | 3718 | 1/1 | 0.88 | 0.34 | - | 68,68,68,68 | 0 |
| 84 | MG | 5 | 3969 | 1/1 | 0.85 | 0.49 | - | 70,70,70,70 | 0 |
| 84 | MG | 1 | 3794 | 1/1 | 0.85 | 0.32 | - | 68,68,68,68 | 0 |
| 84 | MG | O2 | 202 | 1/1 | 0.88 | 0.32 | - | 55,55,55,55 | 0 |
| 84 | MG | 3 | 202 | 1/1 | 0.54 | 0.24 | - | 89,89,89,89 | 0 |
| 84 | MG | 1 | 3704 | 1/1 | 0.79 | 0.32 | - | 55,55,55,55 | 0 |
| 84 | MG | 1 | 3598 | 1/1 | 0.95 | 0.42 | - | 52,52,52,52 | 0 |
| 84 | MG | 5 | 3447 | 1/1 | 0.99 | 0.34 | - | 49,49,49,49 | 0 |
| 84 | MG | C1 | 201 | 1/1 | 0.75 | 0.20 | - | 103,103,103,103 | 0 |
| 84 | MG | 2 | 1968 | 1/1 | 0.87 | 0.29 | - | 95,95,95,95 | 0 |
| 84 | MG | 5 | 3653 | 1/1 | 0.85 | 0.26 | - | 76,76,76,76 | 0 |
| 84 | MG | 1 | 3500 | 1/1 | 0.90 | 0.51 | - | 68,68,68,68 | 0 |
| 84 | MG | 5 | 4096 | 1/1 | 0.93 | 0.34 | - | 54,54,54,54 | 0 |
| 84 | MG | 1 | 3804 | 1/1 | 0.69 | 0.57 | - | 91,91,91,91 | 0 |
| 84 | MG | 5 | 3915 | 1/1 | 0.78 | 0.49 | - | 78,78,78,78 | 0 |
| 84 | MG | 5 | 4127 | 1/1 | 0.96 | 0.22 | - | 62,62,62,62 | 0 |
| 84 | MG | 5 | 4022 | 1/1 | 0.94 | 0.28 | - | 50,50,50,50 | 0 |
| 84 | MG | 5 | 3794 | 1/1 | 0.67 | 0.23 | - | 61,61,61,61 | 0 |
| 84 | MG | 5 | 3953 | 1/1 | 0.82 | 0.60 | - | 62,62,62,62 | 0 |
| 84 | MG | 1 | 3429 | 1/1 | 0.97 | 0.34 | - | 50,50,50,50 | 0 |
| 84 | MG | 5 | 3907 | 1/1 | 0.87 | 0.33 | - | 41,41,41,41 | 0 |
| 84 | MG | s2 | 302 | 1/1 | 0.55 | 0.34 | - | 81,81,81,81 | 0 |
| 84 | MG | 6 | 1966 | 1/1 | 0.88 | 0.18 | - | 73,73,73,73 | 0 |
| 84 | MG | 1 | 3771 | 1/1 | 0.97 | 0.23 | - | 59,59,59,59 | 0 |
| 84 | MG | 5 | 4145 | 1/1 | 0.94 | 0.13 | - | 54,54,54,54 | 0 |
| 84 | MG | 5 | 3591 | 1/1 | 0.64 | 0.55 | - | 61,61,61,61 | 0 |
| 84 | MG | 1 | 3513 | 1/1 | 0.98 | 0.34 | - | 55,55,55,55 | 0 |
| 84 | MG | 6 | 1930 | 1/1 | 0.98 | 0.22 | - | 70,70,70,70 | 0 |
| 84 | MG | 1 | 3922 | 1/1 | 0.83 | 0.25 | - | 61,61,61,61 | 0 |
| 84 | MG | 5 | 3540 | 1/1 | 0.94 | 0.31 | - | 49,49,49,49 | 0 |
| 84 | MG | 2 | 1949 | 1/1 | 0.89 | 0.32 | - | 102,102,102,102 | 0 |
| 84 | MG | 4 | 202 | 1/1 | 0.65 | 0.31 | - | 59,59,59,59 | 0 |
| 84 | MG | 5 | 3923 | 1/1 | 0.85 | 0.90 | - | 67,67,67,67 | 0 |
| 84 | MG | 7 | 215 | 1/1 | 0.94 | 0.28 | - | 63,63,63,63 | 0 |
| 84 | MG | 5 | 3615 | 1/1 | 0.93 | 0.21 | - | 89,89,89,89 | 0 |
| 84 | MG | 1 | 3421 | 1/1 | 0.95 | 0.25 | - | 50,50,50,50 | 0 |
| 84 | MG | 1 | 3585 | 1/1 | 0.92 | 0.29 | - | 52,52,52,52 | 0 |
| 84 | MG | 5 | 3836 | 1/1 | 0.64 | 0.29 | - | 79,79,79,79 | 0 |
| 84 | MG | 5 | 3750 | 1/1 | 0.96 | 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 | MG | 5 | 3807 | 1/1 | 0.94 | 0.27 | - | 71,71,71,71 | 0 |
| 84 | MG | O7 | 103 | 1/1 | 0.92 | 0.18 | - | 59,59,59,59 | 0 |
| 84 | MG | 1 | 3607 | 1/1 | 0.93 | 0.59 | - | 58,58,58,58 | 0 |
| 84 | MG | 5 | 4105 | 1/1 | 0.97 | 0.32 | - | 56,56,56,56 | 0 |
| 84 | MG | 2 | 1922 | 1/1 | 0.95 | 0.28 | - | 84,84,84,84 | 0 |
| 84 | MG | 5 | 3974 | 1/1 | 0.73 | 0.43 | - | 67,67,67,67 | 0 |
| 84 | MG | 5 | 3688 | 1/1 | 0.84 | 0.39 | - | 73,73,73,73 | 0 |
| 84 | MG | 1 | 3621 | 1/1 | 0.93 | 0.47 | - | 68,68,68,68 | 0 |
| 84 | MG | 6 | 2053 | 1/1 | 0.89 | 0.16 | - | 74,74,74,74 | 0 |
| 84 | MG | 5 | 3691 | 1/1 | 0.83 | 0.43 | - | 74,74,74,74 | 0 |
| 84 | MG | 5 | 3858 | 1/1 | 0.83 | 0.31 | - | 55,55,55,55 | 0 |
| 84 | MG | 5 | 4076 | 1/1 | 0.92 | 0.29 | - | 77,77,77,77 | 0 |
| 84 | MG | 1 | 3879 | 1/1 | 0.76 | 0.69 | - | 63,63,63,63 | 0 |
| 84 | MG | 1 | 3819 | 1/1 | 0.87 | 0.30 | - | 80,80,80,80 | 0 |
| 84 | MG | l3 | 403 | 1/1 | 0.86 | 0.45 | - | 43,43,43,43 | 0 |
| 84 | MG | 1 | 3960 | 1/1 | 0.74 | 0.20 | - | 79,79,79,79 | 0 |
| 84 | MG | 6 | 1940 | 1/1 | 0.77 | 0.81 | - | 69,69,69,69 | 0 |
| 84 | MG | 6 | 2000 | 1/1 | 0.94 | 0.17 | - | 84,84,84,84 | 0 |
| 84 | MG | 6 | 2120 | 1/1 | 0.53 | 0.14 | - | 110,110,110,110 | 0 |
| 84 | MG | 1 | 3954 | 1/1 | 0.95 | 0.14 | - | 71,71,71,71 | 0 |
| 84 | MG | n0 | 205 | 1/1 | 0.92 | 0.16 | - | 47,47,47,47 | 0 |
| 84 | MG | 6 | 1980 | 1/1 | 0.82 | 0.24 | - | 108,108,108,108 | 0 |
| 84 | MG | 5 | 3537 | 1/1 | 0.98 | 0.49 | - | 48,48,48,48 | 0 |
| 84 | MG | c8 | 201 | 1/1 | 0.94 | 0.18 | - | 75,75,75,75 | 0 |
| 84 | MG | 5 | 3911 | 1/1 | 0.93 | 0.32 | - | 43,43,43,43 | 0 |
| 84 | MG | 5 | 3773 | 1/1 | 0.91 | 0.10 | - | 139,139,139,139 | 0 |
| 84 | MG | 5 | 3434 | 1/1 | 0.80 | 0.27 | - | 60,60,60,60 | 0 |
| 84 | MG | 5 | 3662 | 1/1 | 0.98 | 0.22 | - | 50,50,50,50 | 0 |
| 84 | MG | 6 | 2162 | 1/1 | 0.22 | 0.21 | - | 96,96,96,96 | 0 |
| 84 | MG | 5 | 3783 | 1/1 | 0.96 | 0.31 | - | 41,41,41,41 | 0 |
| 84 | MG | 1 | 3514 | 1/1 | 0.76 | 0.61 | - | 63,63,63,63 | 0 |
| 84 | MG | L3 | 402 | 1/1 | 0.85 | 0.58 | - | 60,60,60,60 | 0 |
| 84 | MG | 1 | 3951 | 1/1 | 0.95 | 0.06 | - | 82,82,82,82 | 0 |
| 84 | MG | q3 | 503 | 1/1 | 0.75 | 0.26 | - | 79,79,79,79 | 0 |
| 84 | MG | 5 | 3695 | 1/1 | 0.49 | 0.35 | - | 93,93,93,93 | 0 |
| 84 | MG | 2 | 1903 | 1/1 | 0.97 | 0.33 | - | 90,90,90,90 | 0 |
| 84 | MG | 1 | 3466 | 1/1 | 0.86 | 0.44 | - | 54,54,54,54 | 0 |
| 84 | MG | 5 | 3714 | 1/1 | 0.90 | 0.23 | - | 71,71,71,71 | 0 |
| 84 | MG | 2 | 2012 | 1/1 | 0.91 | 0.11 | - | 127,127,127,127 | 0 |
| 84 | MG | l4 | 1102 | 1/1 | 0.90 | 0.27 | - | 57,57,57,57 | 0 |
| 84 | MG | c3 | 201 | 1/1 | 0.77 | 0.61 | - | 89,89,89,89 | 0 |
| 84 | MG | 5 | 3699 | 1/1 | 0.89 | 0.31 | - | 63,63,63,63 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 5 | 3541 | 1/1 | 0.93 | 0.32 | - | 52,52,52,52 | 0 |
| 84 | MG | 2 | 1948 | 1/1 | 0.92 | 0.47 | - | 82,82,82,82 | 0 |
| 84 | MG | 5 | 3706 | 1/1 | 0.78 | 0.62 | - | 71,71,71,71 | 0 |
| 84 | MG | 6 | 2015 | 1/1 | 0.93 | 0.37 | - | 68,68,68,68 | 0 |
| 84 | MG | 5 | 4075 | 1/1 | 0.95 | 0.12 | - | 97,97,97,97 | 0 |
| 84 | MG | 5 | 3927 | 1/1 | 0.82 | 0.40 | - | 55,55,55,55 | 1 |
| 84 | MG | 1 | 3505 | 1/1 | 0.82 | 0.37 | - | 67,67,67,67 | 0 |
| 84 | MG | 5 | 3980 | 1/1 | 0.83 | 0.39 | - | 52,52,52,52 | 0 |
| 84 | MG | 1 | 3721 | 1/1 | 0.96 | 0.26 | - | 59,59,59,59 | 0 |
| 84 | MG | 15 | 302 | 1/1 | 0.74 | 0.14 | - | 78,78,78,78 | 0 |
| 84 | MG | 1 | 3443 | 1/1 | 0.89 | 0.26 | - | 58,58,58,58 | 0 |
| 84 | MG | 1 | 3983 | 1/1 | 0.92 | 0.20 | - | 61,61,61,61 | 0 |
| 84 | MG | 1 | 3584 | 1/1 | 0.75 | 0.36 | - | 76,76,76,76 | 0 |
| 84 | MG | 5 | 3884 | 1/1 | 0.95 | 0.09 | - | 69,69,69,69 | 0 |
| 84 | MG | 5 | 3778 | 1/1 | 0.92 | 0.24 | - | 92,92,92,92 | 0 |
| 84 | MG | 5 | 3917 | 1/1 | 0.91 | 0.31 | - | 62,62,62,62 | 0 |
| 84 | MG | 5 | 3909 | 1/1 | 0.89 | 0.27 | - | 48,48,48,48 | 1 |
| 84 | MG | 5 | 3594 | 1/1 | 0.71 | 0.47 | - | 77,77,77,77 | 0 |
| 84 | MG | 2 | 1981 | 1/1 | 0.91 | 0.62 | - | 58,58,58,58 | 0 |
| 84 | MG | 1 | 3406 | 1/1 | 0.99 | 0.11 | - | 58,58,58,58 | 0 |
| 84 | MG | 5 | 3479 | 1/1 | 0.98 | 0.32 | - | 48,48,48,48 | 0 |
| 84 | MG | D3 | 202 | 1/1 | 0.81 | 0.51 | - | 67,67,67,67 | 0 |
| 84 | MG | s5 | 301 | 1/1 | 0.89 | 0.38 | - | 74,74,74,74 | 0 |
| 84 | MG | 5 | 3584 | 1/1 | 0.95 | 0.48 | - | 51,51,51,51 | 0 |
| 84 | MG | 6 | 1988 | 1/1 | 0.78 | 0.39 | - | 66,66,66,66 | 0 |
| 84 | MG | 1 | 3631 | 1/1 | 0.96 | 0.12 | - | 76,76,76,76 | 0 |
| 84 | MG | 5 | 4138 | 1/1 | 0.90 | 0.24 | - | 48,48,48,48 | 0 |
| 84 | MG | 6 | 1979 | 1/1 | 0.96 | 0.09 | - | 100,100,100,100 | 0 |
| 84 | MG | 5 | 3463 | 1/1 | 0.94 | 0.28 | - | 49,49,49,49 | 0 |
| 84 | MG | 1 | 3610 | 1/1 | 0.96 | 0.29 | - | 52,52,52,52 | 0 |
| 84 | MG | 4 | 201 | 1/1 | 0.98 | 0.34 | - | 55,55,55,55 | 0 |
| 84 | MG | n5 | 201 | 1/1 | 0.60 | 0.13 | - | 96,96,96,96 | 0 |
| 84 | MG | 1 | 3965 | 1/1 | 0.86 | 0.31 | - | 67,67,67,67 | 1 |
| 84 | MG | 1 | 3735 | 1/1 | 0.85 | 0.45 | - | 77,77,77,77 | 0 |
| 84 | MG | 1 | 3622 | 1/1 | 0.86 | 0.38 | - | 87,87,87,87 | 0 |
| 84 | MG | 1 | 3424 | 1/1 | 0.90 | 0.38 | - | 61,61,61,61 | 0 |
| 84 | MG | 5 | 3922 | 1/1 | 0.82 | 0.30 | - | 56,56,56,56 | 0 |
| 84 | MG | 5 | 3833 | 1/1 | 0.79 | 0.36 | - | 53,53,53,53 | 0 |
| 84 | MG | 3 | 215 | 1/1 | 0.70 | 0.17 | - | 74,74,74,74 | 0 |
| 84 | MG | 5 | 4016 | 1/1 | 0.92 | 0.25 | - | 62,62,62,62 | 0 |
| 84 | MG | 1 | 3669 | 1/1 | 0.80 | 0.30 | - | 78,78,78,78 | 0 |
| 84 | MG | 6 | 1919 | 1/1 | 0.88 | 0.11 | - | 80,80,80,80 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 1 | 3774 | 1/1 | 0.85 | 0.30 | - | 61,61,61,61 | 0 |
| 84 | MG | 1 | 3506 | 1/1 | 0.81 | 0.35 | - | 57,57,57,57 | 0 |
| 84 | MG | 5 | 3460 | 1/1 | 0.90 | 0.20 | - | 49,49,49,49 | 0 |
| 84 | MG | 1 | 3752 | 1/1 | 0.93 | 0.28 | - | 62,62,62,62 | 0 |
| 84 | MG | 1 | 3660 | 1/1 | 0.88 | 0.15 | - | 72,72,72,72 | 0 |
| 84 | MG | 1 | 3458 | 1/1 | 0.93 | 0.39 | - | 64,64,64,64 | 0 |
| 84 | MG | 1 | 3659 | 1/1 | 0.93 | 0.15 | - | 69,69,69,69 | 0 |
| 84 | MG | 1 | 3779 | 1/1 | 0.93 | 0.35 | - | 58,58,58,58 | 0 |
| 84 | MG | sR | 401 | 1/1 | 0.75 | 0.18 | - | 76,76,76,76 | 0 |
| 84 | MG | 1 | 3487 | 1/1 | 0.88 | 0.27 | - | 79,79,79,79 | 0 |
| 84 | MG | 5 | 4101 | 1/1 | 0.83 | 0.21 | - | 75,75,75,75 | 0 |
| 84 | MG | 8 | 215 | 1/1 | 0.96 | 0.44 | - | 58,58,58,58 | 0 |
| 84 | MG | 5 | 4132 | 1/1 | 0.84 | 0.34 | - | 94,94,94,94 | 0 |
| 84 | MG | 5 | 3862 | 1/1 | 0.89 | 0.34 | - | 67,67,67,67 | 0 |
| 84 | MG | 6 | 2056 | 1/1 | 0.94 | 0.24 | - | 83,83,83,83 | 0 |
| 84 | MG | 5 | 3855 | 1/1 | 0.76 | 0.57 | - | 69,69,69,69 | 0 |
| 84 | MG | 5 | 3943 | 1/1 | 0.82 | 0.69 | - | 75,75,75,75 | 0 |
| 84 | MG | 6 | 1987 | 1/1 | 0.81 | 0.31 | - | 79,79,79,79 | 0 |
| 84 | MG | 5 | 3520 | 1/1 | 0.81 | 0.36 | - | 54,54,54,54 | 0 |
| 84 | MG | 2 | 2040 | 1/1 | 0.94 | 0.34 | - | 95,95,95,95 | 0 |
| 84 | MG | 5 | 3547 | 1/1 | 0.95 | 0.49 | - | 54,54,54,54 | 0 |
| 84 | MG | 7 | 219 | 1/1 | 0.72 | 0.17 | - | 62,62,62,62 | 0 |
| 84 | MG | 5 | 4144 | 1/1 | 0.85 | 0.18 | - | 58,58,58,58 | 0 |
| 84 | MG | 6 | 1905 | 1/1 | 0.98 | 0.26 | - | 64,64,64,64 | 0 |
| 84 | MG | c1 | 201 | 1/1 | 0.67 | 0.40 | - | 78,78,78,78 | 0 |
| 84 | MG | 5 | 3601 | 1/1 | 0.72 | 0.46 | - | 89,89,89,89 | 0 |
| 84 | MG | L5 | 301 | 1/1 | 0.77 | 0.13 | - | 89,89,89,89 | 0 |
| 84 | MG | 1 | 3442 | 1/1 | 0.61 | 0.39 | - | 83,83,83,83 | 0 |
| 84 | MG | 5 | 3708 | 1/1 | 0.83 | 0.30 | - | 75,75,75,75 | 0 |
| 84 | MG | 5 | 4015 | 1/1 | 0.82 | 0.40 | - | 59,59,59,59 | 0 |
| 84 | MG | 6 | 2110 | 1/1 | 0.85 | 0.12 | - | 124,124,124,124 | 0 |
| 84 | MG | 1 | 3675 | 1/1 | 0.96 | 0.12 | - | 62,62,62,62 | 0 |
| 84 | MG | 5 | 4130 | 1/1 | 0.74 | 0.21 | - | 81,81,81,81 | 0 |
| 84 | MG | 5 | 3808 | 1/1 | 0.68 | 0.23 | - | 66,66,66,66 | 0 |
| 84 | MG | 5 | 3756 | 1/1 | 0.90 | 0.38 | - | 61,61,61,61 | 0 |
| 84 | MG | 5 | 3874 | 1/1 | 0.87 | 0.27 | - | 70,70,70,70 | 0 |
| 84 | MG | 2 | 2023 | 1/1 | 0.57 | 0.15 | - | 132,132,132,132 | 0 |
| 84 | MG | 5 | 4035 | 1/1 | 0.86 | 0.27 | - | 76,76,76,76 | 0 |
| 84 | MG | 2 | 1916 | 1/1 | 0.98 | 0.16 | - | 90,90,90,90 | 0 |
| 84 | MG | 5 | 4106 | 1/1 | 0.64 | 0.32 | - | 49,49,49,49 | 0 |
| 84 | MG | 6 | 1927 | 1/1 | 0.90 | 0.28 | - | 78,78,78,78 | 0 |
| 84 | MG | l3 | 411 | 1/1 | 0.83 | 0.15 | - | 53,53,53,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 6 | 2028 | 1/1 | 0.90 | 0.12 | - | 99,99,99,99 | 0 |
| 84 | MG | 5 | 3932 | 1/1 | 0.88 | 0.25 | - | 52,52,52,52 | 0 |
| 84 | MG | 6 | 1958 | 1/1 | 0.94 | 0.26 | - | 66,66,66,66 | 0 |
| 84 | MG | 2 | 1921 | 1/1 | 0.93 | 0.20 | - | 91,91,91,91 | 0 |
| 84 | MG | 5 | 3575 | 1/1 | 0.97 | 0.21 | - | 51,51,51,51 | 0 |
| 84 | MG | 5 | 3606 | 1/1 | 0.90 | 0.10 | - | 84,84,84,84 | 0 |
| 84 | MG | 8 | 213 | 1/1 | 0.51 | 0.58 | - | 68,68,68,68 | 0 |
| 84 | MG | 5 | 3977 | 1/1 | 0.89 | 0.27 | - | 67,67,67,67 | 0 |
| 84 | MG | 1 | 3732 | 1/1 | 0.96 | 0.36 | - | 75,75,75,75 | 0 |
| 84 | MG | 4 | 215 | 1/1 | 0.79 | 0.38 | - | 69,69,69,69 | 0 |
| 84 | MG | 6 | 2119 | 1/1 | 0.61 | 0.35 | - | 91,91,91,91 | 0 |
| 84 | MG | 1 | 3842 | 1/1 | 0.46 | 0.98 | - | 92,92,92,92 | 0 |
| 84 | MG | 6 | 1934 | 1/1 | 0.80 | 0.36 | - | 67,67,67,67 | 0 |
| 84 | MG | 5 | 3880 | 1/1 | 0.86 | 0.22 | - | 73,73,73,73 | 0 |
| 84 | MG | 5 | 4003 | 1/1 | 0.68 | 0.26 | - | 77,77,77,77 | 0 |
| 84 | MG | 5 | 3854 | 1/1 | 0.90 | 0.23 | - | 60,60,60,60 | 0 |
| 84 | MG | 1 | 3613 | 1/1 | 0.93 | 0.43 | - | 48,48,48,48 | 0 |
| 84 | MG | 1 | 3789 | 1/1 | 0.96 | 0.28 | - | 80,80,80,80 | 0 |
| 84 | MG | 1 | 3840 | 1/1 | 0.81 | 0.67 | - | 67,67,67,67 | 0 |
| 84 | MG | 6 | 2153 | 1/1 | 0.83 | 0.19 | - | 68,68,68,68 | 0 |
| 84 | MG | M7 | 202 | 1/1 | 0.97 | 0.36 | - | 48,48,48,48 | 0 |
| 84 | MG | 6 | 2013 | 1/1 | 0.98 | 0.26 | - | 76,76,76,76 | 0 |
| 84 | MG | 5 | 3947 | 1/1 | 0.87 | 0.49 | - | 57,57,57,57 | 0 |
| 84 | MG | 6 | 1901 | 1/1 | 0.54 | 0.72 | - | 55,55,55,55 | 0 |
| 84 | MG | 5 | 3916 | 1/1 | 0.94 | 0.20 | - | 51,51,51,51 | 0 |
| 84 | MG | 3 | 203 | 1/1 | 0.95 | 0.12 | - | 103,103,103,103 | 0 |
| 84 | MG | 1 | 3600 | 1/1 | 0.96 | 0.34 | - | 54,54,54,54 | 0 |
| 84 | MG | 1 | 3859 | 1/1 | 0.76 | 0.16 | - | 67,67,67,67 | 0 |
| 84 | MG | 1 | 3909 | 1/1 | 0.80 | 0.29 | - | 73,73,73,73 | 0 |
| 84 | MG | 1 | 3512 | 1/1 | 0.89 | 0.51 | - | 66,66,66,66 | 0 |
| 84 | MG | 2 | 2027 | 1/1 | 0.81 | 0.55 | - | 95,95,95,95 | 0 |
| 84 | MG | 1 | 3668 | 1/1 | 0.76 | 0.32 | - | 74,74,74,74 | 0 |
| 84 | MG | 1 | 3478 | 1/1 | 0.97 | 0.31 | - | 58,58,58,58 | 0 |
| 84 | MG | 1 | 3852 | 1/1 | 0.94 | 0.51 | - | 65,65,65,65 | 0 |
| 84 | MG | 5 | 3545 | 1/1 | 0.98 | 0.23 | - | 49,49,49,49 | 0 |
| 84 | MG | 5 | 3678 | 1/1 | 0.97 | 0.25 | - | 68,68,68,68 | 0 |
| 84 | MG | 5 | 3441 | 1/1 | 0.85 | 0.25 | - | 72,72,72,72 | 0 |
| 84 | MG | 1 | 3457 | 1/1 | 0.81 | 0.24 | - | 63,63,63,63 | 0 |
| 84 | MG | 5 | 3681 | 1/1 | 0.97 | 0.29 | - | 66,66,66,66 | 0 |
| 84 | MG | 1 | 3799 | 1/1 | 0.84 | 0.14 | - | 93,93,93,93 | 0 |
| 84 | MG | 5 | 3582 | 1/1 | 0.97 | 0.30 | - | 54,54,54,54 | 0 |
| 84 | MG | 5 | 3893 | 1/1 | 0.88 | 0.62 | - | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 5 | 4147 | 1/1 | 0.92 | 0.17 | - | 61,61,61,61 | 0 |
| 84 | MG | 5 | 3599 | 1/1 | 0.94 | 0.23 | - | 92,92,92,92 | 0 |
| 84 | MG | 2 | 1919 | 1/1 | 0.83 | 0.29 | - | 84,84,84,84 | 0 |
| 84 | MG | 2 | 2006 | 1/1 | 0.95 | 0.28 | - | 106,106,106,106 | 0 |
| 84 | MG | 4 | 212 | 1/1 | 0.56 | 0.38 | - | 84,84,84,84 | 0 |
| 84 | MG | 6 | 2117 | 1/1 | 0.84 | 0.53 | - | 56,56,56,56 | 0 |
| 84 | MG | 1 | 3579 | 1/1 | 0.69 | 0.25 | - | 71,71,71,71 | 0 |
| 84 | MG | d2 | 201 | 1/1 | 0.92 | 0.22 | - | 80,80,80,80 | 0 |
| 84 | MG | 7 | 203 | 1/1 | 0.80 | 0.36 | - | 52,52,52,52 | 0 |
| 84 | MG | 5 | 4135 | 1/1 | 0.68 | 0.32 | - | 77,77,77,77 | 0 |
| 84 | MG | 2 | 1939 | 1/1 | 0.89 | 0.26 | - | 80,80,80,80 | 0 |
| 84 | MG | 5 | 4133 | 1/1 | 0.88 | 0.28 | - | 114,114,114,114 | 0 |
| 84 | MG | 1 | 3811 | 1/1 | 0.92 | 0.20 | - | 80,80,80,80 | 0 |
| 84 | MG | 5 | 3803 | 1/1 | 0.66 | 0.17 | - | 76,76,76,76 | 0 |
| 84 | MG | 5 | 4112 | 1/1 | 0.78 | 0.18 | - | 52,52,52,52 | 0 |
| 84 | MG | 5 | 3872 | 1/1 | 0.94 | 0.14 | - | 76,76,76,76 | 0 |
| 84 | MG | 1 | 3887 | 1/1 | 0.89 | 0.35 | - | 55,55,55,55 | 0 |
| 84 | MG | 5 | 3544 | 1/1 | 0.98 | 0.29 | - | 61,61,61,61 | 0 |
| 84 | MG | M7 | 205 | 1/1 | 0.83 | 0.30 | - | 59,59,59,59 | 0 |
| 84 | MG | 2 | 2001 | 1/1 | 0.66 | 0.61 | - | 146,146,146,146 | 0 |
| 84 | MG | 7 | 224 | 1/1 | 0.88 | 0.18 | - | 71,71,71,71 | 0 |
| 84 | MG | 1 | 3923 | 1/1 | 0.91 | 0.46 | - | 72,72,72,72 | 0 |
| 84 | MG | 5 | 3850 | 1/1 | 0.88 | 0.24 | - | 58,58,58,58 | 0 |
| 84 | MG | 1 | 3905 | 1/1 | 0.85 | 0.22 | - | 76,76,76,76 | 0 |
| 84 | MG | L4 | 406 | 1/1 | 0.92 | 0.29 | - | 48,48,48,48 | 0 |
| 84 | MG | 2 | 2002 | 1/1 | 0.90 | 0.47 | - | 117,117,117,117 | 0 |
| 84 | MG | m7 | 202 | 1/1 | 0.93 | 0.38 | - | 49,49,49,49 | 0 |
| 84 | MG | 6 | 1914 | 1/1 | 0.87 | 0.08 | - | 114,114,114,114 | 0 |
| 84 | MG | 1 | 3941 | 1/1 | 0.83 | 0.17 | - | 66,66,66,66 | 0 |
| 84 | MG | O7 | 104 | 1/1 | 0.65 | 0.22 | - | 88,88,88,88 | 0 |
| 84 | MG | 6 | 2005 | 1/1 | 0.94 | 0.19 | - | 83,83,83,83 | 0 |
| 84 | MG | 1 | 3790 | 1/1 | 0.84 | 0.33 | - | 78,78,78,78 | 0 |
| 84 | MG | 6 | 2133 | 1/1 | 0.86 | 0.20 | - | 84,84,84,84 | 0 |
| 84 | MG | 5 | 3430 | 1/1 | 0.91 | 0.33 | - | 49,49,49,49 | 0 |
| 84 | MG | 1 | 3858 | 1/1 | 0.96 | 0.37 | - | 46,46,46,46 | 0 |
| 84 | MG | 1 | 3496 | 1/1 | 0.94 | 0.59 | - | 73,73,73,73 | 0 |
| 84 | MG | 6 | 2114 | 1/1 | 0.70 | 0.23 | - | 96,96,96,96 | 0 |
| 84 | MG | 1 | 3427 | 1/1 | 0.95 | 0.27 | - | 51,51,51,51 | 0 |
| 84 | MG | 5 | 3638 | 1/1 | 0.93 | 0.23 | - | 51,51,51,51 | 0 |
| 84 | MG | 8 | 211 | 1/1 | 0.90 | 0.58 | - | 63,63,63,63 | 0 |
| 84 | MG | 6 | 2097 | 1/1 | 0.96 | 0.35 | - | 63,63,63,63 | 0 |
| 84 | MG | 1 | 3452 | 1/1 | 0.89 | 0.18 | - | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | q0 | 202 | 1/1 | 0.95 | 0.18 | - | 51,51,51,51 | 0 |
| 84 | MG | 1 | 3650 | 1/1 | 0.64 | 0.40 | - | 53,53,53,53 | 0 |
| 84 | MG | 5 | 3797 | 1/1 | 0.93 | 0.24 | - | 57,57,57,57 | 0 |
| 84 | MG | 1 | 3987 | 1/1 | 0.91 | 0.20 | - | 60,60,60,60 | 0 |
| 84 | MG | 1 | 3673 | 1/1 | 0.98 | 0.12 | - | 66,66,66,66 | 0 |
| 84 | MG | 5 | 3722 | 1/1 | 0.76 | 0.38 | - | 77,77,77,77 | 0 |
| 84 | MG | 5 | 3470 | 1/1 | 0.92 | 0.35 | - | 54,54,54,54 | 0 |
| 84 | MG | 6 | 2062 | 1/1 | 0.80 | 0.11 | - | 111,111,111,111 | 0 |
| 84 | MG | 5 | 3565 | 1/1 | 0.82 | 0.39 | - | 57,57,57,57 | 0 |
| 84 | MG | l3 | 402 | 1/1 | 0.94 | 0.35 | - | 51,51,51,51 | 0 |
| 84 | MG | 5 | 4128 | 1/1 | 0.84 | 0.32 | - | 68,68,68,68 | 0 |
| 84 | MG | 5 | 3951 | 1/1 | 0.86 | 0.92 | - | 68,68,68,68 | 0 |
| 84 | MG | 4 | 222 | 1/1 | 0.88 | 0.20 | - | 79,79,79,79 | 0 |
| 84 | MG | 6 | 1941 | 1/1 | 0.88 | 0.45 | - | 66,66,66,66 | 1 |
| 84 | MG | 1 | 3624 | 1/1 | 0.84 | 0.23 | - | 74,74,74,74 | 0 |
| 84 | MG | N5 | 201 | 1/1 | 0.94 | 0.15 | - | 95,95,95,95 | 0 |
| 84 | MG | 6 | 2058 | 1/1 | 0.79 | 0.31 | - | 81,81,81,81 | 0 |
| 84 | MG | 5 | 3774 | 1/1 | 0.96 | 0.29 | - | 116,116,116,116 | 0 |
| 86 | ZN | D7 | 101 | 1/1 | 0.57 | 0.21 | - | 264,264,264,264 | 0 |
| 84 | MG | 6 | 1981 | 1/1 | 0.93 | 0.13 | - | 97,97,97,97 | 0 |
| 84 | MG | 5 | 3763 | 1/1 | 0.88 | 0.35 | - | 78,78,78,78 | 0 |
| 84 | MG | 1 | 3651 | 1/1 | 0.92 | 0.25 | - | 59,59,59,59 | 0 |
| 84 | MG | 5 | 3918 | 1/1 | 0.92 | 0.30 | - | 58,58,58,58 | 0 |
| 84 | MG | 5 | 4117 | 1/1 | 0.76 | 0.19 | - | 82,82,82,82 | 0 |
| 84 | MG | 8 | 203 | 1/1 | 0.92 | 0.18 | - | 83,83,83,83 | 1 |
| 84 | MG | l9 | 207 | 1/1 | 0.97 | 0.11 | - | 52,52,52,52 | 0 |
| 84 | MG | m6 | 206 | 1/1 | 0.90 | 0.36 | - | 51,51,51,51 | 0 |
| 84 | MG | M6 | 201 | 1/1 | 0.95 | 0.44 | - | 60,60,60,60 | 0 |
| 84 | MG | 1 | 3663 | 1/1 | 0.77 | 0.29 | - | 69,69,69,69 | 0 |
| 84 | MG | 6 | 1922 | 1/1 | 0.93 | 0.17 | - | 74,74,74,74 | 0 |
| 84 | MG | 5 | 3709 | 1/1 | 0.84 | 0.17 | - | 75,75,75,75 | 0 |
| 84 | MG | 5 | 3746 | 1/1 | 0.89 | 0.41 | - | 40,40,40,40 | 0 |
| 84 | MG | 5 | 3742 | 1/1 | 0.94 | 0.27 | - | 67,67,67,67 | 0 |
| 84 | MG | 1 | 3825 | 1/1 | 0.90 | 0.73 | - | 77,77,77,77 | 0 |
| 84 | MG | 1 | 3454 | 1/1 | 0.75 | 0.37 | - | 61,61,61,61 | 0 |
| 84 | MG | 4 | 216 | 1/1 | 0.98 | 0.12 | - | 69,69,69,69 | 0 |
| 84 | MG | 2 | 1915 | 1/1 | 0.91 | 0.25 | - | 95,95,95,95 | 0 |
| 84 | MG | 5 | 3799 | 1/1 | 0.93 | 0.25 | - | 64,64,64,64 | 0 |
| 84 | MG | 1 | 3597 | 1/1 | 0.94 | 0.37 | - | 46,46,46,46 | 0 |
| 84 | MG | 6 | 1908 | 1/1 | 0.97 | 0.18 | - | 70,70,70,70 | 0 |
| 84 | MG | 1 | 3411 | 1/1 | 0.98 | 0.39 | - | 53,53,53,53 | 0 |
| 84 | MG | 1 | 3783 | 1/1 | 0.99 | 0.21 | - | 61,61,61,61 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 2 | 2016 | 1/1 | 0.81 | 0.39 | - | 72,72,72,72 | 0 |
| 84 | MG | 1 | 3899 | 1/1 | 0.89 | 0.11 | - | 82,82,82,82 | 0 |
| 84 | MG | 1 | 3964 | 1/1 | 0.93 | 0.60 | - | 87,87,87,87 | 0 |
| 84 | MG | 1 | 3645 | 1/1 | 0.90 | 0.55 | - | 55,55,55,55 | 0 |
| 84 | MG | 5 | 3781 | 1/1 | 0.86 | 0.21 | - | 56,56,56,56 | 0 |
| 84 | MG | 1 | 3528 | 1/1 | 0.96 | 0.41 | - | 63,63,63,63 | 0 |
| 84 | MG | 5 | 3928 | 1/1 | 0.91 | 0.22 | - | 46,46,46,46 | 0 |
| 84 | MG | 6 | 2067 | 1/1 | 0.88 | 0.24 | - | 92,92,92,92 | 0 |
| 84 | MG | 1 | 3437 | 1/1 | 0.92 | 0.19 | - | 51,51,51,51 | 0 |
| 84 | MG | 5 | 3580 | 1/1 | 0.96 | 0.43 | - | 48,48,48,48 | 0 |
| 84 | MG | 5 | 4143 | 1/1 | 0.89 | 0.17 | - | 72,72,72,72 | 0 |
| 84 | MG | 6 | 1962 | 1/1 | 0.94 | 0.20 | - | 69,69,69,69 | 0 |
| 84 | MG | 1 | 3862 | 1/1 | 0.91 | 0.20 | - | 63,63,63,63 | 0 |
| 84 | MG | 5 | 3762 | 1/1 | 0.89 | 0.38 | - | 65,65,65,65 | 0 |
| 84 | MG | 6 | 1911 | 1/1 | 0.93 | 0.21 | - | 71,71,71,71 | 0 |
| 84 | MG | 1 | 3444 | 1/1 | 0.77 | 0.68 | - | 70,70,70,70 | 0 |
| 84 | MG | 6 | 2030 | 1/1 | 0.61 | 0.30 | - | 82,82,82,82 | 0 |
| 84 | MG | 6 | 1989 | 1/1 | 0.67 | 0.43 | - | 67,67,67,67 | 0 |
| 84 | MG | 2 | 2010 | 1/1 | 0.79 | 0.29 | - | 98,98,98,98 | 0 |
| 84 | MG | 1 | 3671 | 1/1 | 0.99 | 0.36 | - | 55,55,55,55 | 0 |
| 84 | MG | 5 | 4036 | 1/1 | 0.96 | 0.30 | - | 56,56,56,56 | 0 |
| 84 | MG | 2 | 2022 | 1/1 | 0.82 | 0.09 | - | 132,132,132,132 | 0 |
| 84 | MG | Q2 | 502 | 1/1 | 0.94 | 0.14 | - | 65,65,65,65 | 0 |
| 84 | MG | 5 | 4058 | 1/1 | 0.88 | 0.13 | - | 95,95,95,95 | 0 |
| 84 | MG | 6 | 2128 | 1/1 | 0.68 | 0.32 | - | 77,77,77,77 | 0 |
| 84 | MG | 1 | 3886 | 1/1 | 0.77 | 0.22 | - | 83,83,83,83 | 0 |
| 84 | MG | 1 | 3873 | 1/1 | 0.77 | 0.44 | - | 65,65,65,65 | 0 |
| 84 | MG | 5 | 4073 | 1/1 | 0.72 | 0.12 | - | 97,97,97,97 | 0 |
| 84 | MG | 5 | 3590 | 1/1 | 0.90 | 0.35 | - | 59,59,59,59 | 0 |
| 84 | MG | 5 | 3692 | 1/1 | 0.82 | 0.26 | - | 73,73,73,73 | 0 |
| 84 | MG | 3 | 206 | 1/1 | 0.58 | 0.50 | - | 72,72,72,72 | 0 |
| 84 | MG | 5 | 3994 | 1/1 | 0.99 | 0.21 | - | 48,48,48,48 | 0 |
| 84 | MG | 6 | 2113 | 1/1 | 0.92 | 0.17 | - | 67,67,67,67 | 0 |
| 84 | MG | 6 | 2146 | 1/1 | 0.92 | 0.12 | - | 87,87,87,87 | 0 |
| 84 | MG | 1 | 3464 | 1/1 | 0.92 | 0.32 | - | 51,51,51,51 | 0 |
| 84 | MG | 6 | 2086 | 1/1 | 0.97 | 0.09 | - | 83,83,83,83 | 0 |
| 84 | MG | 1 | 3780 | 1/1 | 0.94 | 0.34 | - | 64,64,64,64 | 0 |
| 84 | MG | 2 | 1952 | 1/1 | 0.84 | 0.47 | - | 99,99,99,99 | 0 |
| 84 | MG | 5 | 3982 | 1/1 | 0.95 | 0.15 | - | 50,50,50,50 | 0 |
| 84 | MG | 1 | 3566 | 1/1 | 0.75 | 0.22 | - | 74,74,74,74 | 0 |
| 84 | MG | 2 | 1993 | 1/1 | 0.89 | 0.21 | - | 99,99,99,99 | 0 |
| 84 | MG | 3 | 205 | 1/1 | 0.86 | 0.20 | - | 61,61,61,61 | 1 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 1 | 3402 | 1/1 | 0.89 | 0.24 | - | 60,60,60,60 | 0 |
| 84 | MG | 5 | 3849 | 1/1 | 0.93 | 0.27 | - | 50,50,50,50 | 0 |
| 84 | MG | 1 | 3699 | 1/1 | 0.82 | 0.53 | - | 82,82,82,82 | 0 |
| 84 | MG | 2 | 2000 | 1/1 | 0.74 | 0.36 | - | 164,164,164,164 | 0 |
| 84 | MG | 1 | 3415 | 1/1 | 0.97 | 0.39 | - | 55,55,55,55 | 0 |
| 84 | MG | 5 | 3802 | 1/1 | 0.77 | 0.15 | - | 75,75,75,75 | 0 |
| 84 | MG | c3 | 203 | 1/1 | 0.91 | 0.10 | - | 108,108,108,108 | 0 |
| 84 | MG | 5 | 3508 | 1/1 | 0.97 | 0.10 | - | 53,53,53,53 | 0 |
| 84 | MG | 4 | 209 | 1/1 | 0.94 | 0.50 | - | 59,59,59,59 | 0 |
| 84 | MG | M3 | 205 | 1/1 | 0.83 | 0.26 | - | 82,82,82,82 | 0 |
| 84 | MG | 6 | 2118 | 1/1 | 0.71 | 0.33 | - | 148,148,148,148 | 0 |
| 84 | MG | 1 | 3662 | 1/1 | 0.80 | 0.29 | - | 78,78,78,78 | 0 |
| 84 | MG | 5 | 3698 | 1/1 | 0.87 | 0.32 | - | 81,81,81,81 | 0 |
| 84 | MG | 5 | 4136 | 1/1 | 0.85 | 0.25 | - | 70,70,70,70 | 0 |
| 84 | MG | m4 | 205 | 1/1 | 0.88 | 0.15 | - | 58,58,58,58 | 0 |
| 84 | MG | 1 | 3754 | 1/1 | 0.92 | 0.68 | - | 68,68,68,68 | 0 |
| 84 | MG | 1 | 3560 | 1/1 | 0.75 | 0.20 | - | 78,78,78,78 | 0 |
| 84 | MG | 1 | 3664 | 1/1 | 0.84 | 0.14 | - | 63,63,63,63 | 0 |
| 84 | MG | 8 | 220 | 1/1 | 0.83 | 0.35 | - | 94,94,94,94 | 0 |
| 84 | MG | 5 | 3633 | 1/1 | 0.97 | 0.30 | - | 45,45,45,45 | 0 |
| 84 | MG | 5 | 3450 | 1/1 | 0.96 | 0.34 | - | 42,42,42,42 | 0 |
| 84 | MG | 5 | 4121 | 1/1 | 0.92 | 0.14 | - | 84,84,84,84 | 0 |
| 84 | MG | 1 | 3853 | 1/1 | 0.80 | 0.30 | - | 60,60,60,60 | 0 |
| 84 | MG | 1 | 3769 | 1/1 | 0.66 | 0.90 | - | 65,65,65,65 | 0 |
| 84 | MG | 5 | 3920 | 1/1 | 0.94 | 0.35 | - | 55,55,55,55 | 0 |
| 84 | MG | 5 | 3719 | 1/1 | 0.96 | 0.24 | - | 66,66,66,66 | 0 |
| 84 | MG | 1 | 3874 | 1/1 | 0.90 | 0.21 | - | 66,66,66,66 | 0 |
| 84 | MG | 5 | 3710 | 1/1 | 0.84 | 0.24 | - | 72,72,72,72 | 0 |
| 84 | MG | 6 | 2035 | 1/1 | 0.78 | 0.21 | - | 82,82,82,82 | 0 |
| 84 | MG | 5 | 3518 | 1/1 | 0.95 | 0.44 | - | 53,53,53,53 | 0 |
| 84 | MG | 1 | 3943 | 1/1 | 0.98 | 0.30 | - | 60,60,60,60 | 0 |
| 84 | MG | 1 | 3938 | 1/1 | 0.97 | 0.30 | - | 62,62,62,62 | 0 |
| 84 | MG | 5 | 3945 | 1/1 | 0.91 | 0.44 | - | 59,59,59,59 | 0 |
| 84 | MG | m7 | 204 | 1/1 | 0.91 | 0.30 | - | 62,62,62,62 | 0 |
| 84 | MG | 2 | 1901 | 1/1 | 0.83 | 0.21 | - | 92,92,92,92 | 0 |
| 84 | MG | 5 | 3635 | 1/1 | 0.81 | 0.29 | - | 55,55,55,55 | 0 |
| 84 | MG | 1 | 3897 | 1/1 | 0.97 | 0.14 | - | 104,104,104,104 | 0 |
| 84 | MG | 6 | 1965 | 1/1 | 0.97 | 0.13 | - | 72,72,72,72 | 0 |
| 84 | MG | 3 | 211 | 1/1 | 0.78 | 0.24 | - | 71,71,71,71 | 0 |
| 84 | MG | 5 | 4082 | 1/1 | 0.90 | 0.14 | - | 71,71,71,71 | 0 |
| 84 | MG | 5 | 3765 | 1/1 | 0.89 | 0.24 | - | 64,64,64,64 | 0 |
| 84 | MG | 5 | 4079 | 1/1 | 0.91 | 0.14 | - | 70,70,70,70 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 84 | MG | 1 | 3864 | 1/1 | 0.89 | 0.21 | - | 61,61,61,61 | 0 |
| 84 | MG | 6 | 1964 | 1/1 | 0.98 | 0.40 | - | 73,73,73,73 | 0 |
| 84 | MG | 12 | 302 | 1/1 | 0.99 | 0.29 | - | 53,53,53,53 | 0 |
| 84 | MG | 1 | 3928 | 1/1 | 0.79 | 0.23 | - | 64,64,64,64 | 0 |
| 84 | MG | 5 | 3574 | 1/1 | 0.79 | 0.61 | - | 58,58,58,58 | 0 |
| 84 | MG | 5 | 4051 | 1/1 | 0.87 | 0.31 | - | 77,77,77,77 | 0 |
| 84 | MG | 1 | 3889 | 1/1 | 0.93 | 0.31 | - | 54,54,54,54 | 0 |
| 84 | MG | 1 | 3698 | 1/1 | 0.81 | 0.55 | - | 69,69,69,69 | 0 |
| 84 | MG | 8 | 205 | 1/1 | 0.77 | 0.17 | - | 111,111,111,111 | 0 |
| 84 | MG | 5 | 3767 | 1/1 | 0.92 | 0.34 | - | 60,60,60,60 | 0 |
| 84 | MG | 1 | 3493 | 1/1 | 0.46 | 0.65 | - | 76,76,76,76 | 0 |
| 84 | MG | 5 | 3725 | 1/1 | 0.81 | 0.37 | - | 71,71,71,71 | 0 |
| 84 | MG | 2 | 1913 | 1/1 | 0.71 | 0.61 | - | 81,81,81,81 | 0 |
| 84 | MG | 5 | 3921 | 1/1 | 0.90 | 0.19 | - | 52,52,52,52 | 0 |
| 84 | MG | 5 | 3891 | 1/1 | 0.84 | 0.70 | - | 75,75,75,75 | 0 |
| 84 | MG | 5 | 3869 | 1/1 | 0.80 | 0.87 | - | 67,67,67,67 | 0 |
| 84 | MG | 6 | 2017 | 1/1 | 0.91 | 0.13 | - | 81,81,81,81 | 0 |
| 84 | MG | 6 | 2124 | 1/1 | 0.81 | 0.26 | - | 76,76,76,76 | 0 |
| 84 | MG | 1 | 3957 | 1/1 | 0.83 | 0.21 | - | 71,71,71,71 | 0 |
| 84 | MG | 5 | 3901 | 1/1 | 0.97 | 0.74 | - | 55,55,55,55 | 0 |
| 84 | MG | q1 | 101 | 1/1 | 0.95 | 0.39 | - | 67,67,67,67 | 0 |
| 84 | MG | 5 | 4040 | 1/1 | 0.69 | 0.29 | - | 74,74,74,74 | 0 |

6.5 Other polymers

There are no such residues in this entry.